Thermal Quantum Field Theory and Perturbative Non-Equilibrium Dynamics

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Abstract

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In this thesis, we develop a perturbative formulation of non-equilibrium thermal quantum field theory, capable of describing the evolution of both temporal and spatial inhomogeneities in relativistic, quantum-statistical ensembles. We begin with a review of the necessary prerequisites from classical thermodynamics, classical and quantum statistical mechanics, quantum field theory and equilibrium thermal field theory. Setting general boundary conditions on the ensemble expectation values of products of interaction-picture creation and annihilation operators, we derive free propagators in which space-time translational invariance is explicitly broken. By means of the Schwinger-Kelydsh, closed-time path formalism, we are then able to introduce a path-integral description that accounts consistently for these temporal and spatial inhomogeneities. Subsequently, we develop a time-dependent perturbation theory that is free of the pathologies previously thought to spoil such approaches to non-equilibrium dynamics.

Following an unambiguous definition of the number density of particles, we derive from first principles perturbative, field-theoretic evolution equations for statistical distribution functions. These evolution equations do not rely on the gradient expansion of so-called Wigner functions, as is necessary in the alternative Kadanoff-Baym approach, and are consistent with the well-known Boltzmann equations in the classical limit. Finally, with reference to a simple toy model, we highlight the appearance of processes otherwise kinematically disallowed in existing approaches to thermal field theory. These evanescent contributions are a consequence of the microscopic violation of energy conservation and are shown to be significant to the early-time evolution of non-equilibrium systems. We observe that the spectral evolution oscillates with time-dependent frequencies, which is interpreted as a signal of non-Markovian, memory effects.

Lay Abstract

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Our everyday experience of the world is of something *macroscopic*, i.e., something containing large objects that we can touch. Intellectually, we can appreciate that these objects are made up of *microscopic* pieces like atoms and molecules, but this remains something intangible to our human senses. For instance, we know that the air around us is a gas of molecules. Nevertheless, when deciding whether to put on a jumper, we don't ask ourselves what each of these molecules is doing. Instead, we simply ask ourselves how warm it is. The temperature of the air as a whole is what matters to us, not the properties of the billions of individual air molecules. Yet, these things must be connected; the temperature must somehow be a consequence of the individual behaviour of these billions of molecules.

However, there are also *macroscopic* objects that are beyond our everyday experience; objects that are unimaginably hot and dense and contain incomprehensible amounts of energy. One example is the infant Universe shortly after the Big Bang. We want to understand the properties of this, the largest object that we know of, in terms of the behaviour of the very smallest objects. These are the elementary particles, the building blocks out of which everything is made. The connection between the *microscopic* properties of these individual elementary particles and the *macroscopic* properties of such massive collections of these particles is the subject of this thesis.

Declaration

I hereby declare that no portion of the work referred to in this thesis has been submitted in support of an application for another degree or qualification of this or any other university or other institute of learning.

Peter William Millington
August, 2012

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to Alison, Jennifer, Haydn, John, Margo and Ralphie

Two roads diverged in a wood, and I—

I took the one less travelled by,

And that has made all the difference.

The Road Not Taken
Robert Frost (1874–1963)

Preface

Peter Millington began his physics studies at William Brookes School and Sixth Form, Much Wenlock, Shropshire, which he attended between 1996 and 2003. In 2003, Peter departed from physics (albeit temporarily) to pursue a career in medicine, taking up a place at the University of Newcastle upon Tyne. On finding himself at a loss without mathematics to play with, Peter soon saw his error of judgement, making the decision to apply for a transfer to study physics at the University of Newcastle upon Tyne. As fate would have it, Newcastle's physics department was due to close at the end of that academic year.

Peter turned his sights upon the then Victoria University of Manchester, where he began as a student of the newly-amalgamated University of Manchester in September 2004. With the award of the Herbert Lloyd Tate Scholarship for his performance at A-Level, Peter embarked upon the studies of his undergraduate masters in physics. His early interests were skewed heavily towards astrophysics and cosmology, spending the summer of 2006 working with the Pulsar Group at Jodrell Bank Observatory under Profs. Andrew Lyne and Michael Kramer. Shortly after, Peter was awarded the Moseley Prize for Physics for his academic achievement and the Delta Travel Prize for his essay on entropy, sparking an interest in thermodynamics that led to his third-year supervision by Dr. Peter Lucas of the Condensed Matter Group. With his thirst for theoretical understanding growing, Peter requested to study his masters year under the supervision of Prof. Apostolos Pilaftsis. Here, Peter was introduced to theoretical particle physics in the context of extra-dimensional theories. After being awarded the Platt Prize for Physics for his theoretical work,

Peter graduated master of physics first class with honours in 2008.

Turning down the offer of undertaking a research degree with Manchester's Condensed Matter Group, Peter chose to continue his post-graduate studies under the supervision of Prof. Apostolos Pilaftsis. The project that they were set to tackle would turn out to touch base with each of Peter's seemingly-fickle interests: astrophysics, cosmology, thermodynamics, condensed matter physics and theoretical particle physics. This project was *the application of thermal quantum field theory to the evolution of systems out of thermodynamic equilibrium.*

Peter William Millington
August, 2012

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Firstly, I would like to take this opportunity to thank my supervisor, Prof. Apostolos Pilaftsis for letting me loose on such a challenging and rewarding area of research. His meticulous and discerning approach to physics is one that I can only hope to emulate; without his insightful guidance, his rigorous expectations and his patience in the light of my own stubbornness, this project could not have come to all that follows. Secondly, to my advisor, Prof. Jeff Forshaw, I will always be grateful, not only for his continued encouragement and his enthusiasm for my research, but also for the faith that he has held in me throughout my career as a student of the University of Manchester. Indeed, it is to Jeff's support that I owe the opportunity to pursue a career as a professional physicist.

Many thanks go to Lisa Alexander-Nunneley, Tim Coughlin, Frank Deppisch, Rosa Duran-Delgado, Jimmy Garland, Simone Marzani, Luke McDermott, Viraf Mehta, Andrew Pilkington, Alex Schofield and Daniele Teresi for many illuminating discussions and a great deal of encouragement. Thank you also to Prof. Björn Garbrecht of the Institut für Theoretische Teilchenphysik und Kosmologie, RWTH Aachen and the organisers of the 2010 workshop on Out-of-Equilibrium Quantum Fields in the Early Universe; to Prof. Edmund Iancu of the Institut de Physique Théorique, CEA-Saclay; and to Prof. Michel Le Bellac of the Institut Non Linéaire de Nice. Thank you to Prof. Terry Wyatt, for his interest in my project and his support in my post-doctoral applications; to Sabah Salih, for his endless computing assistance; to Prof. Fred Loebinger, for his invaluable advice and immutable enthusiasm; and to Anne Morrow, for her seemingly-infinite patience.

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I would also like to thank Dr. Carsten van de Bruck and Prof. Elizabeth Winstanley of the Astro-Particle and Cosmology Group at the University of Sheffield and the Lancaster, Manchester, Sheffield Consortium for Fundamental Physics for not only giving me the opportunity of a position of Research Associate, but also for affording me the flexibility to complete this project with the time and attention that it deserved.

Finally, I would like to thank my friends and my family for their love, support and patience throughout my studies. Thank you to my beautiful wife, Alison; my sister, Jennifer and her partner, Haydn; my parents, John and Margo; to Carol and Alwyn; and Darren and Sarah. To you, Alison, I owe the most of all: thank you for your sense of humour, for knowing when I need reassurance, and for knowing when I need telling what for; thank you for reminding me to eat and to sleep, and for always being there to stand by me. Without you, I would be far less than the person that I hope myself to be.

This document was typeset in LaTeX and uses the SLAC SPIRES `utphys` BibTeX style file. Feynman diagrams were drawn using `FeynMP` and metapost. Plots were drawn using `Wolfram Mathematica`. The word count was generated using TeXcount. I owe and rightly acknowledge a debt of gratitude to the army of LaTeX users whose online tutorials, references and forum posts have proven to be an invaluable resource.

This work was supported by a studentship from the Science and Technology Facilities Council (STFC).

Note to the Reader

The proliferation of 'time'-related objects is somewhat unavoidable in the analysis described in this thesis. As such, the reader's attention is drawn to the list of symbols included on page 31. In particular, we emphasise the distinction between the macroscopic time t and the microscopic time $\tilde{t}$, differentiated by a tilde. The purely-imaginary time of the Matsubara formalism will be denoted by the Greek character τ and the complex time of the Schwinger-Keldysh, closed-time path formalism by the Gothic character $\mathfrak{t}$.

Every effort has been made to ensure that this thesis is as self-contained as practicable. However, a comprehensive review of thermal field quantum theory (or perhaps, more appropriately, *theories*) is far beyond the scope of this discussion. We concentrate therefore on including only that which is necessary to the pedagogy of the exposition of our approach. Nevertheless, when it is suitable to do so, references to further material are included.

Final Submission

Since the original submission of this thesis, the material contained has subsequently been published in:

Perturbative Non-Equilibrium Thermal Field Theory
Peter Millington and Apostolos Pilaftsis
arXiv: 1211.3152

List of Abbreviations

CJT	Cornwall-Jackiw-Tomboulis (effective action)	36
EEV	ensemble expectation value	36
CTP	closed-time path (formalism)	137
FD	Feynman-Dyson (series)	156
ITF	imaginary-time formalism	36
KB	kadanoff-baym equations	37
KMS	Kubo-Martin-Schwinger (relation)	118
LIPS	Lorentz-invariant phase space	124
SD	Schwinger-Dyson (equation)	154
VEV	vacuum expectation value	112

List of Symbols

β	inverse thermodynamic temperature	62
$\mathcal{C}$	closed-time path contour	137
χ	complex scalar field	183
Δ_{F}	Feynman propagator	112
Δ_{D}	Dyson propagator	129
$\Delta_{>(<)}$	positive-(negative-)frequency Wightman propagator	113
$\Delta_{\mathrm{R(A)}}$	retarded(advanced) propagator	128
Δ	Pauli-Jordan propagator (commutator of fields)	126
Δ_1	Hadamard propagator (anti-commutator of fields)	129
$\Delta_{\mathcal{P}}$	principal-part propagator	130
$\bar{\Delta}$	imaginary-time/Matsubara propagator	120
ϵ	pole prescriptions	110
ε	signum function	119
f	statistical distribution function	70
$\tilde{f}$	statistical function	144/162
f_{B}	Bose-Einstein distribution	101
f_β	the Boltzmann distribution	72
F	Helmholtz free energy/statistical function	59/211
G	Gibbs free energy/Green's function	59/107
Γ	effective action/Breit-Wigner width	151/170
H	Hamiltonian/enthalpy/Boltzmann's "H"	48/59/70
J, j	external sources	137/108

$\tilde{t}$	microscopic real time	78
$\mathfrak{t}$	complex time	109
τ	imaginary time	105
T	kinetic energy/thermodynamic temperature	47/58
T	time-ordering operator	87
$\bar{\mathrm{T}}$	anti-time ordering operator	88
T_τ	imaginary-time ordering operator	116
$\mathrm{T}_\mathcal{C}$	path-ordering operator	139
θ	unit step function/polar angle	110/227
u	evanescent action	227
U	potential energy/total internal energy	47/57
$\hat{U}$	evolution operator	82
V	thermodynamic volume/potential	56
W	work/statistical weight/density matrix amplitudes	57/65/165
$\mathcal{W}$	generating functional of connected Green's functions	151
Ξ	grand canonical partition function	63
Z	canonical partition function/wavefunction renormalisation	93/126
$\mathcal{Z}$	generating functional	108

1 Introduction

With modern experimental particle physics continuing to push at both the energy and intensity frontiers, we are increasingly concerned with the dynamics of dense systems of ultra-relativistic particles. One such system is the deconfined phase of quantum chromo dynamics (QCD) — the quark gluon plasma (QGP) [1] — the existence of which has been inferred from the observation of jet quenching (see for instance [2]) in Pb-Pb collisions by the ATLAS [3], CMS [4] and ALICE [5] experiments at the LHC of CERN in Geneva. Aside from these terrestrial, but nevertheless exotic systems, an understanding of these ultra-relativistic many-body dynamics is also of interest in theoretical astro-particle physics and cosmology. Predictions about the evolution of the early Universe rely upon our understanding of the dynamics of the exotic states of matter that were present in the unimaginably-high energy densities that immediately followed the Big Bang. Furthermore, these systems will in general begin their evolution far from thermodynamic equilibrium.

The Wilkinson Microwave Anisotropy Probe (WMAP) [6,7] measured a baryon-to-photon ratio at the present epoch of $\eta = n_B/n_\gamma = 6.116^{+0.197}_{-0.249} \times 10^{-10}$, where $n_B = n_b - n_{\bar{b}}$ is the difference in the number densities of baryons and anti-baryon. This observed baryon asymmetry of the Universe (BAU) — the asymmetry between the present-day numbers of baryons and anti-baryons — is consistent with the predictions of Big-Bang nucleosynthesis (BBN) [8]. The generation of this asymmetry requires the presence in the early Universe of out-of-equilibrium processes and the violation of baryon number (B), charge (C) and charge-parity (CP). These are the so-called Sakharov conditions [9]. One such set of processes is prescribed by the

baryogenesis via leptogenesis scenario [10, 11], in which an initial excess in lepton number (L), provided by the decay of heavy right-handed Majorana neutrinos, is converted to a baryon number excess through the $B + L$-violating sphaleron interactions [12] of the Weinberg-Salam electroweak theory [13, 14]. The description of these phenomena requires a consistent approach to the non-equilibrium dynamics of particle number densities. Such a treatment may also be relevant to reheating and preheating [15–17] at the end of the inflationary epoch.

The classical evolution of particle number densities is described by the Boltzmann transport equation, see for instance [18–21] and semi-classical approaches may be achieved by substituting the classical Boltzmann factors with quantum-statistical, Bose-Einstein or Fermi-Dirac distribution functions, in the case of bosons and fermions respectively. However, these approaches cannot systematically take into account the finite-width and off-shell effects provided by a complete field-theoretic description.

The first such framework for calculating ensemble expectation values (EEVs) of field operators was provided by Matsubara [22] in the so-called imaginary-time formalism (ITF) of thermal field theory, derived by interpreting the canonical density operator as an evolution operator in negative imaginary time. Consistent real time Green's functions may then be obtained by appropriate, but subtle, analytic continuation. The ITF remains however limited to the description of processes occurring at thermodynamic equilibrium.

The calculation of EEVs directly in real time is achieved using so-called real-time formalisms. In particular, for non-equilibrium systems, one uses the closed-time path (CTP) [23, 24] or in-in formalism due to Schwinger and Keldysh. The correspondence of these results with those obtained by the imaginary-time formalism are discussed extensively in the literature, see for instance [25–31]. A perturbative expansion of the in-in generating functional is then provided by the Corwall-Jackiw-Tomboulis (CJT) effective action [32,33] as applied to the CTP formalism by Calzetta and Hu [34, 35].

The extension of this description to the calculation of the out-of-equilibrium evolution of particle number densities is often achieved by the derivation of so-called quantum-corrected or quantum Boltzmann equations [36–43]. These approaches rely upon the Wigner transformation and gradient expansion [44] of a system of Kadanoff-Baym (KB) [45, 46] equations, originally applied in the non-relativistic regime [47, 48]. Often one must also make quasi-particle Ansätzen for the forms of the propagators.

In this thesis, we describe a perturbative approach to non-equilibrium dynamics of many-body quantum field-theoretic systems. This approach is based upon a minor modification of the Schwinger-Keldysh CTP formalism. Appealing to the remaining freedom in the canonical commutation relations of the interaction-picture creation and annihilation operators, we are able to derive the most general form of time-dependent free propagators, in which space-time translational invariance is explicitly broken. Subsequently, we argue that a perturbation theory based upon these non-homogeneous propagators is free of the pinching singularities thought to spoil perturbative approaches to non-equilibrium quantum field theory. With the introduction of an unambiguous definition of the number density of particles, we derive perturbative evolution equations for statistical distribution functions, which do not rely on gradient expansion. Furthermore, we argue that this gradient expansion is inappropriate for the early-time evolution of these non-equilibrium systems.

With reference to a simple toy model, we show that these time-evolution equations are consistent with the Boltzmann transport equation and the truncated gradient expansion of the Kadanoff-Baym equations. We show that the systematic incorporation of finite-time effects and the consistent treatment of generalised decay kinematics lead to the appearance of processes otherwise kinematically disallowed in existing approaches. These evanescent processes result from the microscopic violation of energy conservation at early times. The contributions of this evanescent regime are significant to the early-time evolution of these systems. Finally, we investigate the spectral evolution of the particle width, in which we observe oscillations with time-dependent frequencies. This is interpreted as a signal of non-Markovian,

memory effects and evidence of a truly out-of-equilibrium description.

This thesis is divided into two parts. Part I contains a review of material pertinent to the subsequent formulation of our approach to non-equilibrium quantum field theory. We revisit the central ideas of classical mechanics, thermodynamics and statistical mechanics; their first quantisation in the form of *quantum* statistical mechanics; and finally their second quantisation, with reference to the approaches of equilibrium thermal field theory. In Part II, we develop the aforementioned formalism applicable to the non-equilibrium dynamics of many-body field-theoretic systems.

The content of this thesis is briefly outlined as follows; more detailed summaries are provided in the introductions to Parts I and II and at the start of each chapter where appropriate. In Chapter 3, we set out from Hamilton's principle and the resulting formulation of classical mechanics. Following a brief review of key ideas from thermodynamics and statistical mechanics, we arrive at the Boltzmann transport equation, the quantum field-theoretic generalisation of which is the aim of this thesis. Moving to quantum mechanics, we proceed in Chapter 4 to a review of quantum statistical mechanics, with particular reference to the quantum harmonic oscillator. Here, we introduce many of the formal ideas required for our later discussions. Subsequently, in Chapter 5, we introduce the path-integral representation of the quantum harmonic oscillator and derive the form of its propagators. In Chapter 6, we outline the ITF and the introduction of thermal propagators in the quantum-statistical limit. Finally, in Chapter 7, we move to quantum field theory with the quantisation of the scalar field. This takes us to the equilibrium description of thermal field theory and the conclusion of Part I.

Part II contains the generalisations of these ideas to non-equilibrium systems, setting out from a description of the CTP formalism in Chapter 9 and its minor modification, we outline the generalisation to non-homogeneous backgrounds in Chapter 10. As a check of the consistency of our approach, Chapter 11 describes the thermodynamic equilibrium limit and the correspondence with the familiar results of

the ITF. Chapter 13 outlines the generalisations of these discussions to the complex scalar field. In Chapter 12, we argue that the perturbation theory is free of pinching singularities. Subsequently, in Chapter 14, we define the number density of particles, allowing us then to derive the perturbative time-evolution equations described in Chapter 15. In Chapter 16, we introduce the techniques required to compute loop integrals containing the non-homogeneous free propagators. These results are then used to investigate the dynamics of a simple toy model in Chapter 17. Finally, in Chapter 18, we conclude our discussions.

A number of appendices are also included. Appendix A lists the definitions and properties of, as well as relevant relations between, the various propagators used throughout our analysis. In Appendix B, we illustrate the form of the most general Guassian-like density matrix. For comparison with the results of Chapter 15, we derive the familiar form of the Kadanoff-Baym equations in Appendix C.

The material presented in Chapter 7 and Part II is based heavily upon a forthcoming publication [49]. References, whose use was more general in the writing of this thesis, are indicated at the beginning of relevant chapters.

Part I

Equilibrium Mechanics

2 Introduction to Part I

As we have identified, the aim of this part is to cover the prerequisites necessary for the pedagogy of the exposition of the approach to non-equilibrium dynamics described in Part II. In attempting to write down what is essentially a second quantisation of statistical mechanics, we implicitly rely on central ideas from classical mechanics, thermodynamics and statistical mechanics, as well as quantum mechanics, quantum statistical mechanics and finally quantum field theory. As such there are a number of key ideas that we must revisit: the introduction and interpretation of statistical distribution functions as applied to systems of particles; the concept of observables and the calculation of their ensemble expectation values (EEVs); the path integral and the introduction of the propagators with which we will ultimately perform the calculations of interest.

Part I then is broken up into roughly three general areas: the first is concerned with classical theory; the second moves on to quantum mechanics; and the third introduces us to the ideas of quantum field theory. As pedagogical as we intend to be, we must allow ourselves a starting point: this is the founding principle of classical mechanics — the principle of least action. Chapter 3 moves through the Hamiltonian and Lagrangian formulations of mechanics, leading on to a derivation of the Liouville theorem and the introduction of the classical distribution function. We pass then to discussions of the statistical distribution functions of systems of classical particles, closing with a discussion of the Boltzmann transport equation. In Chapter 4 and with reference to the quantum harmonic oscillator, we introduce the ideas of quantum mechanics and quantum statistical mechanics. Subsequently,

we devote Chapter 5 to the derivation of the path integral, introduced by Richard Feynman [50], the use of which will be fundamental to the discussions of Part II. Before proceeding finally to the ideas of quantum field theory in Chapter 7, we describe in Chapter 6 the inclusion of thermal effects, with particular reference to the imaginary-time approach to equilibrium thermal field theory. In order to keep this first part to a reasonable length, a number of areas of thermal field theory are omitted from our discussions. Nevertheless, where appropriate, suitable references are indicated.

3 Classical Prerequisites

In this chapter, we review the classical foundations on which our later discussions are built. Setting out from a revision of Hamilton's formulation of mechanics, we revisit the ideas of classical statistical mechanics and its relation to classical thermodynamics. We proceed by introducing the classical distribution function and deriving its equation of motion — the Liouville equation. Introducing the familiar thermodynamic potentials, we make use of Liouville's theorem to derive the classical distribution function of a gas of particles in thermodynamic equilibrium — the Gibb's distribution. Arriving at the concept of a statistical ensemble, we are able to bridge the gap between the microscopic description of statistical mechanics and the macroscopic description of thermodynamics by means of Boltzmann's hypothesis for the definition of the entropy. With the subsequent introduction of the classical partition function, we obtain a complete microscopic description of the macroscopic properties of classical equilibrium systems.

Having successfully derived the collective properties of our gas, we look again at the properties of the individual particles that comprise it. Employing Boltzmann's H theorem — the law of increase of entropy — we derive the equilibrium statistical distribution function of these particles — the Boltzmann distribution. Finally, allowing then for interactions between the particles and the departure from equilibrium, we derive the Boltzmann transport equation, which describes the approach to equilibrium of the statistical distribution function. It is a self-consistent quantum field-theoretic analogue of this time-evolution equation that is the ultimate goal of this work and it is for this reason that we justify this classical introduction.

Of course, the content of this chapter is in no way new. A number of texts have been used in its preparation: in particular, those by J. B. Marion & S. T. Thornton [51], L. D. Landau, E. M. Lifshitz & L. P. Pitaevskii [52], J. W. Halley [53] and R. Bowley & M. Sánchez [54]; and for the discussion of the Boltzmann equation, the texts by G. H. Wannier [55] and V. Garzó & A. Santos [56].

3.1 Hamilton's Principle

Let us consider an *isolated* system $\mathscr{U}$, which we shall for definiteness take to be a gas of $N_{\mathscr{U}}$ *distinguishable* particles, each of which is free to move in three spatial dimensions, such that $\mathscr{U}$ comprises $3N_{\mathscr{U}}$ independent degrees of freedom. An isolated system is one that is completely separate from its surroundings in the sense that it is unable to exchange either energy or particles with those surroundings. With the k-th degree of freedom, we associate the coordinate q_k and its time derivative $\dot{q}_k$. These are the components of the positions and velocities of all $N_{\mathscr{U}}$ particles. We may then fully specify the state of the system $\mathscr{U}$ at a time t in terms of $6N_{\mathscr{U}}$ parameters: the set of $3N_{\mathscr{U}}$ coordinates $\{q_k \,|\, k \in \mathbb{N},\ k \leq 3N_{\mathscr{U}}\}$ and their time-derivatives $\{\dot{q}_k |\, k \in \mathbb{N},\ k \leq 3N_{\mathscr{U}}\}$.

The starting point for our description of the dynamics of this system is *Hamilton's principle*, which we may state as follows:

> *The dynamics of a system are such that the time integral of the difference of the kinetic and potential energies is minimised.*

We introduce the classical *action*

$$S[q_k, t_i, t_f] = \int_{t_i}^{t_f} \mathrm{d}t\, L(q_k, \dot{q}_k, t), \tag{3.1.1}$$

where $t_f - t_i$ is the time interval over which the dynamics of the system $\mathscr{U}$ take

place. The quantity

$$L(q_k, \dot{q}_k, t) = T(q_k, \dot{q}_k, t) - U(q_k, \dot{q}_k, t) \tag{3.1.2}$$

is the *Lagrangian*, which is nothing other than the difference of the total kinetic and potential energies, which we donote by T and U respectively. Hamilton's principle is then the statement that the dynamics of the system $\mathscr{U}$ are such that the action S is minimised—*the principle of least action*. (Indeed, we may want to consider whether it is necessary for the action to be minimised or sufficient for it to be extremised.) We note that the action has dimensionality $[S] = \mathrm{E} \times \mathrm{T}$, that is energy $\times$ time, or equivalently $\mathrm{M} \times \mathrm{L}^2 \times \mathrm{T}^{-1}$, mass $\times$ length-squared $\div$ time.

It follows therefore that the dynamics of the system $\mathscr{U}$ may be obtained by solving the variational integral equation

$$\delta S[q_k, t_f, t_i] = \delta \int_{t_i}^{t_f} \mathrm{d}t\, L(q_k, \dot{q}_k, t) = 0. \tag{3.1.3}$$

The lower-case Greek delta denotes the functional variation, i.e., we are to vary the functions $q_k(t)$ in order to extremise the action. Considering then the small variations δq_k and $\delta \dot{q}_k$, we may write

$$\int_{t_i}^{t_f} \mathrm{d}t \sum_{k=1}^{3N_{\mathscr{U}}} \left(\frac{\partial L}{\partial q_k} \delta q_k + \frac{\partial L}{\partial \dot{q}_k} \delta \dot{q}_k \right) = 0. \tag{3.1.4}$$

Integrating by parts in the second term, choosing the variation to vanish at the boundaries of integration, i.e., $\delta q_k(t_f) = \delta q_k(t_i) = 0$, we obtain

$$\sum_{k=1}^{3N_{\mathscr{U}}} \int_{t_i}^{t_f} \mathrm{d}t \left(\frac{\partial L}{\partial q_k} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{q}_k} \right) \delta q_k = 0, \tag{3.1.5}$$

where we have swapped the order of integration and summation. Since the δq_k are arbitrary up to the constraint at the boundaries of integration, it follows that the parentheses must vanish independently for each degree of freedom. We then obtain

the set of $3N_{\mathscr{U}}$ *Euler-Lagrange equations*

$$\frac{\partial L}{\partial q_k} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_k} = 0, \tag{3.1.6}$$

the solutions of which, given a set of $6N_{\mathscr{U}}$ boundary conditions, completely specify the dynamics of the system $\mathscr{U}$.

The total time derivative of the Lagrangian is

$$\frac{\mathrm{d}L}{\mathrm{d}t} = \frac{\partial L}{\partial t} + \sum_{k=1}^{3N_{\mathscr{U}}} \left(\frac{\partial L}{\partial q_k}\dot{q}_k + \frac{\partial L}{\partial \dot{q}_k}\ddot{q}_k \right). \tag{3.1.7}$$

For an isolated system, the Lagrangian cannot depend explicitly on time and, as such, the partial derivative with respect to time vanishes. Using the Euler-Lagrange equations in (3.1.6), we may then write the total time derivative as

$$\frac{\mathrm{d}L}{\mathrm{d}t} = \sum_{k=1}^{3N_{\mathscr{U}}} \left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_k}\dot{q}_k + \frac{\partial L}{\partial \dot{q}_k}\ddot{q}_k \right), \tag{3.1.8}$$

or, equivalently,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{k=1}^{3N_{\mathscr{U}}} \frac{\partial L}{\partial \dot{q}_k}\dot{q}_k - L \right) = 0. \tag{3.1.9}$$

We define by the parentheses a quantity H, which is the *Legendre transform*

$$H(p_k, q_k) = \max_{\dot{q}_\ell} \left(\sum_{k=1}^{3N_{\mathscr{U}}} p_k \dot{q}_k - L \right), \tag{3.1.10}$$

where p_k is the generalised momentum of the k-th degree of freedom and the extremisation yields

$$p_k = \frac{\partial L}{\partial \dot{q}_k}. \tag{3.1.11}$$

It follows straightforwardly from the Euler-Lagrange equations in (3.1.6) that

$$\dot{p}_k = \frac{\partial L}{\partial q_k}. \tag{3.1.12}$$

The quantity H is the *Hamiltonian*. For our isolated system $\mathscr{U}$, this is just the

total energy $T + U$, which, by (3.1.9), must be conserved. The p_k are the $3N_{\mathscr{U}}$ components of the *conjugate momenta*.

The total differential of the Hamiltonian is

$$\mathrm{d}H = \sum_{k=1}^{3N_{\mathscr{U}}} \left(\frac{\partial H}{\partial p_k} \mathrm{d}p_k + \frac{\partial H}{\partial q_k} \mathrm{d}q_k \right) + \frac{\partial H}{\partial t} \mathrm{d}t, \tag{3.1.13}$$

or, in terms of the Legendre transform of the Lagrangian in (3.1.10),

$$\mathrm{d}H = \sum_{k=1}^{3N_{\mathscr{U}}} \left(\dot{q}_k \mathrm{d}p_k + p_k \mathrm{d}\dot{q}_k - \frac{\partial L}{\partial q_k} \mathrm{d}q_k - \frac{\partial L}{\partial \dot{q}_k} \mathrm{d}\dot{q}_k \right) - \frac{\partial L}{\partial t} \mathrm{d}t. \tag{3.1.14}$$

Using (3.1.11) and (3.1.12), the second and fourth terms in the parentheses cancel and we may rewrite the total differential as

$$\mathrm{d}H = \sum_{k=1}^{3N_{\mathscr{U}}} \left(\dot{q}_k \mathrm{d}p_k - \dot{p}_k \mathrm{d}q_k \right) - \frac{\partial L}{\partial t} \mathrm{d}t. \tag{3.1.15}$$

Comparing (3.1.13) and (3.1.15), we obtain *Hamilton's equations of motion*

$$\dot{q}_k = \frac{\partial H}{\partial p_k}, \tag{3.1.16a}$$

$$\dot{p}_k = -\frac{\partial H}{\partial q_k}. \tag{3.1.16b}$$

For completeness, we note that the partial derivatives with respect to time are related via

$$\frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}, \tag{3.1.17}$$

all of which are of course zero for the isolated system $\mathscr{U}$.

We have obtained two descriptions of the dynamics of our system $\mathscr{U}$: the first comprises $3N_{\mathscr{U}}$ second-order differential equations, the Euler-Lagrange equations; and the second comprises $6N_{\mathscr{U}}$ first-order differential equations, Hamilton's equations of motion. Herein, lies a problem: if, in reality, $\mathscr{U}$ comprises a large number of interacting particles, then this system of $6N_{\mathscr{U}}$ coupled first-order differential equa-

tions rapidly becomes intractable. However, the fact that this number of degrees of freedom is so large will turn out to provide the solution to this seemingly insoluble problem; it will allow us to treat this system statistically.

3.2 Liouville's Theorem

Let $\mathscr{S} \subset \mathscr{U}$ be some small *subsystem* of the larger isolated system $\mathscr{U}$, comprising $N_{\mathscr{S}} \ll N_{\mathscr{U}}$ particles and having $3N_{\mathscr{S}}$ independent degrees of freedom, where the number of particles $N_{\mathscr{S}}$ is still sufficiently large that we cannot hope to describe the dynamics by solving the classical equations of motion. We may consider the subsystem $\mathscr{S}$ to be in contact with a reservoir $\mathscr{R}$ formed by the complement of $\mathscr{S}$ in $\mathscr{U}$, i.e., $\mathscr{R} = \mathscr{U} \setminus \mathscr{S}$, see Figure 3.1.

Choosing to describe the system in terms of the Hamiltonian formulation, we associate with the k-th degree of freedom the coordinate q_k and the conjugate momentum p_k. At a given time t, the state of the subsystem $\mathscr{S}$ is completely specified by the set of $3N_{\mathscr{S}}$ coordinates and $3N_{\mathscr{S}}$ momenta, which we may consider as specifying the coordinates of a point or *phase point* in some $6N_{\mathscr{S}}$-dimensional *phase space*. Hereafter, we will drop the subscript $\mathscr{S}$ on quantities associated with the subsystem $\mathscr{S}$ for convenience.

On microscopic time scales, i.e., those comparable with the characteristic time between collisions in the gas, τ_c say, the microscopic arrangement of the subsystem $\mathscr{S}$ will evolve rapidly in time. It seems intuitive however that many of these microscopic arrangements or *microstates* will lead to equivalent macroscopic properties, which will vary only slowly in comparison to these microscopic fluctuations. Given some observable $\mathcal{O}(t)$, our aim then is to find a means of calculating the *time average* over these stochastic fluctuations:

$$\bar{\mathcal{O}}(t) = \frac{1}{\tau} \int_{t-\tau/2}^{t+\tau/2} \mathrm{d}t' \, \mathcal{O}(t'), \tag{3.2.1}$$

where $\tau \gg \tau_c$. Nevertheless, in order to evaluate this time average directly, we would

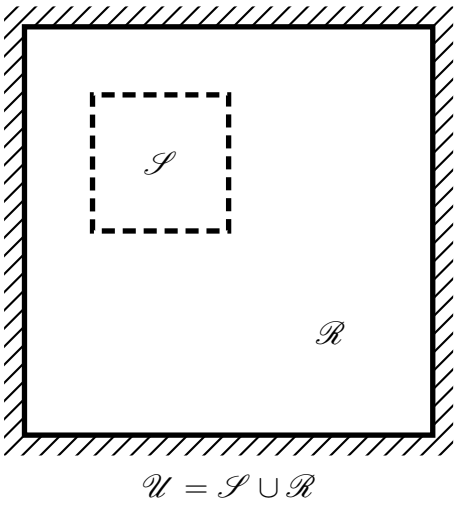


Figure 3.1: A schematic representation of the isolated system $\mathscr{U}$, partitioned into the open subsystem $\mathscr{S}$ and the reservoir $\mathscr{R} = \mathscr{U} \setminus \mathscr{S}$. The hatched square represents the fixed, impermeable adiabatic boundaries of the system $\mathscr{U}$, across which neither particle exchange nor heat transfer are permitted. The dashed square represents the open boundary of the subsystem $\mathscr{S}$, across which both particle exchange and heat transfer are permitted.

still require complete knowledge of the microscopic evolution of the system, which we have identified as an impossibility.

We return then to our phase space. As a result of these microscopic fluctuations, the phase point occupied by $\mathscr{S}$ will traverse some path or *phase trajectory* in phase space. Suppose then that we observe $\mathscr{S}$ for some period of time τ between $t - \tau/2$ and $t + \tau/2$, where $\tau \gg \tau_c$. This time must be sufficiently large that the phase trajectory has traversed the entire phase space, and equivalently $\mathscr{S}$ has passed through every possible microstate, a number of times. Concentrating on a small $6N$-dimensional hypervolume $\Delta\Omega_{6N}$ between q_k and $q_k = q_k + \Delta q_k$ and p_k and $p_k = p_k + \Delta p_k$, where

$$\Delta\Omega_{6N} = \prod_{k=1}^{3N} \Delta q_k \, \Delta p_k, \tag{3.2.2}$$

we observe that $\mathscr{S}$ occupies this hypervolume for a time $\Delta\tau$. Given a subsequent

observation, the probability of finding $\mathscr{S}$ in this hypervolume must then be

$$\Delta\mathbb{P}(q_k, p_k, q'_k, p'_k, t) = \frac{\Delta\tau(q_k, p_k, q'_k, p'_k, t)}{\tau}. \tag{3.2.3}$$

Given that $\Delta\Omega_{6N}$ is small, we may perform a Taylor expansion of this probability around $q'_k = q_k$ and $p'_k = p_k$. The first non-vanishing contribution will be that in which we vary with respect to all $6N$ dimensions of the hypervolume, in which case

$$\Delta\mathbb{P}(q_k, p_k, q'_k, p'_k, t) \approx \left[\left(\prod_{k=1}^{3N} \partial_{q'_k}\,\partial_{p'_k}\right)\frac{\Delta\tau(q_k, p_k, q'_k, p'_k, t)}{\tau}\right]_{\substack{q'_k=q_k\\p'_k=p_k}} \Delta\Omega_{6N}. \tag{3.2.4}$$

In the infinitesimal limit, we may associate with the infinitesimal phase space hypervolume between q_k and $q_k + \mathrm{d}q_k$ and p_k and $p_k + \mathrm{d}p_k$ a particular microstate of the subsystem, which we take to occupy a hypervolume h^{3N}, where the constant h has dimensions of action, that is $\mathrm{M} \times \mathrm{L}^2 \times \mathrm{T}^{-1}$. We may interpret the constant h as the width of a microstate in each of the two-dimensional hypersurfaces of the phase space. The symbol chosen for this constant is not accidental: in the quantum mechanical case, it will turn out to be precisely Planck's constant. The probability of finding $\mathscr{S}$ in a given microstate is then given by

$$\mathrm{d}\mathbb{P}(q_k, p_k, t) = \rho(q_k, p_k, t)\frac{\mathrm{d}\Omega_{6N}}{h^{3N}}, \tag{3.2.5}$$

where

$$\mathrm{d}\Omega_{6N} = \prod_{k=1}^{3N} \mathrm{d}q_k\,\mathrm{d}p_k. \tag{3.2.6}$$

We have defined

$$\rho(q_k, p_k, t) = \left[\left(\prod_{k=1}^{3N} h\,\partial_{q'_k}\,\partial_{p'_k}\right)\frac{\Delta\tau(q_k, p_k, q'_k, p'_k, t)}{\tau}\right]_{\substack{q'_k=q_k\\p'_k=p_k}}, \tag{3.2.7}$$

which is the number density of representative points in phase space or the *density in phase space*, which we shall refer to as the *classical distribution function*.

If we are finding these continuous probability distributions disconcerting, it is worth noting that we could also have proceeded by dividing the phase space up into a lattice comprising a large number of discrete hypervolumes Ω_i. Observing that $\mathscr{S}$ occupied the i-th hypervolume for a time $\tau_i(t)$ of the total time τ, again between $t-\tau/2$ and $t+\tau/2$, the probability of finding $\mathscr{S}$ in this hypervolume is

$$\mathbb{P}_i(t) = \frac{\tau_i(t)}{\tau}. \tag{3.2.8}$$

The subsystem must be somewhere in phase space and it is clear then that the sum over all probabilities must unity, i.e.,

$$\sum_i \mathbb{P}_i(t) = 1. \tag{3.2.9}$$

Let us suppose then that we are interested again in our observable quantity $\mathcal{O}$, which varies slowly over each discrete hypervolume. In this case, we may write the expectation of this observable, which we denote $\langle \mathcal{O}(t) \rangle$, as

$$\langle \mathcal{O}(t) \rangle = \sum_i \mathbb{P}_i(t) \mathcal{O}_i, \tag{3.2.10}$$

where $\mathcal{O}_i$ is the value of the observable if $\mathscr{S}$ occupies the i-th hypervolume. In the continuum limit, taking the lattice spacing to be infinitesimally small, it follows that the expectation of our observable quantity $\mathcal{O}$ is just

$$\langle \mathcal{O}(t) \rangle = \int \mathrm{d}\mathbb{P}(q_k, p_k, t)\, \mathcal{O}(q_k, p_k) = \int \frac{\mathrm{d}\Omega_{6N}}{h^{3N}}\, \rho(q_k, p_k, t) \mathcal{O}(q_k, p_k), \tag{3.2.11}$$

where the distribution function must be subject to the normalisation

$$\int \mathrm{d}\mathbb{P}(q_k, p_k, t) = \int \frac{\mathrm{d}\Omega_{6N}}{h^{3N}}\, \rho(q_k, p_k, t) = 1. \tag{3.2.12}$$

It seems reasonable that this *statistical average* is entirely equivalent to the *time average* in (3.2.1). If we are able to find the form of the distribution function $\rho(q_k, p_k, t)$ without having to solve the system of classical equations of motion, then we have

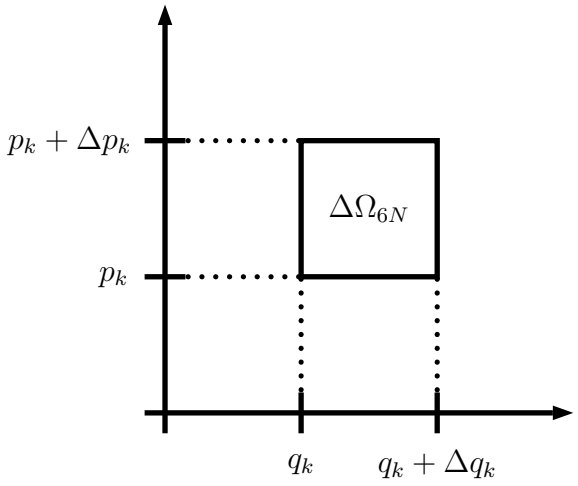


Figure 3.2: A schematic representation of the phase-space hypervolume $\Delta\Omega_{6N}$.

succeeded in finding a palatable means of modelling our many-body system. The equivalence of these two types of average relies on the validity of our assumption that the phase trajectory of the system passes through, or at least passes arbitrarily close to, every point in phase space. This assumption is the so-called *ergodic hypothesis* due to Boltzmann [57, 58].

On macroscopic time scales, the subsystem $\mathscr{S}$ will also evolve in time due to its interactions with the reservoir $\mathscr{R}$. These interactions will alter the likelihood that $\mathscr{S}$ is found in any given microstate and as such the distribution function will also evolve in time. However, $\rho(q_k, p_k, t)$ may only change by the net flux of representative points in or out of the hypervolume between q_k and $q_k + \mathrm{d}q_k$ and p_k and $p_k + \mathrm{d}p_k$, i.e.,

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = 0, \tag{3.2.13}$$

where $\mathbf{u} = \sum_{k=1}^{3N} (\dot{q}_k \hat{\mathbf{q}}_k + \dot{p}_k \hat{\mathbf{p}}_k)$ is the phase-space velocity of these representative points and $\hat{\mathbf{q}}_k$ and $\hat{\mathbf{p}}_k$ are $3N$-dimensional unit vectors. This is the *continuity equation*. We have omitted the arguments of $\rho(q_k, p_k, t)$ for convenience. Using the identity

$$\boldsymbol{\nabla} \cdot (\rho \mathbf{u}) = (\boldsymbol{\nabla} \rho) \cdot \mathbf{u} + \rho \boldsymbol{\nabla} \cdot \mathbf{u}, \tag{3.2.14}$$

this may be written in full as

$$\frac{\partial \rho}{\partial t} + \sum_{k=1}^{3N} \left[\frac{\partial \rho}{\partial q_k} \dot{q}_k + \frac{\partial \rho}{\partial p_k} \dot{p}_k + \rho \left(\frac{\partial \dot{q}_k}{\partial q_k} + \frac{\partial \dot{p}_k}{\partial p_k} \right) \right] = 0. \tag{3.2.15}$$

Using Hamilton's equations of motion (3.1.16), the latter parenthesis is identically zero and we are left with

$$\frac{\partial \rho}{\partial t} + \sum_{k=1}^{3N} \left(\frac{\partial \rho}{\partial q_k} \dot{q}_k + \frac{\partial \rho}{\partial p_k} \dot{p}_k \right) = 0. \tag{3.2.16}$$

After again using Hamilton's equations of motion and introducing the symmetric *Poisson brackets*

$$\{A, B\}_{q_k, p_k} = \frac{\partial A}{\partial q_k} \frac{\partial B}{\partial p_k} - \frac{\partial B}{\partial q_k} \frac{\partial A}{\partial p_k}, \tag{3.2.17}$$

this may be rewritten in the form of the *Liouville equation*

$$\frac{\partial \rho}{\partial t} - \sum_{k=1}^{3N} \{H, \rho\}_{q_k, p_k} = 0. \tag{3.2.18}$$

Looking again at (3.2.15), we see that this is nothing other than the total time derivative, such that

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = 0. \tag{3.2.19}$$

We may state this result as follows:

> *The classical distribution function of a system must remain constant along the phase trajectories of that system.*

This is *Liouville's theorem.*

Returning to (3.2.16), we interpret $\dot{p}_k$ as the k-th component of the $3N$-dimensional generalised force $\mathbf{F} = \sum_{k=1}^{3N} \dot{p}_k \hat{\mathbf{p}}_k$ and $\dot{q}_k$ as the k-th component of the $3N$-dimensional generalised velocity $\mathbf{v} = \sum_{k=1}^{3N} \dot{q}_k \hat{\mathbf{q}}_k$. We have denoted by $\mathbf{v}$ the generalised velocity to distinguish it from the $6N$-dimensional phase-space velocity

u. We then obtain the *Vlasov equation*

$$\frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{q}} \rho + \mathbf{F} \cdot \nabla_{\mathbf{p}} \rho = 0, \tag{3.2.20}$$

where the left-most two terms are the so-called *drift terms* and the right-most term is the so-called *force term*.

3.3 Thermodynamic Potentials

Let us suppose now that the subsystem $\mathscr{S}$ is in a state of *thermodynamic equilibrium*, such that it appears static on *macroscopic* scales. Clearly, on *microscopic* scales, the motion of individual particles remains far from static. In this case, the description of the macroscopic state or *macrostate* of $\mathscr{S}$ in terms of our $6N$ microscopic parameters seems somewhat undesirable. A far more reasonable approach might be to describe the state by its macroscopic, collective properties, that is by appropriate *thermodynamic variables*, which are functions only of the state of $\mathscr{S}$, i.e., *functions of state*, independent of the history by which it reached equilibrium.

The subsystem $\mathscr{S}$ is *open* in the sense that it may exchange both energy and particles with the reservoir $\mathscr{R}$. Let us imagine that we partition $\mathscr{S}$ from $\mathscr{R}$ by some partially permeable and conductive vessel. It follows therefore that there are three ways in which $\mathscr{R}$ may effect a change on $\mathscr{S}$: by the transfer of *heat*; the action of *chemical work*, through the addition or removal of particles and the action of *mechanical work*, through changes in the volume of the vessel. Given that $\mathscr{R}$ is sufficiently large, we may assume that $\mathscr{S}$ cannot effect any change of state on $\mathscr{R}$.

For now, let us assume that the vessel is impermeable, whilst still permitting heat exchange between $\mathscr{S}$ and $\mathscr{R}$. It follows that the total particle number N in $\mathscr{S}$ is fixed and $\mathscr{S}$ is said to be *closed*. Suppose then that $\mathscr{S}$ expands from an initial volume V_i to a final volume V_f, resulting say from the removal of some compressive force exerted on the vessel by the reservoir. We allow this expansion to proceed slowly in infinitesimal steps of volume $\mathrm{d}V$, each resulting from an infinitesimal reduction

in this compressive force. We may then assume that $\mathscr{S}$ remains in thermodynamic equilibrium in each step of the expansion. We refer to such a process as *quasi-static*. After each step, it seems reasonable that we may restore the compressive force in the same quasi-static manner, slowly returning $\mathscr{S}$ to its initial state. We then refer to this process as *reversible*.

In expanding by a volume $\mathrm{d}V$, $\mathscr{S}$ must do an amount of *reversible work* $đW$ on $\mathscr{R}$, the magnitude of which is $P\mathrm{d}V$, where P is the *thermodynamic pressure*. We have, however, not restricted the flow of heat between $\mathscr{S}$ and $\mathscr{R}$ and, indeed, further information is required in order to determine whether this expansion takes place *adiabatically*, that is without heat exchange. In general, therefore, the infinitesimal amount of reversible work $đW$ must be accompanied by some infinitesimal, reversible flow of heat $đQ$. It follows then, by conservation of energy, that the *total internal energy* U of $\mathscr{S}$ changes by an amount

$$\mathrm{d}U = đQ + đW, \tag{3.3.1}$$

where $đW = -P\mathrm{d}V$, since any increase in volume must reduce the total internal energy. This is the *first law of thermodynamics*. The horizontal bar through the differentials on the right-hand side denote that these are *inexact* differentials, that is there do not exist *anti-derivative* operations that yield the total work done or the total heat transferred. These quantities depend not only on the initial and final states, but also the details of the states through which the system moves during this change of state. In other words, work and heat are not functions of state.

In writing the differential work in terms of the volume and pressure, we have already rewritten part of the right-hand side of (3.3.1) in terms of functions of state. What remains is to write the differential heat in terms of an *exact* differential. We introduce a new function of state: the *entropy* S, which we define through

$$\mathrm{d}S = \frac{đQ}{T}, \tag{3.3.2}$$

where T is the *thermodynamic temperature*. The entropy will turn out to be a measure of the disorder of $\mathscr{S}$. We may now write the first law of thermodynamics entirely in terms of exact differentials:

$$\mathrm{d}U = T\mathrm{d}S - P\mathrm{d}V. \tag{3.3.3}$$

If we allow $\mathscr{S}$ to exchange particles with $\mathscr{R}$, we must also allow for the effect of some infinitesimal change in the total particle number $\mathrm{d}N$. In this case, the first law may be written

$$\mathrm{d}U = T\mathrm{d}S - P\mathrm{d}V + \mu\mathrm{d}N, \tag{3.3.4}$$

where we have introduced the *chemical potential* μ, which is simply a measure of the energy required to add a particle to $\mathscr{S}$. It is clear then that the total internal energy is a function of the entropy S, volume V and particle number N, all of which are *extensive* variables, those that scale with the size of the system. A system in thermodynamic equilibrium is therefore one in which the entropy, volume and particle number do not change with time. True thermodynamic equilibrium then necessitates simultaneous kinetic, mechanical and chemical equilibrium. By considering the total differential

$$\mathrm{d}U(S,V,N) = \left(\frac{\partial U}{\partial S}\right)_{V,N}\mathrm{d}S + \left(\frac{\partial U}{\partial V}\right)_{S,N}\mathrm{d}V + \left(\frac{\partial U}{\partial N}\right)_{S,V}\mathrm{d}N, \tag{3.3.5}$$

where the subscripts remind us that the partial derivatives are evaluated with all other variables held constant, we may define the *intensive* variables: temperature T, pressure P and chemical potential μ — those which do not scale with the size of the system — as

$$T = \left(\frac{\partial U}{\partial S}\right)_{V,N}, \quad P = \left(\frac{\partial U}{\partial V}\right)_{S,N}, \quad \mu = \left(\frac{\partial U}{\partial N}\right)_{S,V}. \tag{3.3.6}$$

Hence, kinetic, mechanical or chemical equilibrium are attained when the temperature, pressure or total particle number, respectively, have reached constant values.

Thermodynamic Potential	**Total Differential**	**Natural Variables**
Total Internal Energy, U	$\mathrm{d}U = T\mathrm{d}S - P\mathrm{d}V + \mu\mathrm{d}N$	S, V, N
Enthalpy, H	$\mathrm{d}H = T\mathrm{d}S + V\mathrm{d}P + \mu\mathrm{d}N$	S, P, N
Helmholtz Free Energy, F	$\mathrm{d}F = -S\mathrm{d}T - P\mathrm{d}V + \mu\mathrm{d}N$	T, V, N
Gibbs Free Energy, G	$\mathrm{d}G = -S\mathrm{d}T + V\mathrm{d}P + \mu\mathrm{d}N$	T, P, N
Grand Potential, Φ	$\mathrm{d}\Phi = -S\mathrm{d}T - P\mathrm{d}V - N\mathrm{d}\mu$	T, V, μ

Table 3.1: Summary of the key thermodynamic potentials and their natural variables.

For processes that take place at constant entropy (*isoentropic*), constant volume (*isochoric* or *isovolumetric*) or particle number (*isosmotic*), it is clear that the total internal energy is a useful quantity for calculations. For *isobaric* processes however, taking place at constant pressure, it is convenient to define a new *thermodynamic potential* by the Legendre transform

$$H = U + PV, \tag{3.3.7}$$

such that

$$\mathrm{d}H = T\mathrm{d}S + V\mathrm{d}P + \mu\mathrm{d}N. \tag{3.3.8}$$

This quantity is known as the *enthalpy*. For processes occurring at constant volume and constant temperature (*isothermal*), it is convenient to define the *Helmholtz free energy*

$$F = U - TS, \tag{3.3.9}$$

and for processes at constant pressure and constant temperature, the *Gibbs free energy*

$$G = H - TS. \tag{3.3.10}$$

Finally, for open subsystems in which we are interested in the total particle number

N, it will prove useful to define the *grand potential*

$$\Phi = F - \mu N. \tag{3.3.11}$$

Table 3.1 summarises the differential forms of these thermodynamic potentials and lists their natural variables.

In the presence of s different particle species, the generalisation of these definitions is reasonably straightforward. We simply replace the terms μN in the Legendre transforms and $\mu \mathrm{d}N$ in the total differential forms with summations over all particle species, i.e.,

$$\mu N \to \sum_{i=1}^{s} \mu_i N_i, \tag{3.3.12a}$$

$$\mu \mathrm{d}N \to \sum_{i=1}^{s} \mu_i \, \mathrm{d}N_i. \tag{3.3.12b}$$

3.4 Entropy and the Gibb's Distribution

Thus far we have introduced two seemingly disparate descriptions of our subsystem $\mathscr{S}$: the first, based upon the *microscopic* properties of the individual constituents of the subsystem and the second, based upon only *macroscopic*, collective properties of the subsystem as a whole. Not surprisingly, the next step is to find a connection between these two descriptions.

In Section 3.2, we established Liouville's theorem: the statement that the classical distribution function must remain constant along the phase trajectories of the system. It follows therefore that this distribution function can depend only on those quantities that also remain constant along those trajectories. These are the constants or *integrals of motion*, which for our gas of particles are the total energy, three-dimensional linear momentum and three-dimensional angular momentum, the latter two of which correspond to the collective motion of the system. Choosing the boundaries of the system $\mathscr{U}$ to be fixed in some inertial, non-accelerating reference

frame, we may neglect this collective motion and the density in phase space of the subsystem $\mathscr{S}$ must then be a function only of the total energy $E_N(q_k, p_k)$. The subscript N reminds us that this is the total energy of all N particles.

However, we can restrict the form of the distribution function further. Let us consider two congruous subsystems: $\mathscr{S}_1$ and $\mathscr{S}_2$, each with respective distribution functions ρ_1 and ρ_2 and whose volumes are fixed by impermeable vessels, such that they are both closed. If $\mathscr{S}_1$ and $\mathscr{S}_2$ are themselves sufficiently large, then we may neglect the contributions from interactions occurring at the boundary between them and, as such, the state of one subsystem cannot effect the state of the other. In which case, $\mathscr{S}_1$ and $\mathscr{S}_2$ are said to be *statistically independent*. Given the law of addition for independent probabilities, it follows that the combined distribution function of the two subsystems $\mathscr{S}_1 \cup \mathscr{S}_2$ must be the product of their individual distribution functions, i.e.,

$$\rho_{1\cup 2} = \rho_1 \rho_2. \tag{3.4.1}$$

We conclude therefore that the logarithm of the distribution function of a subsystem must be an additive function of the relevant integrals of motion. For $\mathscr{S}$, we have only to consider the total energy and we may write

$$\ln \rho(q_k, p_k) = -\alpha - \beta E_N(q_k, p_k), \tag{3.4.2}$$

where α and β are constants. We have chosen the overall sign suggestively in anticipation that we should be less likely to find the subsystem in a state of higher energy than one of lower energy. Exponentiating this result, the distribution function of our closed subsystem is

$$\rho(q_k, p_k) = \frac{1}{Z} e^{-\beta E_N(q_k, p_k)}, \tag{3.4.3}$$

where the constant Z is such that the normalisation in (3.2.12) is satisfied, i.e.,

$$Z = \int \frac{\mathrm{d}\Omega_{6N}}{h^{3N}}\, e^{-\beta E_N(q_k, p_k)}. \tag{3.4.4}$$

The density in phase space in (3.4.3), pertaining to the closed subsystem, is referred to as the *canonical distribution*. The normalisation Z, which represents a sum over all possible states, is known as the *canonical partition function*.

The expectation of the logarithm of the distribution function in (3.4.2) is

$$\int \frac{\mathrm{d}\Omega_{6N}}{h^{3N}}\,\rho(q_k,p_k)\ln\rho(q_k,p_k) = -\alpha - \beta\int \frac{\mathrm{d}\Omega_{6N}}{h^{3N}}\,\rho(q_k,p_k)E_N(q_k,p_k). \tag{3.4.5}$$

The integral on the right hand side is just the expectation of the total energy, which, if the system is in equilibrium, must be nothing other than the thermodynamic, total internal energy

$$U = \langle E_N\rangle = \int \frac{\mathrm{d}\Omega_{6N}}{h^{3N}}\,\rho(q_k,p_k)E_N(q_k,p_k). \tag{3.4.6}$$

For our closed subsystem of fixed volume and particle number, the first law of thermodynamics has the form

$$\mathrm{d}U = T\mathrm{d}S, \tag{3.4.7}$$

cf. (3.3.3). Comparing (3.4.7) with the total differential of (3.4.5), we infer that

$$\mathrm{d}S = -\beta T\,\mathrm{d}\langle\ln\rho\rangle. \tag{3.4.8}$$

The entropy must therefore be related to the expectation of the logarithm of the distribution function as follows:

$$S = -k_\mathrm{B}\left\langle\ln\rho\right\rangle, \tag{3.4.9}$$

up to some overall additive constant, where k_B is Boltzmann's constant. The constant

$$\beta = \frac{1}{k_\mathrm{B}T}, \tag{3.4.10}$$

is then the *inverse thermodynamic temperature* having units of energy, in which case the exponent of the distribution function is dimensionless as required.

Considering again our two congruous subsystems, we now allow particle ex-

change across the boundary between them. Nevertheless, if the subsystems are sufficiently large, then we may also neglect this contribution and consider these subsystems to be *quasi-closed*. In this case, they remain statistically independent, as were the closed subsystems above, and the form of the logarithm of the distribution function is exactly as in (3.4.2). However, for these quasi-closed subsystems of fixed volume, the first law of thermodynamics is

$$\mathrm{d}U = T\mathrm{d}S + \mu\mathrm{d}N. \tag{3.4.11}$$

It follows then that the distribution function must take the form

$$\rho(q_k, p_k) = \frac{1}{\Xi}\, e^{-\beta[E_n(q_k,p_k)-\mu n]}, \tag{3.4.12}$$

where the constant α in (3.4.2) has become a function of the total particle number n. This distribution function is referred to as the *grand canonical distribution*. Again, we must always find the subsystem to be in one of the possible microstates. However, as well as all possible energies, these microstates now cover all possible total particle numbers n, which differ from the macroscopic total particle number $N = \langle n \rangle$. It follows then that this distribution function must satisfy the normalisation

$$\sum_n \int \frac{\mathrm{d}\Omega_{6n}}{h^{3n}}\, \rho(q_k, p_k) = 1, \tag{3.4.13}$$

where we now sum over all possible numbers of particles, in which case

$$\Xi = \sum_n \int \frac{\mathrm{d}\Omega_{6n}}{h^{3n}}\, e^{-\beta[E_n(q_k,p_k)-\mu n]}. \tag{3.4.14}$$

This normalisation again represents a sum over all possible states and is known as the *grand canonical partition function*.

Looking again at (3.4.5), it would appear more convenient to rewrite the integral over phase space as an integral over the energies E_N of the microstates. We can then forget about the impractical set of microscopic coordinates and momenta

entirely. In this form, the expectation of the energy of a closed subsystem becomes

$$U = \int \mathrm{d}E_N \, \rho(E_N) \frac{1}{h^{3N}} \frac{\partial \Omega_{6N}}{\partial E_N} E_N, \tag{3.4.15}$$

where $\rho(E_N)$ is the canonical distribution in (3.4.3). From this integral, we see that the probability of finding $\mathscr{S}$ in a microstate of energy between E_N and $E_N + \mathrm{d}E_N$ is

$$\mathrm{d}\mathbb{P}(E_N) = \rho(E_N) \frac{1}{h^{3N}} \frac{\partial \Omega_{6N}}{\partial E_N} \mathrm{d}E_N, \tag{3.4.16}$$

The canonical distribution $\rho(E_N)$ is the number density of microstates in phase space and

$$\mathrm{d}w_N \equiv \frac{1}{h^{3N}} \frac{\partial \Omega_{6N}}{\partial E_N} \mathrm{d}E_N \tag{3.4.17}$$

is the total number of microstates with energy in the interval between E_N and $E_n + \mathrm{d}E_N$. It follows that the product

$$\rho(E_N) \frac{\mathrm{d}w_N}{\mathrm{d}E_N} \tag{3.4.18}$$

is then the density of microstates in the space of energies.

If the closed subsystem $\mathscr{S}$ is in thermodynamic equilibrium with total internal energy U, the energy probability distribution

$$\frac{\mathrm{d}\mathbb{P}(E_N)}{\mathrm{d}E_N} = \rho(E_N) \frac{\mathrm{d}w_N}{\mathrm{d}E_N} \tag{3.4.19}$$

must be highly peaked near $E_N = U$ with some finite width ΔU. If all microstates in the energy interval ΔU are equally likely — the assumption of *equal a priori probability* — then the energy probability distribution must be constant over that interval. In this case, the total probability must be equal to the area of a rectangle with height $\rho(U) \frac{\mathrm{d}w_N}{\mathrm{d}U}$ and width ΔU, which must also be normalised to unity. Hence,

$$\int \mathrm{d}E_N \, \rho(E_N) \frac{\mathrm{d}w_N}{\mathrm{d}E_N} \approx \rho(U) \frac{\mathrm{d}w_N}{\mathrm{d}U} \Delta U = 1, \tag{3.4.20}$$

where

$$W(U) \equiv \Delta w_N = \frac{\mathrm{d}w_N}{\mathrm{d}U}\Delta U \tag{3.4.21}$$

is just the total number of microstates with energy in the interval ΔU, that is the number of microstates consistent with the macrostate of total internal energy U. It follows therefore that

$$W(U) = \frac{1}{\rho(U)}, \tag{3.4.22}$$

which we refer to as the *statistical weight* of the macrostate of total internal energy U. Since all microstates are equally likely, the probability of finding the system in any one of the $W(U)$ microstates given that it is in a macrostate of energy U is simply $W^{-1}(U)$.

Using Liouville's theorem, we argued that the logarithm of the distribution function must be a linear function of the energy and, as such, the following equality holds:

$$S = -k_{\mathrm{B}} \ln \rho(U) = -k_{\mathrm{B}} \left\langle \ln \rho(E_N) \right\rangle . \tag{3.4.23}$$

Using (3.4.22), the entropy of a given macrostate may be expressed in terms of its statistical weight as

$$S = k_{\mathrm{B}} \ln W(U). \tag{3.4.24}$$

Hence, the entropy of a given macrostate is the natural logarithm of the total number of microstates consistent with that macrostate. This is *Boltzmann's hypothesis*. This is a significant result: the question of calculating the distribution function of a system and subsequently its thermodynamic properties is now one of counting microstates, i.e., a question only of combinatorics.

For an open subsystem, we must also sum over all possible total particle numbers n, replacing the canonical distribution with the grand canonical distribution in (3.4.23). Nevertheless, the energy probability distribution must also be dominated by particle numbers n near the thermodynamic total particle number N, in which

case the generalisation of (3.4.20) reads as

$$\sum_n \int \mathrm{d}E_n \, \rho(E_n, n) \frac{\mathrm{d}w_n}{\mathrm{d}E_n} \approx \rho(U, N) \frac{\mathrm{d}w_N}{\mathrm{d}U} \Delta U = 1, \tag{3.4.25}$$

differing only by the replacement of the canonical distribution by the grand canonical distribution. We may conclude therefore that the arguments followed above for the closed subsystem also hold for an open subsystem.

The introduction of the statistical weight W allows us to construct a different picture of our statistical average. Rather than observing a single system for a sufficiently large period of time, we can instead consider observing a sufficiently large number of identically-prepared systems instantaneously. We imagine populating phase space with copies of the subsystem, all prepared in the same way and each in one of the possible microstates. This set of copies is called a *statistical ensemble*.

If the copies are prepared with the same energy, volume and particle number and are isolated from one another then the ensemble is said to be *microcanonical*. This is true of the isolated system $\mathscr{U}$, for which the distribution function must be narrowly peaked at a particular value $U_{\mathscr{U}}$ and thus have the form of a delta function:

$$\rho = W^{-1} \delta(U - U_{\mathscr{U}}). \tag{3.4.26}$$

This is known as the *microcanonical distribution*. The *microcanonical partition function* W is just the statistical weight of the macrostate with energy $U_{\mathscr{U}}$, that is

$$W = e^{S/k_{\mathrm{B}}}. \tag{3.4.27}$$

For the closed subsystem $\mathscr{S}$, we must allow for the energy to be exchanged with the reservoir $\mathscr{R}$. The copies of the subsystem must then be allowed to exchange energy. Such an ensemble is said to be *canonical* and is described by the *Gibb's distribution*

$$\rho(U) = e^{-S(U)/k_{\mathrm{B}}}, \tag{3.4.28}$$

obtained by exponentiating (3.4.23). Using the definition of the Helmholtz free energy in (3.3.9), we may write the Gibb's distribution in the following form:

$$\rho(U) = e^{\beta(F-U)}. \tag{3.4.29}$$

Comparing this with (3.4.3), we see that the canonical partition function may be written in terms of the Helmholtz free energy as

$$Z = e^{-\beta F} \tag{3.4.30}$$

and therefore

$$F = -k_{\mathrm{B}} T \ln Z. \tag{3.4.31}$$

Hence, it is through the canonical partition function that we are able to calculate the thermodynamic potentials directly.

For an open subsystem, we must allow the copies in our ensemble to exchange both energy and particles. This is known as the *grand canonical ensemble*. In this case, the Gibb's distribution still takes the form in (3.4.28), where the entropy is now a function of both the total internal energy U and the total particle number N. In this case, we may use the definition of the grand potential in (3.3.11) to write the grand canonical Gibb's distribution as

$$\rho(U, N) = e^{\beta(\Phi - U + \mu N)}. \tag{3.4.32}$$

It follows then that the grand potential may be written in terms of the grand canonical partition function as

$$\Phi = -k_{\mathrm{B}} T \ln \Xi. \tag{3.4.33}$$

Thus, for open subsystems, it is through the grand canonical partition function that we make connection with the thermodynamic potentials.

Until now, we have considered the N particles in our gas to be distinguishable. That is to say that we may distinguish two particles whose positions and momenta

Statistical Ensemble	**Type of System**	**Fixed Variables**	**Partition Function**
microcanonical	isolated system	all	$W = e^{S/k_\mathrm{B}}$
canonical	closed subsystem	particle number	$Z = e^{FT/k_\mathrm{B}}$
grand canonical	open subsystem	none	$\Xi = e^{\Phi T/k_\mathrm{B}}$

Table 3.2: Summary of the three statistical ensembles and their partition functions.

are identical. For point-like particles, this does not seem a reasonable proposition. If we want to treat *indistinguishable* particles then our integrals over all microstates must be replaced by integrals over all *physically-distinct* microstates. There are $N!$ ways to arrange N particles and as such the number of physically distinct microstates is reduced by the same factor. It follows that for indistinguishable particles, the definitions of the canonical and grand canonical partition functions become

$$Z = \frac{1}{N!} \int \frac{\mathrm{d}\Omega_{6N}}{h^{6N}} \, e^{-\beta E_N(q_k, p_k)}, \tag{3.4.34a}$$

$$\Xi = \sum_n \frac{1}{n!} \int \frac{\mathrm{d}\Omega_{6n}}{h^{3n}} \, e^{-\beta[E_n(q_k, p_k) - \mu n]}. \tag{3.4.34b}$$

In summary, having introduced statistical ensembles comprising copies of the subsystem in each of the possible microstates, we have found a means of calculating macroscopic thermodynamic quantities from a microscopic description of the subsystem. The various statistical ensembles are summarised in Table 3.2. This connection is made through the partition function, which may be determined from the statistical weights of the various macrostates. What remains is for us to calculate these statistical weights directly by counting available microstates.

3.5 The Boltzmann Distribution

Let us consider again our subsystem $\mathscr{S}$ of N particles, which we shall now assume to be *indistinguishable*. For this subsystem, the microstates are just the possible microscopic states of the individual particles. In this case, the particles themselves constitute a canonical ensemble and groups of particles with the same energy, a grand canonical ensemble. It is reasonable therefore to ask for the probability of finding a single particle with energy between E and $E + \mathrm{d}E$. Our task then is to count the number of physically-distinct ways in which we can distribute these N particles amongst the available microstates, which are presumably infinite in number.

Suppose then that there are g_i microstates all of which have a discrete energy E_i, so that there are g_i ways in which a particle may have the energy E_i. We will eventually take the continuous limit, but for now we wish to count discrete microstates. There are then $g_i^{N_i}$ ways in which N_i particles can have energy E_i: there are g_i ways to place the first particle, g_i ways to place the second and so on. However, these particles are indistinguishable and as such we must remove those arrangements that differ only by permutation. The number of permutations of N_i particles is simply $N_i!$. As such, the total number of physically-distinct ways of placing N_i particles into microstates with energy E_i is simply

$$W_i = \frac{g_i^{N_i}}{N_i!}. \tag{3.5.1}$$

Hence, the statistical weight of a macrostate of total internal energy U, where

$$U = \sum_i N_i E_i, \tag{3.5.2}$$

is just

$$W(U) = \prod_i W_i = \prod_i \frac{g_i^{N_i}}{N_i!}. \tag{3.5.3}$$

Following Boltzmann, we define the quantity

$$H = \ln W = \sum_i \ln\, W_i, \tag{3.5.4}$$

which of course is related to the entropy of the subsystem. This H is not to be confused with the Hamiltonian. Substituting then for (3.5.1), this quantity takes the form

$$H = \sum_{i=1}^{\infty} \big(N_i \ln g_i - \ln N_i!\big). \tag{3.5.5}$$

For N_i large, we may use Stirling's approximation for the logarithm of the factorial

$$\ln N_i! = N_i \ln N_i - N_i, \tag{3.5.6}$$

in which case

$$H = -\sum_{i=1}^{\infty} \big(N_i \ln \frac{N_i}{g_i} - N_i\big). \tag{3.5.7}$$

The ratio $f_i \equiv N_i/g_i$ is just the average number of particles in each microstate of energy E_i, which we shall refer to as the *statistical distribution function*. We may then rewrite

$$H = -\sum_{i=1}^{\infty} g_i\big(f_i \ln f_i - f_i\big) \tag{3.5.8}$$

We shall assert that the system moves to extremise this quantity. This is *Boltzmann's H theorem* and a statement of the law of increase of entropy, otherwise known as the *second law of thermodynamics*. It follows that we must solve

$$\frac{\partial}{\partial f_i} \sum_{j=1}^{\infty} g_j\big(f_j \ln f_j - f_j\big) = 0, \tag{3.5.9}$$

subject to the constraints

$$N = \sum_{i=1}^{\infty} g_i f_i, \tag{3.5.10}$$

and

$$U = \sum_{i=1}^{\infty} g_i f_i E_i. \tag{3.5.11}$$

By the method of Lagrange undetermined multipliers, we must solve therefore the auxiliary equation

$$\frac{\delta}{\delta f_i}\sum_{j=1}^{\infty} g_j\big(f_j \ln f_j - f_j + \alpha f_j + \beta f_j E_j\big) = 0, \tag{3.5.12}$$

where α and β are constants. Using the functional derivative

$$\frac{\delta f_j}{\delta f_i} = \delta_{ij}, \tag{3.5.13}$$

where δ_{ij} is the Kronecker delta, equal to unity for $i = j$ and zero otherwise, we find

$$-\ln f_i = \alpha + \beta E_i \tag{3.5.14}$$

or, exponentiating,

$$f_i = e^{-(\alpha+\beta E_i)}. \tag{3.5.15}$$

The entropy of this system is

$$S = k_{\mathrm{B}} H = -k_{\mathrm{B}} \sum_{i=1}^{\infty} g_i (f_i \ln f_i - f_i), \tag{3.5.16}$$

the total differential of which is

$$\mathrm{d}S = -k_{\mathrm{B}} \sum_{i=1}^{\infty} g_i (\alpha + \beta E_i) \mathrm{d}f_i. \tag{3.5.17}$$

Comparing again with the first law of thermodynamics, we conclude that $\alpha = -\beta\mu$ and $\beta = 1/k_{\mathrm{B}}T$, where μ and T are the chemical potential and thermodynamic temperature as before. Thus, we have

$$f_i = e^{-\beta(E_i-\mu)}. \tag{3.5.18}$$

This is the *Boltzmann distribution*, describing the average number of particles in a particular microstate of energy E_i.

Thus, we have the answer to our original question: the probability of finding a particle with energy between E and $E + \mathrm{d}E$ is just

$$\mathrm{d}\mathbb{P}(E) = \frac{1}{Z} g(E) f_\beta(E) \mathrm{d}E, \tag{3.5.19}$$

where the partition function may be written as

$$Z = \int \mathrm{d}E \, g(E) f_\beta(E). \tag{3.5.20}$$

Herein, we denote the continuous Boltzmann distribution by $f_\beta(E) = e^{-\beta(E-\mu)}$. $g(E)$ is the number of microstates with energy between E and $E + \mathrm{d}E$.

3.6 The Boltzmann Transport Equation

The energy of the single-particle microstate E must depend only the position and momentum of that single particle, i.e., $E \equiv E(\mathbf{q}, \mathbf{p})$. It follows then from the Vlasov equation in (3.2.20), that the Boltzmann distribution f_β, must satisfy the following equation of motion:

$$\frac{\partial f_\beta}{\partial t} + \mathbf{v} \cdot \boldsymbol{\nabla}_{\mathbf{q}} f_\beta + \mathbf{F} \cdot \boldsymbol{\nabla}_{\mathbf{p}} f_\beta = 0, \tag{3.6.1}$$

the solution of which we have established above. This is the so-called *collisionless Boltzmann equation*.

Suppose then that we perturb our gas of particles, such that the statistical distribution deviates from the Boltzmann distribution. The system will only return to equilibrium if the particles that comprise it our allowed to interact. It is clear then that the collisionless Boltzmann equation is insufficient to describe this process of *thermalisation*. For a system out of equilibrium, the statistical distribution function will depend explicitly on time. Recalling that the left-hand side of the collisionless Boltzmann equation is nothing other than the total derivative of the distribution function, it is clear that the right-hand side will no longer be zero. Instead, it will comprise terms that depend upon the interactions between the particles in the gas

— the so-called *collision terms*.

Before considering these collisions further, we shall assume our gas of particles to be *ideal*. By this, we mean that the particles are of negligible size in comparison to the distance between them and that the time between collisions is long in comparison to the characteristic length of those collisions. In fact, we shall take the particles to be point-like and the collisions to be instantaneous. It follows then that we may consider the particles to be free, in the sense that we may consider any potential energy due to the collisions to be negligible. In this case, the energy of a particle of momentum $\mathbf{p}$ is just the non-relativistic kinetic energy

$$E(\mathbf{p}) = \frac{\mathbf{p}^2}{2m}, \tag{3.6.2}$$

where m is the mass of the particle.

We shall allow then for binary collisions between the particles of our gas and consider collisions that scatter particles into or out of the volume element $\mathrm{d}^3\mathbf{p}$ taking place instantaneously at a time t and position $\mathbf{q}$. For either of these processes, we have two incoming particles of momentum $\mathbf{k}_1$ and $\mathbf{k}_2$ and two outgoing particles of momentum $\mathbf{k}_1'$ and $\mathbf{k}_2'$, where the total momentum must be conserved throughout the collision. Assuming that these collisions are elastic, the total kinetic energy must also be conserved. We then obtain the kinematic constraints

$$\mathbf{k}_1' + \mathbf{k}_2' = \mathbf{k}_1 + \mathbf{k}_2, \tag{3.6.3a}$$

$$\mathbf{k}_1'^{\,2} + \mathbf{k}_2'^{\,2} = \mathbf{k}_1^2 + \mathbf{k}_2^2, \tag{3.6.3b}$$

where the second equality results from (3.6.2), since all the particles are assumed to have the same mass. Thus, the 12 degrees of freedom (the 3 components of 4 momenta) are subject to 4 constraints: 3 from the conservation of momentum and 1 from the conservation of energy. Of the remaining 8 degrees of freedom, 3 are the components of a momentum $\mathbf{p}$ that we will fix, leaving 5 degrees of freedom over which we must sum to obtain the total cross-section for the collisions of interest.

Using (3.6.3), we may show also that the magnitude of the relative initial and final momenta are also conserved, that is

$$k^2 = (\mathbf{k}_1' - \mathbf{k}_2')^2 = (\mathbf{k}_1 - \mathbf{k}_2)^2. \tag{3.6.4}$$

It follows that the cross-section for an individual collision must be a function of the magnitude k and not the magnitudes of both the initial and final relative momenta, since these quantities are not independent. Each individual cross-section will however depend upon the angles between both pairs of initial and final momenta, of which their are 4: 2 polar and 2 azimuthal. In which case, it is clear that to calculate the total cross-section for such collisions, we must sum over one of the initial momenta, $\mathbf{k}_1$ say, and the angular degrees of freedom of one other momentum. We may parametrise this angular dependence by the solid angle Ω, swept out between the two relative momenta $\mathbf{k}_1' - \mathbf{k}_2'$ and $\mathbf{k}_1 - \mathbf{k}_2$. In all, this comprises 5 integrals as we anticipated.

The cross-section for an individual process will depend upon the relative flux of the incoming particles, which is just k/m, and the differential cross-section $\sigma' = \mathrm{d}\sigma/\mathrm{d}\Omega$, with which we parametrise the angular dependence of the collision. Both of these quantities are symmetric under the interchange of the initial and final states. However, the cross-section will also depend upon the availability of the incoming particles, which will *not* be symmetric under this interchange. The number of particles with momenta between $\mathbf{k}$ and $\mathbf{k} + \mathrm{d}^3\mathbf{k}$ is just $f(\mathbf{k}, \mathbf{q}, t)\mathrm{d}^3\mathbf{k}$.

Fixing the out-going momentum $\mathbf{k}_2' = \mathbf{p}$, the total cross-section for the scattering of particles into the volume $\mathrm{d}^3\mathbf{p}$ is

$$\mathrm{d}^3\mathbf{k}_2 \int \frac{\mathrm{d}^3\mathbf{k}_1}{h^3}\, \mathrm{d}\Omega\, \frac{k}{m}\sigma' f(\mathbf{k}_1, \mathbf{q}, t) f(\mathbf{k}_2, \mathbf{q}, t). \tag{3.6.5}$$

The total cross-section for the inverse process, whereby a particle is scattered out of the volume $\mathrm{d}^3\mathbf{p}$, is obtained by interchanging the initial and final states, such that

$\mathbf{k_1} \to \mathbf{k}_1'$ and $\mathbf{k_2} \to \mathbf{k}_2'$. Recalling that $\mathbf{k}_2' = \mathbf{p}$, we find

$$\mathrm{d}^3\mathbf{p} \int \frac{\mathrm{d}^3\mathbf{k}_1'}{h^3}\, \mathrm{d}\Omega\, \frac{k}{m}\sigma' f(\mathbf{k}_1', \mathbf{q}, t) f(\mathbf{p}, \mathbf{q}, t). \tag{3.6.6}$$

The Jacobian of the transformation $\mathbf{k}_1 \to \mathbf{k}_1'$, $\mathbf{k}_2 \to \mathbf{k}_2'$ is unity. In which case, we may rewrite (3.6.5) as

$$\mathrm{d}^3\mathbf{p} \int \frac{\mathrm{d}^3\mathbf{k}_1'}{h^3}\, \mathrm{d}\Omega\, \frac{k}{m}\sigma' f(\mathbf{k}_1, \mathbf{q}, t) f(\mathbf{k}_2, \mathbf{q}, t). \tag{3.6.7}$$

The differential cross-section σ' has dimensions of L^2 and so these results have the dimensions of T^{-1}. Thus, (3.6.7) may be interpreted as the rate of increase of the number density of particles with momentum between $\mathbf{p}$ and $\mathbf{p} + \mathrm{d}^3\mathbf{p}$ due to scattering into the volume $\mathrm{d}^3\mathbf{p}$. Conversely, (3.6.6) is the corresponding rate of decrease, resulting from the inverse process. The net increase in the number density is therefore the difference of (3.6.7) and (3.6.6), which is nothing other than the total time derivative of the statistical distribution function $f(\mathbf{p}, \mathbf{q}, t)$, i.e.,

$$\frac{\mathrm{d}f(\mathbf{p}, \mathbf{q}, t)}{\mathrm{d}t} = \int \frac{\mathrm{d}^3\mathbf{k}_1}{h^3}\, \mathrm{d}\Omega\, \frac{k}{m}\sigma' \Big[f(\mathbf{k}_1, \mathbf{q}, t) f(\mathbf{k}_2, \mathbf{q}, t) - f(\mathbf{k}_1', \mathbf{q}, t) f(\mathbf{p}, \mathbf{q}, t) \Big]. \tag{3.6.8}$$

The dimensionality of this expression is consistent with the interpretation of the statistical distribution function $f(\mathbf{p}, \mathbf{q}, t)$ as a number density in phase space. It follows then that the total number of particles per unit volume between $\mathbf{q}$ and $\mathbf{q} + \mathrm{d}^3\mathbf{q}$ is

$$n(\mathbf{q}, t) = \int \frac{\mathrm{d}^3\mathbf{p}}{h^3}\, f(\mathbf{p}, \mathbf{q}, t); \tag{3.6.9}$$

and the total number of particles is

$$N(t) = \int \mathrm{d}^3\mathbf{q}\, n(\mathbf{q}, t) = \int \mathrm{d}^3\mathbf{q} \int \frac{\mathrm{d}^3\mathbf{p}}{h^3}\, f(\mathbf{p}, \mathbf{q}, t). \tag{3.6.10}$$

The total time derivative in (3.6.8) must be equal to the left-hand side of the collisionless Boltzmann equation in (3.6.1), in which we must replace the equilibrium Boltzmann distribution by the time-dependent distribution function $f(\mathbf{p}, \mathbf{q}, t)$. We

then arrive at the *Boltzmann transport equation*

$$\frac{\partial f(\mathbf{p},\mathbf{q},t)}{\partial t} + \mathbf{v}\cdot\boldsymbol{\nabla}_{\mathbf{q}} f(\mathbf{p},\mathbf{q},t) + \mathbf{F}\cdot\boldsymbol{\nabla}_{\mathbf{p}} f(\mathbf{p},\mathbf{q},t) = \int \frac{\mathrm{d}^3\mathbf{k}_1'}{h^3}\,\mathrm{d}\Omega\,|\mathbf{v}-\mathbf{v}_1'|\sigma'\big[f(\mathbf{k}_1,\mathbf{q},t)f(\mathbf{k}_2,\mathbf{q},t) - f(\mathbf{k}_1',\mathbf{q},t)f(\mathbf{p},\mathbf{q},t)\big], \quad (3.6.11)$$

where the velocities $\mathbf{v} = \mathbf{p}/m$ and $\mathbf{v}_1' = \mathbf{k}_1'/m$ and $\mathbf{k}_2 = \mathbf{p} + \mathbf{k}_1' - \mathbf{k}_1$ by momentum conservation.

We have obtained a first-order differential equation describing the time evolution of the statistical distribution function, corresponding to the number density of our N particles in phase space. If this system is perturbed from thermodynamic equilibrium, we anticipate that its return to equilibrium will be driven by the collision terms, proceeding until those terms vanish. As a final check therefore, let us replace the time-dependent distribution function in the binary collision terms by the Boltzmann distribution and show that they do indeed vanish as we expect. After making this substitution, we obtain the difference of two exponentials:

$$e^{-\beta(\mathbf{p}^2+\mathbf{k}_1{}'^2)/2m} - e^{-\beta(\mathbf{k}_1^2+\mathbf{k}_2^2)/2m}. \quad (3.6.12)$$

By conservation of energy, the exponents of these two terms are identical and the rates of scatterings into and out of the phase space volume $\mathrm{d}^3\mathbf{p}$ are equal. Thus, the exponential form of the Boltzmann distribution and the conservation of energy are sufficient to ensure that the collision terms vanish and we conclude that the Boltzmann distribution also describes the equilibrium distribution of our idealised gas of interacting particles.

The aim of the remainder of this thesis is to generalise these statistical distribution functions and their transport equations to quantum field theory.

4 Quantum Statistical Mechanics

Before proceeding to the full quantum field-theoretic description of the macroscopic phenomena introduced in the previous chapter, we should first review the corresponding quantum-mechanical approach — *quantum statistical mechanics.*

In this chapter, we will set out from the first quantisation of classical mechanics in the familiar wave picture due to Erwin Schrödinger. Having introduced the familiar states, operators and observables, we will emphasise the time-dependence of the various pictures: the Schrödinger, Heisenberg and interaction pictures. After defining the quantum mechanical density operator, we move on to many-body quantum systems, introducing the quantum statistical density operator and its relation to the partition function. Finally, by considering the archetypal quantum harmonic oscillator, we derive the statistical distribution function of integer-spin quanta, i.e., bosons — the Bose-Einstein distribution.

For a comprehensive discussion of the concepts introduced in this chapter, the reader is directed to the text by J. J. Sakurai [59].

4.1 Quantisation

The classical numbers q and p, corresponding to one-dimensional coordinates of position and momentum, are now superseded by the quantum mechanical position and momentum operators $\hat{q}$ and $\hat{p}$. These operators allow us to make measurements of the positions and momenta of a quantum state, which is described in the Schrödinger

picture of quantum mechanics by a wavefunction $\psi(q,\tilde{t})$. The modulus squared of this wavefunction

$$|\psi(q,\tilde{t})|^2 = \psi^*(q,\tilde{t})\psi(q,\tilde{t}) \tag{4.1.1}$$

is the probability density that, at a time $\tilde{t}$, the quantum state will be found at a position between q and $q+\mathrm{d}q$. The quantum state must be somewhere and as such the wavefunction satisfies the normalisation

$$\int_{-\infty}^{+\infty} \mathrm{d}q\, \psi^*(q,\tilde{t})\psi(q,\tilde{t}) = 1. \tag{4.1.2}$$

The expectation value of a general operator $\hat{O}$ is then

$$\langle O\rangle = \int_{-\infty}^{+\infty} \mathrm{d}q\, \psi^*(q,\tilde{t})\hat{O}\psi(q,\tilde{t}). \tag{4.1.3}$$

The 'time' appearing in this wavefunction has deliberately been denoted with a tilde. This is to differentiate these *microscopic times* from the *macroscopic times* of thermodynamics. This may seem particularly pedantic, but our motivation is this: the second law of thermodynamics — the law of increase of entropy. This law seemingly gives the 'time' of thermodynamics a preferred direction. By this, we do not mean that time must always run in the same direction — we hope to avoid a philosophical discussion of the *arrow of time* – and in fact, we made use of reversible processes to derive the first law of thermodynamics. Instead, we mean that processes occurring out of thermodynamic equilibrium, i.e., those which do not take place quasi-statically, cannot be reversed exactly. In other words, the process and its inverse are asymmetric. In this case, our 'preferred direction' is a rather ambiguous statement of the violation of *time-reversal symmetry* on macroscopic scales. On the other hand, the microscopic equations of motion — including those of Newton, Hamilton and Lagrange — are entirely symmetric under this time reversal. This then is our justification for distinguishing these two times: dependence upon microscopic times is constrained to be symmetric under time reversal, whereas dependence upon macroscopic times is not.

The wavefunction evolves according to the Schrödinger equation

$$\hat{H}\psi(q,\tilde{t}) = i\hbar\frac{\partial}{\partial\tilde{t}}\psi(q,\tilde{t}), \tag{4.1.4}$$

where $\hat{H}$ is the Hamiltonian operator, which will be some combination of the position and momentum operators. The constant $\hbar$ is Planck's constant h divided by 2π, having the units of action. The Hamiltonian operator allows us to make a measurement of the energy of a quantum state and the presumption therefore is that the wavefunction describes a state of definite energy. Looking again at the expectation value in (4.1.3), it is clear that a suitable representation of the position operator is simply the position q. We may obtain the coordinate representation of the momentum operator by differentiating the Schrödinger equation with respect to this position:

$$\frac{\partial\hat{H}}{\partial q}\psi(q,\tilde{t}) = i\hbar\frac{\partial^2}{\partial\tilde{t}\partial q}\psi(q,\tilde{t}), \tag{4.1.5}$$

where we have commuted the partial derivatives on the right-hand side. From Hamilton's equations of motion (3.1.16b), the partial derivative of the Hamiltonian is related to the partial time derivative of the momentum. We then obtain

$$\hat{p} = -i\hbar\frac{\partial}{\partial q}. \tag{4.1.6}$$

From this coordinate representation of the momentum operator, we may derive the *canonical commutation relation*

$$\left[\hat{q},\hat{p}\right] = \hat{q}\hat{p} - \hat{p}\hat{q} = i\hbar. \tag{4.1.7}$$

This commutation relation expresses a fundamental incompatibility between simultaneous measurements of the position and momenta of a quantum state — the *Heisenberg uncertainty principle*. The uncertainties in any such measurements must satisfy

$$\Delta q\Delta p \geq \frac{\hbar}{2}. \tag{4.1.8}$$

This result presents us with a problem. The statistical approach of the previous chapter relied on our ability to write down the statistical distribution function $f(\mathbf{q}, \mathbf{p}, t)$, which depends simultaneously upon both position and momentum. This is seemingly forbidden by the uncertainty principle. We have however already established the solution. Each representative point in phase space (representative of a given microstate) was smeared out by a factor of the constant h, which had the dimensions of action. This smearing out is exactly what is required by the uncertainty principle and this h must be Planck's constant. It follows therefore that the microstates of quantum mechanical systems are the quantum states themselves.

Introducing the *braket* notation due to Dirac, we may write the coordinate-space wavefunction as the inner product between vectors of a Hilbert space

$$\psi(q, \tilde{t}) = \langle q|\psi(\tilde{t})\rangle \,. \tag{4.1.9}$$

The basis vectors $|q\rangle$ are eigenstates of the position operator $\hat{q}$, satisfying the eigenvalue equation

$$\hat{q}\,|q\rangle = q\,|q\rangle \,, \tag{4.1.10}$$

where the eigenvalue q is the observable position of the state $|q\rangle$. We may also introduce the momentum-space wavefunction

$$\psi(p, \tilde{t}) = \langle p|\psi(\tilde{t})\rangle, \tag{4.1.11}$$

representing the probability that a quantum state has the momentum p. The basis vectors $|p\rangle$ are eigenstates of the momentum operator $\hat{p}$, satisfying the eigenvalue equation

$$\hat{p}\,|p\rangle = p\,|p\rangle \,. \tag{4.1.12}$$

These position and momentum eigenstates form complete orthonormal bases, satis-

fying the orthogonality conditions

$$\langle q|q'\rangle = \delta(q-q'), \tag{4.1.13a}$$

$$\langle p|p'\rangle = 2\pi\hbar\delta(p-p'). \tag{4.1.13b}$$

and the completeness relations

$$\int_{-\infty}^{+\infty} \mathrm{d}q\ |q\rangle\langle q| = \mathbb{I}, \tag{4.1.14a}$$

$$\int_{-\infty}^{+\infty} \frac{\mathrm{d}p}{2\pi\hbar}\ |p\rangle\langle p| = \mathbb{I}. \tag{4.1.14b}$$

The appearance of Planck's constant in the denominator of the momentum integration is consistent with our treatment of the classical phase space in the previous chapter, cf. (3.2.5), such that the volume element

$$\frac{\mathrm{d}q\,\mathrm{d}p}{2\pi\hbar} \tag{4.1.15}$$

is dimensionless. The position and momentum eigenstates have respective dimensions of $\mathrm{L}^{-1/2}$ and $\mathrm{L}^{1/2}$.

By inserting into (4.1.9) the completeness relation of the momentum eigenstates, we may relate the coordinate- and momentum-space wavefunctions via

$$\psi(q,\tilde{t}) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}p}{2\pi\hbar}\ \langle q|p\rangle\,\psi(p,\tilde{t}). \tag{4.1.16}$$

Using the canonical commutation relation (4.1.7) and the coordinate representation of the momentum operator (4.1.6), we may show that the kernel

$$\langle q|p\rangle = e^{iqp/\hbar} \tag{4.1.17}$$

is that of the inverse Fourier transform. Hence, the position- and momentum-space

wavefunctions are related by

$$\psi(q,\tilde{t}) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}p}{2\pi\hbar}\, e^{iqp/\hbar}\, \psi(p,\tilde{t}), \tag{4.1.18}$$

as we would anticipate.

In braket notation, the expectation value of the operator $\hat{O}$ may be written in the form

$$\langle O(\tilde{t})\rangle = \langle\psi(\tilde{t})|\hat{O}|\psi(\tilde{t})\rangle\,. \tag{4.1.19}$$

We see that all time-dependence is contained in the state vectors $|\psi(\tilde{t})\rangle$. This defines the so-called *Schrödinger picture*, in which basis vectors and operators are *time-independent* and state vectors are *time-dependent*. The evolution of the state vector $|\psi(\tilde{t})\rangle$ is determined by

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}\tilde{t}}\,|\psi(\tilde{t})\rangle = \hat{H}\,|\psi(\tilde{t})\rangle\,. \tag{4.1.20}$$

The Hamiltonian is time-independent and it follows straightforwardly that the state vector at a time $\tilde{t}$ may be related to the state vector at an earlier time $\tilde{t}_i$ by

$$|\psi(\tilde{t})\rangle = e^{-i\hat{H}(\tilde{t}-\tilde{t}_i)/\hbar}\,|\psi(\tilde{t}_i)\rangle\,. \tag{4.1.21}$$

This defines the *evolution operator*

$$\hat{U}(\tilde{t},\tilde{t}_i) = e^{-i\hat{H}(\tilde{t}-\tilde{t}_i)/\hbar}, \tag{4.1.22}$$

whose action is to evolve the state vector forwards in time from $\tilde{t}_i$ to $\tilde{t}$.

We may now write the expectation value of an operator in an alternate form:

$$\langle O(\tilde{t})\rangle = {}_{\mathrm{S}}\langle\psi(\tilde{t}_i)|e^{i\hat{H}_{\mathrm{S}}(\tilde{t}-\tilde{t}_i)/\hbar}\hat{O}_{\mathrm{S}}e^{-i\hat{H}_{\mathrm{S}}(\tilde{t}-\tilde{t}_i)/\hbar}|\psi(\tilde{t}_i)\rangle_{\mathrm{S}}. \tag{4.1.23}$$

We have been careful to indicate by a subscript S that the state vectors and operators are understood in the *Schrödinger picture*. From this expression, we may define a new picture in which all of the time dependence is in the operators. This is the

so-called *Heisenberg picture*. The *time-independent* Heisenberg-picture state vector is defined as

$$|\psi\rangle_{\mathrm{H}} \equiv |\psi(\tilde{t}_i)\rangle_{\mathrm{S}}, \tag{4.1.24}$$

which depends implicitly on the time $\tilde{t}_i$. The *time-dependent*, Heisenberg-picture operator is

$$\hat{O}_{\mathrm{H}}(\tilde{t}) \equiv e^{i\hat{H}_{\mathrm{S}}(\tilde{t}-\tilde{t}_i)/\hbar}\hat{O}_{\mathrm{S}}e^{-i\hat{H}_{\mathrm{S}}(\tilde{t}-\tilde{t}_i)/\hbar}, \tag{4.1.25}$$

in which case the expectation value in the Heisenberg picture is

$$\langle O(\tilde{t})\rangle = {}_{\mathrm{H}}\langle\psi|\hat{O}_{\mathrm{H}}(\tilde{t})|\psi\rangle_{\mathrm{H}}. \tag{4.1.26}$$

The Heisenberg-picture operator evolves according to the *Heisenberg equation of motion*

$$\frac{\mathrm{d}}{\mathrm{d}\tilde{t}}\hat{O}_{\mathrm{H}}(\tilde{t}) = \frac{i}{\hbar}\big[\hat{H}_{\mathrm{H}}, \hat{O}_{\mathrm{H}}(\tilde{t})\big]. \tag{4.1.27}$$

The full Hamiltonian commutes with itself and the Heisenberg- and Schrödinger-picture Hamiltonians are identical. In corollary, the full Hamiltonian remains *time-independent* in the Heisenberg picture. Returning to (4.1.9), the equivalence of these two pictures requires that the coordinate-space basis vectors are *time-dependent* in the Heisenberg picture, that is to say

$$|q(\tilde{t})\rangle_{\mathrm{H}} = e^{i\hat{H}_{\mathrm{S}}(\tilde{t}-\tilde{t}_i)/\hbar}|q\rangle_{\mathrm{S}}, \tag{4.1.28}$$

evolving with the complex-conjugate of the Schrödinger equation. The coordinate space wave-function may then be written in terms of basis and state vectors in the Heisenberg picture as

$$\psi(q,\tilde{t}) = {}_{\mathrm{H}}\langle q(\tilde{t})|\psi\rangle_{\mathrm{H}}. \tag{4.1.29}$$

4.2 The Interaction Picture

Finally, let us suppose that we are interested in the evolution of states as a result of interactions, as will indeed be the case for the rest of this thesis. We divide the full Hamiltonian into free and interaction parts, i.e.,

$$\hat{H}_{\mathrm{S}} \equiv \hat{H}_{\mathrm{S}}^{0} + \hat{H}_{\mathrm{S}}^{\mathrm{int}}. \tag{4.2.1}$$

We may then define *time-dependent*, interaction-picture state vectors according to

$$|\psi(\tilde{t})\rangle_{\mathrm{I}} \equiv e^{i\hat{H}_{\mathrm{S}}^{0}(\tilde{t}-\tilde{t}_i)/\hbar}|\psi(\tilde{t})\rangle_{\mathrm{S}} = e^{-i\hat{H}_{\mathrm{S}}^{\mathrm{int}}(\tilde{t}-\tilde{t}_i)/\hbar}|\psi(\tilde{t}_i)\rangle_{\mathrm{S}}, \tag{4.2.2}$$

whose evolution is driven entirely by the interaction part of the Hamiltonian. The interaction-picture basis states are

$$|q(\tilde{t})\rangle_{\mathrm{I}} \equiv e^{i\hat{H}_{\mathrm{S}}^{0}(\tilde{t}-\tilde{t}_i)/\hbar}|q\rangle_{\mathrm{S}} \tag{4.2.3}$$

and the interaction-picture operator is

$$\hat{O}_{\mathrm{I}}(\tilde{t}) \equiv e^{i\hat{H}_{\mathrm{S}}^{0}(\tilde{t}-\tilde{t}_i)/\hbar}\hat{O}_{\mathrm{S}}e^{-i\hat{H}_{\mathrm{S}}^{0}(\tilde{t}-\tilde{t}_i)/\hbar}, \tag{4.2.4}$$

both of which are now *time dependent*.

From (4.2.4), the free part of the Hamiltonian remains *time-independent* in the interaction picture. The interaction part of the Hamiltonian, on the other hand, becomes *time-dependent*, since the free and interaction parts of the Hamiltonian do not necessarily commute. The interaction part

$$\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}) = e^{i\hat{H}_{\mathrm{S}}^{0}(\tilde{t}-\tilde{t}_i)/\hbar}\hat{H}_{\mathrm{S}}^{\mathrm{int}}e^{-i\hat{H}_{\mathrm{S}}^{0}(\tilde{t}-\tilde{t}_i)/\hbar}. \tag{4.2.5}$$

may be written by virtue of the Baker-Campbell-Hausdorff formula as

$$\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}) = \mathrm{Ad}_{i\hat{H}_{\mathrm{S}}^{0}(\tilde{t}-\tilde{t}_i)/\hbar}\hat{H}_{\mathrm{S}}^{\mathrm{int}}, \tag{4.2.6}$$

where $\mathrm{Ad}_X \equiv e^{\mathrm{ad}_X}$ and ad_X is the adjoint representation of the commutator

$$\mathrm{ad}_X(Y) = [X, Y]. \tag{4.2.7}$$

It follows that the evolution of the interaction-picture state vector is determined by the equation of motion

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}\tilde{t}} |\psi(\tilde{t})\rangle_{\mathrm{I}} = \hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}) |\psi(\tilde{t})\rangle_{\mathrm{I}}, \tag{4.2.8}$$

where we emphasise the time dependence of the interaction part of the Hamiltonian. The basis states evolve under the free part of the Hamiltonian according to

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}\tilde{t}} |q(\tilde{t})\rangle_{\mathrm{I}} = -\hat{H}_{\mathrm{I}}^{0} |q(\tilde{t})\rangle_{\mathrm{I}}; \tag{4.2.9}$$

and the operator, according to

$$\frac{\mathrm{d}}{\mathrm{d}\tilde{t}} \hat{O}_{\mathrm{I}}(\tilde{t}) = \frac{i}{\hbar} \big[\hat{H}_{\mathrm{I}}^{0}, \hat{O}_{\mathrm{I}}(\tilde{t})\big]. \tag{4.2.10}$$

In order to solve (4.2.8), we return to the evolution operator, which in the interaction picture may be written in terms of the interaction-part of the Hamiltonian in Schrödinger-picture as

$$\hat{U}(\tilde{t}, \tilde{t}_i) = e^{-i\hat{H}_{\mathrm{S}}^{\mathrm{int}}(\tilde{t} - \tilde{t}_i)}, \tag{4.2.11}$$

which evolves the interaction-picture state vector $|\psi(\tilde{t}_i)\rangle_{\mathrm{I}}$ from a time $\tilde{t}_i$ to a time $\tilde{t}$, i.e.,

$$|\psi(\tilde{t})\rangle_{\mathrm{I}} = \hat{U}(\tilde{t}, \tilde{t}_i) |\psi(\tilde{t}_i)\rangle_{\mathrm{I}}. \tag{4.2.12}$$

For convenience, we have not included a subscript I on this evolution operator but we emphasise its distinction from (4.1.22). If follows from (4.2.8) that $\hat{U}(\tilde{t}, \tilde{t}_i)$ must satisfy

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}\tilde{t}} \hat{U}(\tilde{t}, \tilde{t}_i) = \hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}) \hat{U}(\tilde{t}, \tilde{t}_i), \tag{4.2.13}$$

subject to the boundary condition

$$\hat{U}(\tilde{t}, \tilde{t}) = \mathbb{I} \tag{4.2.14}$$

for all times $\tilde{t}$. Furthermore, we may convince ourselves that $\hat{U}$ is Markovian, satisfying

$$\hat{U}(\tilde{t},\tilde{t}_1)\hat{U}(\tilde{t}_1,\tilde{t}_i)=\hat{U}(\tilde{t},\tilde{t}_i). \tag{4.2.15}$$

In this case, it would appear that the evolution between $\tilde{t}_1$ and $\tilde{t}$ is independent of the evolution between $\tilde{t}_1$ and $\tilde{t}_i$. In other words, at least microscopically, there is no memory of the previous history of the evolution. Of course, for a macroscopic system evolving out of thermodynamic equilibrium, we cannot yet exclude such *memory effects* and indeed this non-Markovian macroscopic evolution should signal departure from equilibrium.

The inverse of the evolution operator $\hat{U}^{-1}(\tilde{t},\tilde{t}_i)$, which evolves the interaction-picture state vector back from the time $\tilde{t}$ to the time $\tilde{t}_i$, is defined via the inverse relation

$$\hat{U}^{-1}(\tilde{t},\tilde{t}_i)\hat{U}(\tilde{t},\tilde{t}_i)=\mathbb{I}, \tag{4.2.16}$$

since, at least microscopically, the evolution may always be reversed. Given the Markovian property in (4.2.15), it follows that

$$\hat{U}^{-1}(\tilde{t},\tilde{t}_i)=\hat{U}(\tilde{t}_i,\tilde{t}). \tag{4.2.17}$$

Differentiating (4.2.16) and using (4.2.13), $\hat{U}^{-1}(\tilde{t},\tilde{t}_i)$ is the solution to

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}\tilde{t}}\hat{U}^{-1}(\tilde{t},\tilde{t}_i)=-\hat{U}^{-1}(\tilde{t},\tilde{t}_i)\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}), \tag{4.2.18}$$

from which we may confirm that $\hat{U}(\tilde{t},\tilde{t}_i)$ is unitary with

$$\hat{U}^{-1}(\tilde{t},\tilde{t}_i)=\hat{U}^{\dagger}(\tilde{t},\tilde{t}_i)=e^{i\hat{H}_{\mathrm{S}}^{\mathrm{int}}(\tilde{t}-\tilde{t}_i)/\hbar}, \tag{4.2.19}$$

where $\dagger$ denotes the Hermitian conjugate of the operator—the complex conjugate of the transpose of the operator. We have also used the fact that the Hamiltonian is necessarily Hermitian, that is Hermitian self-conjugate, such that it has real eigenvalues. The unitary property ensures that the total probability is conserved during

the evolution.

We have so far written the explicit form of the evolution operator in terms of Schrödinger-picture operators only. In order to express $\hat{U}(\tilde{t},\tilde{t}_i)$ in terms of interaction-picture operators, we return to (4.2.13), transforming the equation of motion into the form of a Volterra integral equation of the second kind:

$$\hat{U}(\tilde{t},\tilde{t}_i) = \mathbb{I} - \frac{i}{\hbar}\int_{\tilde{t}_i}^{\tilde{t}} \mathrm{d}\tilde{t}_1\, \hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1)\hat{U}(\tilde{t}_1,\tilde{t}_i), \tag{4.2.20}$$

where we have used the boundary condition in (4.2.14). By repeatedly reinserting this result into itself—the successive approximation method—we obtain the Neumann series (see for instance [60])

$$\hat{U}(\tilde{t},\tilde{t}_i) = \mathbb{I} - \frac{i}{\hbar}\int_{\tilde{t}_i}^{\tilde{t}} \mathrm{d}\tilde{t}_1\, \hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1) + \Big(-\frac{i}{\hbar}\Big)^2 \int_{\tilde{t}_i}^{\tilde{t}} \mathrm{d}\tilde{t}_1 \int_{\tilde{t}_i}^{\tilde{t}_1} \mathrm{d}\tilde{t}_2\, \hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1)\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_2) + \cdots \tag{4.2.21}$$

Let us look more closely at the third term in (4.2.21). In the $\tilde{t}_1$-$\tilde{t}_2$ plane, the region of integration is the triangle bounded by $\tilde{t}_1 = \tilde{t}$, $\tilde{t}_1 = \tilde{t}_2$ and $\tilde{t}_2 = \tilde{t}_i$. By changing the order of integration, we may show that

$$\int_{\tilde{t}_i}^{\tilde{t}} \mathrm{d}\tilde{t}_1 \int_{\tilde{t}_i}^{\tilde{t}_1} \mathrm{d}\tilde{t}_2\, \hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1)\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_2) = \int_{\tilde{t}_i}^{\tilde{t}} \mathrm{d}\tilde{t}_2 \int_{\tilde{t}_2}^{\tilde{t}} \mathrm{d}\tilde{t}_1\, \hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1)\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_2). \tag{4.2.22}$$

Subsequently making the change of variables $\tilde{t}_1 \leftrightarrow \tilde{t}_2$ on the right-hand side, we obtain the identity

$$\int_{\tilde{t}_i}^{\tilde{t}} \mathrm{d}\tilde{t}_1 \int_{\tilde{t}_i}^{\tilde{t}_1} \mathrm{d}\tilde{t}_2\, \hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1)\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_2) = \int_{\tilde{t}_i}^{\tilde{t}} \mathrm{d}\tilde{t}_1 \int_{\tilde{t}_1}^{\tilde{t}} \mathrm{d}\tilde{t}_2\, \hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_2)\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1). \tag{4.2.23}$$

On the left-hand side, $\tilde{t}_1 \geq \tilde{t}_2$, where as, on the right-hand side, $\tilde{t}_2 \geq \tilde{t}_1$. Noticing that the Hamiltonian operators are always ordered with the left-most having the largest (or latest) time, we introduce the *time-ordering operator*

$$\mathrm{T}\big[\hat{O}(\tilde{t}_1)\hat{O}(\tilde{t}_2)\cdots\hat{O}(\tilde{t}_n)\big] = \hat{O}(\tilde{t}_1)\hat{O}(\tilde{t}_2)\cdots\hat{O}(\tilde{t}_n),\ \tilde{t}_1 \geq \tilde{t}_2 \geq \cdots \geq \tilde{t}_n. \tag{4.2.24}$$

By adding to both sides of (4.2.23) a duplicate of the left-hand side, we may write

$$\begin{aligned}\int_{\tilde{t}_i}^{\tilde{t}}\mathrm{d}\tilde{t}_1\int_{\tilde{t}_i}^{\tilde{t}_1}\mathrm{d}\tilde{t}_2\,\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1)\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_2) &= \frac{1}{2}\Bigg[\int_{\tilde{t}_i}^{\tilde{t}}\mathrm{d}\tilde{t}_1\int_{\tilde{t}_1}^{\tilde{t}}\mathrm{d}\tilde{t}_2\,\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_2)\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1)\\ &\qquad\qquad+\int_{\tilde{t}_i}^{\tilde{t}}\mathrm{d}\tilde{t}_1\int_{\tilde{t}_i}^{\tilde{t}_1}\mathrm{d}\tilde{t}_2\,\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1)\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_2)\Bigg]\\ &= \frac{1}{2}\int_{\tilde{t}_i}^{\tilde{t}}\mathrm{d}\tilde{t}_1\left[\int_{\tilde{t}_1}^{\tilde{t}}\mathrm{d}\tilde{t}_2+\int_{\tilde{t}_i}^{\tilde{t}_1}\mathrm{d}\tilde{t}_2\right]\mathrm{T}\big[\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1)\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_2)\big]\\ &= \frac{1}{2}\int_{\tilde{t}_i}^{\tilde{t}}\mathrm{d}\tilde{t}_1\int_{\tilde{t}_i}^{\tilde{t}}\mathrm{d}\tilde{t}_2\,\mathrm{T}\big[\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1)\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_2)\big],\end{aligned}\tag{4.2.25}$$

such that all integrations now run from $\tilde{t}_i$ to $\tilde{t}$. It follows that the Neumann series (4.2.20) may be recast in the form

$$\hat{U}(\tilde{t},\tilde{t}_i)=\mathbb{I}-\frac{i}{\hbar}\int_{\tilde{t}_i}^{\tilde{t}}\mathrm{d}\tilde{t}_1\,\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1)+\frac{1}{2!}\Big(-\frac{i}{\hbar}\Big)^2\int_{\tilde{t}_i}^{\tilde{t}}\mathrm{d}\tilde{t}_1\int_{\tilde{t}_i}^{\tilde{t}}\mathrm{d}\tilde{t}_2\,\mathrm{T}\big[\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1)\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_2)\big]+\cdots.\tag{4.2.26}$$

Recognising this series as the expansion of the exponential function, we obtain the solution

$$\hat{U}(\tilde{t},\tilde{t}_i)=\mathrm{T}\left[\exp\left(-\frac{i}{\hbar}\int_{\tilde{t}_i}^{\tilde{t}}\mathrm{d}\tilde{t}'\,\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}')\right)\right].\tag{4.2.27}$$

There is however an implicit assumption in this result. The validity of the expansion requires that the integral in the exponent is small in comparison to $\hbar$. Therefore, either the time interval $\tilde{t}-\tilde{t}_i$ must be comparably short; the interactions must be comparably weak, so that there contribution to the energy is small; or both.

The equation of motion of the inverse evolution operator has the integral form

$$\hat{U}^{-1}(\tilde{t},\tilde{t}_i)=\mathbb{I}+\frac{i}{\hbar}\int_{\tilde{t}_i}^{\tilde{t}}\mathrm{d}\tilde{t}_1\,\hat{U}^{-1}(\tilde{t}_1,\tilde{t}_i)\hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}_1).\tag{4.2.28}$$

Following the same procedure as above, repeatedly inserting this expression into itself, we will end up with the rightmost (as opposed to the leftmost) operator having the largest time. As such, we must introduce the *anti-time-ordering operator*

$$\bar{\mathrm{T}}\big[\hat{O}(\tilde{t}_1)\hat{O}(\tilde{t}_2)\cdots\hat{O}(\tilde{t}_n)\big]=\hat{O}(\tilde{t}_n)\cdots\hat{O}(\tilde{t}_2)\hat{O}(\tilde{t}_1),\ \tilde{t}_1\geq\tilde{t}_2\geq\cdots\geq\tilde{t}_n.\tag{4.2.29}$$

We then obtain

$$\hat{U}^{-1}(\tilde{t},\tilde{t}_i) = \bar{\mathrm{T}}\left[\exp\left(\frac{i}{\hbar}\int_{\tilde{t}_i}^{\tilde{t}} \mathrm{d}\tilde{t}'\, \hat{H}_{\mathrm{I}}^{\mathrm{int}}(\tilde{t}')\right)\right]. \tag{4.2.30}$$

4.3 The Density Operator

In the previous chapter, our statistical description of macroscopic systems stemmed from the density in phase space or classical distribution function. Our aim in this section is to introduce the corresponding object in quantum statistical mechanics: *the density operator*.

Let us consider a closed quantum mechanical subsystem $\mathscr{S}$ in thermodynamic equilibrium, which is at time $\tilde{t}$ described by the state vector $|\Psi(\tilde{t})\rangle_{\mathrm{S}}$. This subsystem is to be the quantum analogue of our gas of particles. The state vector $|\Psi(\tilde{t})\rangle_{\mathrm{S}}$ is a coherent sum over all possible quantum states of $\mathscr{S}$, where those quantum states constitute the microstates of $\mathscr{S}$. The expectation value of the Schrödinger-picture operator $\hat{O}_{\mathrm{S}}$ is then

$$\langle O(\tilde{t})\rangle = {}_{\mathrm{S}}\langle\Psi(\tilde{t})|\hat{O}_{\mathrm{S}}|\Psi(\tilde{t})\rangle_{\mathrm{S}}. \tag{4.3.1}$$

We introduce the complete orthonormal set of state vectors $\{|\psi_i(\tilde{t})\rangle_{\mathrm{S}}\}$, which are the accessible microstates of $\mathscr{S}$. These state vectors satisfy the orthonormality condition

$${}_{\mathrm{S}}\langle\psi_i(\tilde{t})|\psi_j(\tilde{t})\rangle_{\mathrm{S}} = \delta_{ij}, \tag{4.3.2}$$

and the completeness relation

$$\sum_i |\psi_i(\tilde{t})\rangle_{\mathrm{S}}\,{}_{\mathrm{S}}\langle\psi_i(\tilde{t})| = \mathbb{I}, \tag{4.3.3}$$

where δ_{ij} is again the Kronecker delta. Inserting the orthonormality condition (4.3.3) to the left and right of the operator in (4.3.1), the expectation value may be rewritten as

$$\langle O(\tilde{t})\rangle = \sum_{ij} a_i^*(\tilde{t})a_j(\tilde{t})\,{}_{\mathrm{S}}\langle\psi_i(\tilde{t})|\hat{O}_{\mathrm{S}}|\psi_j(\tilde{t})\rangle_{\mathrm{S}}, \tag{4.3.4}$$

where the amplitudes are given by

$$a_i(\tilde{t}) = {}_{\mathrm{S}}\langle\psi_i(\tilde{t})|\Psi(\tilde{t})\rangle_{\mathrm{S}}. \tag{4.3.5}$$

This is the probability amplitude that $\mathscr{S}$ is in the i-th microstate at a time $\tilde{t}$. We have then the coherent decomposition

$$|\Psi(\tilde{t})\rangle_{\mathrm{S}} = \sum_i a_i(\tilde{t})|\psi_i(\tilde{t})\rangle_{\mathrm{S}}. \tag{4.3.6}$$

Alternatively, we may write this expectation value as

$$\langle O(\tilde{t})\rangle = \operatorname{tr}\hat{\varrho}_{\mathrm{S}}(\tilde{t})\hat{O}_{\mathrm{S}}, \tag{4.3.7}$$

defining the *quantum-mechanical density operator*

$$\hat{\varrho}_{\mathrm{S}}(\tilde{t}) = \sum_{ij} a_i^*(\tilde{t})a_j(\tilde{t})|\psi_j(\tilde{t})\rangle_{\mathrm{S}}\,{}_{\mathrm{S}}\langle\psi_i(\tilde{t})| = |\Psi(\tilde{t})\rangle_{\mathrm{S}}\,{}_{\mathrm{S}}\langle\Psi(\tilde{t})|, \tag{4.3.8}$$

where we have made use of the cyclicity of the trace

$$\operatorname{tr} ABC = \operatorname{tr} CAB = \operatorname{tr} BCA. \tag{4.3.9}$$

We note that this density operator is *time-dependent* in the Schrödinger picture, evolving according to the *quantum Liouville* or *von Neumann equation*

$$\frac{\mathrm{d}}{\mathrm{d}\tilde{t}}\hat{\varrho}_{\mathrm{S}}(\tilde{t}) + \frac{i}{\hbar}\big[\hat{H}_{\mathrm{S}}, \hat{\varrho}_{\mathrm{S}}(\tilde{t})\big] = 0, \tag{4.3.10}$$

such that $\hat{\varrho}_{\mathrm{S}}(\tilde{t}) = e^{-i\hat{H}_{\mathrm{S}}(\tilde{t}-\tilde{t}_i)/\hbar}\hat{\varrho}_{\mathrm{S}}(\tilde{t}_0)e^{i\hat{H}_{\mathrm{S}}(\tilde{t}-\tilde{t}_i)/\hbar}$. The Poisson brackets of the classical Liouville equation (3.2.18) have been replaced by the commutator of operators. We note that this differs by an overall sign from the Heisenberg equation of motion, cf. (4.1.27). This is as we should expect since, in the Heisenberg-picture, the density operator is *time-independent* and the evolution is passed on to the operators, which must evolve contrary to the Schrödinger-picture density operator for the two pictures

to remain equivalent. The interaction-picture density operator, on the other hand, evolves according to

$$\frac{\mathrm{d}}{\mathrm{d}\tilde{t}}\hat{\varrho}_{\mathrm{I}}(\tilde{t}) = -\frac{i}{\hbar}\big[\hat{H}^{\mathrm{int}}_{\mathrm{I}}(\tilde{t}), \hat{\rho}_{\mathrm{I}}(\tilde{t})\big] = \hat{\mathcal{L}}(\tilde{t})\hat{\varrho}(\tilde{t}), \tag{4.3.11}$$

where we have introduced the Liouvillian $\hat{\mathcal{L}}(\tilde{t}) = \mathrm{ad}_{-i\hat{H}^{\mathrm{int}}_{\mathrm{I}}/\hbar}(\tilde{t})$.

We have specified that the subsystem $\mathscr{S}$ is in a state of thermodynamic equilibrium. As such, the only time evolution should be that intrinsic to the state vectors themselves, described by the Schrödinger equation. It follows then that the amplitudes $a_i(t)$ must be time-independent. However, these amplitudes are microscopic quantities and must therefore be subject to random, stochastic fluctuations. The period τ of these fluctuations must be cut off at some characteristic time-scale, τ_c say, which, by the uncertainty principle, must be of order $\hbar/k_{\mathrm{B}}T$, where k_{B} is the Boltzmann constant and T is the thermodynamic temperature of the system $\mathscr{S}$. Working in natural units with $\hbar$ and k_{B} set to unity, we conclude that τ must be less than of order the inverse thermodynamic temperature $\beta = 1/T$. In which case, our interest is in the time-average of these quantum-mechanical expectation values over periods of order β. By the ergodic hypothesis, see Section 3.2, we shall refer to these time-averaged observables as *ensemble expectation values* (EEVs).

Returning to (4.3.7), let us now assume that the commutator $\big[\hat{H}_{\mathrm{S}}, \hat{O}_{\mathrm{S}}\big]$ vanishes, such that $\hat{O}_{\mathrm{S}}$ is diagonal in the basis of state vectors. As a result, the matrix element

$$O_{ij} = {}_{\mathrm{S}}\langle\psi_i(\tilde{t})|\hat{O}_{\mathrm{S}}|\psi_j(\tilde{t})\rangle_{\mathrm{S}} \tag{4.3.12}$$

is time-independent, vanishing for $i \neq j$. In this case, we may write the expectation value as

$$\langle O(\tilde{t})\rangle = \varrho_{ii}(\tilde{t})O_{ii}, \tag{4.3.13}$$

where the summation over i is implicit and

$$\varrho_{ii}(\tilde{t}) = |a_i(\tilde{t})|^2. \tag{4.3.14}$$

The only remaining time-dependence is that due to the random, microscopic fluctuations. We then define the EEV

$$\langle O \rangle_\beta = \rho_{ii}(\beta) O_{ii}, \tag{4.3.15}$$

where

$$\rho_{ii}(\beta) \approx \frac{1}{\beta} \int_0^\beta \mathrm{d}\tilde{t}\, \varrho_{ii}(\tilde{t}) = \frac{1}{\beta} \int_0^\beta \mathrm{d}\tilde{t}\, |a_i(\tilde{t})|^2 \tag{4.3.16}$$

is the *quantum-statistical density matrix*. It follows that the quantum-statistical density *operator* may be written in the form

$$\hat{\rho}_{\mathrm{S}}(\beta) = \rho_{ii}(\beta) |\psi_i(\tilde{t})\rangle_{\mathrm{S}\,\mathrm{S}} \langle \psi_i(\tilde{t})|, \tag{4.3.17}$$

which is time-independent as we expected. Of course, this object need not be diagonal and in general

$$\hat{\rho}_{\mathrm{S}}(\beta, \tilde{t}) = \rho_{ij}(\beta) |\psi_i(\tilde{t})\rangle_{\mathrm{S}\,\mathrm{S}} \langle \psi_j(\tilde{t})|, \tag{4.3.18}$$

where the sum over i and j remains implicit and the density operator is now time-dependent. Recalling that the state vectors correspond to the microstates of $\mathscr{S}$, it follows that the elements of the density matrix ρ_{ii} are the statistical weights of the corresponding macrostates.

The quantum-statistical density operator, hereafter referred to as simply the *density operator*, is an incoherent sum over the microstates of $\mathscr{S}$. It is important to note that we have therefore removed the possibility, in general, of constructing this density operator out of some thermal state vector $|\Psi(\tilde{t}); \beta\rangle_{\mathrm{S}}$, that is to say

$$\hat{\rho}_{\mathrm{S}}(\beta) \neq |\Psi(\tilde{t}); \beta\rangle_{\mathrm{S}\,\mathrm{S}} \langle \Psi(\tilde{t}); \beta|, \tag{4.3.19}$$

where

$$|\Psi(\tilde{t}); \beta\rangle_{\mathrm{S}} = \sum_i a_i(\beta) |\psi_i(\tilde{t})\rangle_{\mathrm{S}}. \tag{4.3.20}$$

Indeed, such a coherent approach to equilibrium quantum statistical mechanics is formulated in *thermo field dynamics* [61–63]. However, our aim is to describe systems

out of equilibrium in which a coherent decomposition of this form is certainly not appropriate, although generalisations of such approaches to non-equilibrium systems have been discussed [64–67].

4.4 The Partition Function

The final step is to connect the density operator to the thermodynamic quantities discussed in the previous chapter. As we have identified, the elements of the diagonal density matrix are the statistical weights of the corresponding macrostates. We anticipate then that the definition of the entropy, which must have the form of an EEV, is

$$S = -k_{\mathrm{B}} \mathrm{tr}\, \hat{\rho} \ln \hat{\rho}. \tag{4.4.1}$$

The logarithm of the operator is understood as an expansion in terms of a diagonal matrix representation, in which case

$$S = -k_{\mathrm{B}} \sum_i \rho_{ii} \ln \rho_{ii}. \tag{4.4.2}$$

The law of increase in entropy then results in the canonical form of the elements of the density matrix

$$\rho_{ii} = \frac{1}{Z} e^{-\beta E_i}, \tag{4.4.3}$$

where E_i is the energy of the i-th quantum state. The normalisation Z is the canonical partition function, which may now be written as explicitly as a *sum over states*

$$Z = \sum_i e^{-\beta E_i}. \tag{4.4.4}$$

This may be in turn written in the form of a trace:

$$Z = \mathrm{tr}\, e^{-\beta \hat{H}}, \tag{4.4.5}$$

where $\hat{H}$ is the Hamiltonian operator. We then arrive at the form of the canonical density operator

$$\hat{\rho}(\beta) = \frac{1}{Z} e^{-\beta \hat{H}}. \tag{4.4.6}$$

We now have a means of calculating EEVs of operators in quantum mechanics. For our closed subsystem $\mathscr{S}$, which is in thermodynamic equilibrium at temperature T, the EEV of a general operator $\hat{O}$ is

$$\langle O \rangle_\beta = \frac{1}{Z} \operatorname{tr} e^{-\beta \hat{H}} \hat{O}. \tag{4.4.7}$$

The trace is then evaluated in any complete orthonormal basis by inserting the orthonormality condition before the trace and between the operators, using both the cyclicity and linearity of the trace operation. There are no indications as to the picture in which this EEV is to be understood, since it is picture-independent: we can insert unity (in the form of a product of evolution operators and their inverses) and use the cyclicity of the trace to map between pictures. The only requirement then is that the operators appearing within the trace are understood in the *same* picture.

Hereafter, it will be convenient to redefine the density operator so that it does not include its normalisation and so that this normalisation must always be specified explicitly. With this convention, the canonical density operator becomes

$$\hat{\rho} = e^{-\beta \hat{H}} \tag{4.4.8}$$

and the canonical partition function,

$$Z = \operatorname{tr} \hat{\rho}. \tag{4.4.9}$$

The EEV of a general operator $\hat{O}$ may then be written

$$\langle O \rangle_\beta = \frac{\operatorname{tr} \hat{\rho} \hat{O}}{\operatorname{tr} \hat{\rho}}. \tag{4.4.10}$$

This definition will lend itself more naturally to the forthcoming discussions.

4.5 The Quantum Harmonic Oscillator

Before continuing our discussions of quantum statistical mechanics further, it will be helpful to consider a specific example. This example, not surprisingly, will be the archetypal harmonic oscillator. This will lead us to a definition of the number operator and its equilibrium EEV — the distribution function of integer-spin, bosonic quantum states known as the Bose-Einstein distribution.

The Hamiltonian operator of the one-dimensional quantum harmonic oscillator of mass m and angular frequency ω is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2, \tag{4.5.1}$$

where $\hat{q}$ and $\hat{p}$ are the position and momentum operators introduced previously. Our aim is to solve the Schrödinger equation (4.1.4) explicitly. A discussion of this solution and its generalisation to three-dimensional quantum harmonic oscillator is provided in [68].

Separating variables, we write the wavefunction of the quantum harmonic oscillator as a product of coordinate- and time-dependent terms

$$\psi(q, \tilde{t}) = \psi(q)U(\tilde{t}). \tag{4.5.2}$$

We then obtain the *time-independent Schrödinger equation* (TISE)

$$\hat{H}\psi(q) = E\,\psi(q), \tag{4.5.3}$$

where the constant E is the energy of the state $\psi(q, \tilde{t})$. The time-dependence $U(\tilde{t})$ satisfies

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}\tilde{t}}U(\tilde{t}) = EU(\tilde{t}), \tag{4.5.4}$$

from which we obtain

$$U(\tilde{t}) = e^{-iE\tilde{t}/\hbar}, \tag{4.5.5}$$

where any constants due to explicit boundary conditions have been absorbed into the normalisation of $\psi(q)$. Comparing with the evolution operator, we justify our choice of notation.

The TISE may be written explicitly as

$$\left[\frac{\partial^2}{\partial q^2} - \left(\frac{m\omega}{\hbar}\right)^2 q^2 + \frac{2mE}{\hbar^2}\right]\psi(q) = 0. \tag{4.5.6}$$

This may be cast in a soluble form by making the Ansatz

$$\psi(q) = Ae^{-\frac{m\omega}{2\hbar}q^2}P(q), \tag{4.5.7}$$

where $P(q)$ is some polynomial of q. The constant A will be fixed by normalisation of the time-independent wavefunction via

$$\int_{-\infty}^{+\infty} \mathrm{d}q\, |\psi(q)|^2 = 1, \tag{4.5.8}$$

since the modulus-squared of the time-dependent part is unity. Substituting for this Ansatz, the TISE may be cast in terms of the polynomial $P(q)$:

$$\left[\frac{\partial^2}{\partial q^2} - 2\frac{m\omega}{\hbar}q\frac{\partial}{\partial q} + \frac{2m}{\hbar^2}\Big(E - \frac{1}{2}\hbar\omega\Big)\right]P(q) = 0. \tag{4.5.9}$$

Defining a new variable x through

$$x^2 = \frac{m\omega}{\hbar}q^2, \tag{4.5.10}$$

we obtain

$$\left[\frac{\partial^2}{\partial x^2} - 2x\frac{\partial}{\partial x} + \frac{2}{\hbar\omega}\Big(E - \frac{1}{2}\hbar\omega\Big)\right]P(x) = 0. \tag{4.5.11}$$

This is the *Hermite differential equation*, for which solutions exist only if $E - \frac{1}{2}\hbar\omega$ is

an integer multiple of $\hbar\omega$. Thus, we find that the energies of the quantum harmonic oscillator are *quantised*, taking discrete values

$$E_n = \hbar\omega\Big(n + \frac{1}{2}\Big), \tag{4.5.12}$$

where $n \in \mathbb{N}_0$. Each solution may be interpreted as comprising n quanta, each an oscillator of frequency ω and with energy $\hbar\omega$. Note that the lowest energy state with $n = 0$ — the *vacuum* — has a finite energy $\frac{1}{2}\hbar\omega$, referred to as the *zero-point energy*. The polynomials $P(y)$ are the Hermite polynomials $H_n(y)$ [69], which form an orthogonal basis with the weight function

$$w(x) = e^{-x^2}, \tag{4.5.13}$$

such that

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-x^2} H_n(x) H_m(x) = \sqrt{\pi} 2^n n! \delta_{nm}. \tag{4.5.14}$$

For future reference, we note that these polynomials satisfy the recursion relations

$$H_{n+1}(x) = 2xH_n(x) - \frac{\mathrm{d}H_n}{\mathrm{d}x}, \tag{4.5.15a}$$

$$\frac{\mathrm{d}H_n}{\mathrm{d}x} = 2nH_{n-1}(x). \tag{4.5.15b}$$

After normalising, we find the constant

$$A = \frac{1}{\sqrt{2^n n!}}\Big(\frac{m\omega}{\pi\hbar}\Big)^{1/4} \tag{4.5.16}$$

and hence the time-dependent wavefunctions of the one-dimensional quantum harmonic oscillator are

$$\psi_n(q, \tilde{t}) = \frac{1}{\sqrt{2^n n!}}\Big(\frac{m\omega}{\pi\hbar}\Big)^{1/4} H_n(\sqrt{m\omega/\hbar}\, q) \exp\Big(-\frac{m\omega}{2\hbar} q^2\Big) \exp\Big(\frac{iE_n\tilde{t}}{\hbar}\Big). \tag{4.5.17}$$

Given the orthogonality of the Hermite polynomials, these wavefunctions form an

orthonormal set, satisfying

$$\int_{-\infty}^{+\infty} \mathrm{d}q\, \psi_n^*(q,\tilde{t})\psi_m(q,\tilde{t}) = \delta_{nm}, \tag{4.5.18}$$

as required.

Having established the quantisation of the harmonic oscillator, we return to the braket notation introduced previously. The time-independent wavefunctions may then be written as

$$\psi_n(q) = \langle q|\, n\rangle\,. \tag{4.5.19}$$

The time-independent energy eigenstates $|n\rangle \equiv |\psi_n\rangle$, denoted simply by the discrete *quantum number* $n \in \mathbb{N}_0$, satisfy the energy eigenvalue equation

$$\hat{H}\,|n\rangle = E_n\,|n\rangle\,, \tag{4.5.20}$$

and together form a complete orthonormal basis with

$$\sum_{n=0}^{\infty} |n\rangle\langle n| = \mathbb{I}, \tag{4.5.21a}$$

$$\langle n|m\rangle = \delta_{nm}. \tag{4.5.21b}$$

We have already identified that the state $|n\rangle$ comprises n quanta of energy $\hbar\omega$. It follows then that the Hamiltonian must have the form

$$\hat{H} = \hbar\omega\Big(\hat{n} + \frac{1}{2}\Big), \tag{4.5.22}$$

where $\hat{n}$ is an operator which counts the number of quanta — the *number operator*. Thus, the energy eigenstate $|n\rangle$ is an eigenstate of the number operator $\hat{n}$ with eigenvalue n, i.e.,

$$\hat{n}\,|n\rangle = n\,|n\rangle\,. \tag{4.5.23}$$

Looking again at the Hamiltonian in (4.5.1), written in terms of the position

and momentum operators, we see that it may be factorised as follows:

$$\hat{H} = \hbar\omega\Big[\Big(\sqrt{\frac{m\omega}{2\hbar}}\hat{q} - \frac{\hat{p}}{\sqrt{2m\hbar\omega}}i\Big)\Big(\sqrt{\frac{m\omega}{2\hbar}}\hat{q} + i\frac{\hat{p}}{\sqrt{2m\hbar\omega}}\Big) + \frac{1}{2}\Big], \tag{4.5.24}$$

where the zero-point contribution has resulted from the use of the canonical commutation relation in (4.1.7). Introducing the dimensionless operators

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{q} + i\frac{\hat{p}}{\sqrt{2m\hbar\omega}}, \tag{4.5.25a}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{q} - i\frac{\hat{p}}{\sqrt{2m\hbar\omega}}, \tag{4.5.25b}$$

the Hamiltonian may be written in the more condensed form

$$\hat{H} = \hbar\omega\Big(\hat{a}^\dagger\hat{a} + \frac{1}{2}\Big). \tag{4.5.26}$$

We conclude that the number operator is

$$\hat{n} = \hat{a}^\dagger\hat{a}. \tag{4.5.27}$$

The canonical commutation relation translates to the algebra

$$\big[\hat{a}, \hat{a}^\dagger\big] = 1 \tag{4.5.28}$$

of these new operators, the action of which we will now determine.

Acting explicitly on the time-independent wavefunctions, using their coordinate representations and the recursion relations of the Hermite polynomials (4.5.15), we find that

$$\hat{a}\psi_n(q) = \sqrt{n}\psi_{n-1}(q), \tag{4.5.29a}$$

$$\hat{a}^\dagger\psi_n = \sqrt{n+1}\psi_{n+1}, \tag{4.5.29b}$$

and, equivalently, it follows that

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle\,, \tag{4.5.30a}$$

$$\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle\,. \tag{4.5.30b}$$

We interpret then $\hat{a}^\dagger$ as a *creation operator*, whose operation on an energy eigenstate adds a quanta of energy to the system; and $\hat{a}$ as an *annihilation operator*, whose operation removes a quanta of energy from the system. Note that we can construct the n^{th} state as

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\,|0\rangle\,, \tag{4.5.31}$$

where $|0\rangle$ is the *vacuum state*.

We can quickly show that these operators satisfy the commutators

$$[\hat{H}, \hat{a}^\dagger] = \hbar\omega\hat{a}^\dagger, \quad [\hat{H}, \hat{a}] = -\hbar\omega\hat{a}. \tag{4.5.32}$$

Hence, by the Heisenberg equation of motion, we find the time-dependent position and momentum operators

$$\hat{q}(t) = \left(\frac{\hbar}{2m\omega}\right)^{1/2}(\hat{a}e^{-i\omega t} + \hat{a}^\dagger e^{i\omega t}), \tag{4.5.33a}$$

$$\hat{p}(t) = -i\left(\frac{m\omega\hbar}{2}\right)^{1/2}(\hat{a}e^{-i\omega t} - \hat{a}^\dagger e^{i\omega t}), \tag{4.5.33b}$$

satisfying Hamilton's equations of motion, in which case $\hat{p}$ is indeed the quantum analogue of the conjugate momentum.

4.6 The Bose-Einstein Distribution

We are now in a position to ask for the EEV of the number of quanta of a quantum harmonic oscillator in thermodynamic equilibrium. This is just

$$\langle n \rangle_\beta = \frac{1}{Z} \mathrm{tr}\, e^{-\beta \hat{H}} \hat{n}, \tag{4.6.1}$$

where the partition function is

$$Z = \mathrm{tr}\, e^{-\beta \hat{H}}. \tag{4.6.2}$$

Evaluating the trace in the basis of energy eigenstates, using the orthonormality conditions in (4.5.21), the partition function may be written

$$Z = e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n} = \frac{e^{\beta\hbar\omega/2}}{e^{\beta\hbar\omega} - 1}. \tag{4.6.3}$$

The remaining trace in the numerator of (4.6.1) yields

$$= e^{-\beta\hbar\omega/2} \sum_{n=0}^{\infty} n e^{-\beta\hbar\omega n} = \frac{e^{\beta\hbar\omega/2}}{(e^{\beta\hbar\omega} - 1)^2}. \tag{4.6.4}$$

Hence, the EEV of the number density is

$$\langle n \rangle_\beta = f_{\mathrm{B}}(\hbar\omega) = \frac{1}{e^{\beta\hbar\omega} - 1}. \tag{4.6.5}$$

This is the *Bose-Einstein distribution*, describing the number density of integer-spin particles, i.e., bosons, with energy between $\hbar\omega$ and $\hbar\omega + \mathrm{d}\hbar\omega$. Note that in the low-temperature limit, in which β is large, we recover the classical Boltzmann distribution $f_\beta(\hbar\omega)$.

5 Correlation Functions

In this chapter, we introduce a description of the quantum harmonic oscillator based upon the *path integral* introduced by Richard Feynman [50] (see also [70–72]). This representation will be fundamentally important to the derivation of our approach to non-equilibrium quantum field theory and, as a result, we have chosen to devote a full chapter to its explanation.

5.1 The Path Integral

Let us consider again the state of the quantum harmonic oscillator described by the wavefunction $\psi(q_f, \tilde{t}_f) = \langle q_f, \tilde{t}_f | \psi \rangle$ at some time $\tilde{t}_f$, here written in the Heisenberg picture, where for generality we have not indicated the quantum number n. We may insert a complete set of position eigenstates at some earlier time $\tilde{t}_i < \tilde{t}_f$, such that

$$\psi(q_f, \tilde{t}_f) = \int_{-\infty}^{+\infty} \mathrm{d}q_i \; \langle q_f(\tilde{t}_f) | \tilde{q}_i(\tilde{t}_i) \rangle \, \psi(q_i, \tilde{t}_i). \tag{5.1.1}$$

The inner product $D(q_f, \tilde{t}_f; q_i, \tilde{t}_i) = \langle q_f(\tilde{t}_f) | q_i(\tilde{t}_i) \rangle$ may be interpreted as the probability amplitude for a transition from the state $\psi(q_i, \tilde{t}_i)$ to the state $\psi(q_f, \tilde{t}_f)$, occurring with probability

$$\mathbb{P}(q_f, \tilde{t}_f; q_i, \tilde{t}_i) = |D(q_f, \tilde{t}_f; q_i, \tilde{t}_i)|^2. \tag{5.1.2}$$

Further subdividing the time-interval $\tilde{t}_f - \tilde{t}_i$ and requiring that the 'path' of our wavefunction pass through a given point q at some time $\tilde{t}$, where $\tilde{t}_i < \tilde{t} < \tilde{t}_f$, we

develop the *Markov train*

$$\psi(q_f,\tilde{t}_f)=\iint_{-\infty}^{+\infty}\mathrm{d}q\,\mathrm{d}q_i\,D(q_f,\tilde{t}_f;q,\tilde{t})D(q,\tilde{t};q_i,\tilde{t}_i)\psi(q_i,\tilde{t}_i). \tag{5.1.3}$$

We can imagine continuing to subdivide the time interval into N infinitesimally-small intervals $\delta\tilde{t}=(\tilde{t}_f-\tilde{t}_i)/N$. In the continuum limit $N\to\infty$, our integrations over all the intermediate spatial configurations become an integral over all possible 'paths' by which the system can evolve, or as Feynman put it "a sum over all histories." Symbolically, we write

$$\int\ldots\int_{-\infty}^{+\infty}\prod_{j=0}^{N-1}\mathrm{d}q_j\to\int[\mathrm{d}q], \tag{5.1.4}$$

where $q_0\equiv q_i(\tilde{t}_i)$ and $q_N\equiv q_f(\tilde{t}_f)$.

Let us consider then one infinitesimal interval between $\tilde{t}_j$ and $\tilde{t}_{j+1}$. In terms of time-independent position eigenstates, which we emphasise still depend implicitly on the time $\tilde{t}_i$, we may write

$$\langle q_{j+1}(\tilde{t}_{j+1})|q_j(\tilde{t}_j)\rangle=\langle q_{j+1}|e^{-i\hat{H}(\tilde{t}_{j+1}-\tilde{t}_j)/\hbar}|q_j\rangle\,, \tag{5.1.5}$$

where $\hat{H}$ is the full Hamiltonian. Taylor-expanding the exponent, we obtain

$$\langle q_{j+1}|[1-\tfrac{\delta\tilde{t}}{\hbar}\hat{H}+\mathcal{O}(\delta\tilde{t})^2]|q_j\rangle\,, \tag{5.1.6}$$

which, using the orthonormality of the basis of position eigenstates, becomes

$$\delta(q_{j+1}-q_j)-\tfrac{\delta t}{\hbar}\,\langle q_{j+1}|\hat{H}|q_j\rangle+\mathcal{O}(\delta t)^2, \tag{5.1.7}$$

where we subsequently replace the delta function by the Fourier representation

$$\int_{-\infty}^{+\infty}\frac{\mathrm{d}p_j}{2\pi\hbar}\exp\left[\frac{i}{\hbar}p_j(q_{j+1}-q_j)\right], \tag{5.1.8}$$

where p_j is the conjugate momenta. In order to proceed further, we recall that the

Hamiltonian of the quantum harmonic oscillator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2, \tag{5.1.9}$$

Inserting a complete set of momentum eigenstates, we may write

$$\langle q_{j+1}|\hat{p}^2|q_j\rangle = \int_{-\infty}^{+\infty} \frac{\mathrm{d}p_j}{2\pi\hbar}\, \langle q_{j+1}|\hat{p}^2|p_j\rangle \langle p_j|q_j\rangle\,. \tag{5.1.10}$$

We then find

$$\langle q_{j+1}|\hat{p}^2|\hat{q}_j\rangle = \int_{-\infty}^{+\infty} \frac{\mathrm{d}p_j}{2\pi\hbar}\, p_j^2 \exp\left[\frac{i}{\hbar}p_j(q_{j+1}-q_j)\right]. \tag{5.1.11}$$

Furthermore, we may write

$$\frac{1}{2}m\omega^2 \langle q_{j+1}|\hat{q}^2|q_j\rangle = \frac{1}{2}m\omega^2 q_j^2 \langle q_{j+1}|q_j\rangle = \frac{1}{2}m\omega^2 q_j^2\delta(q_{j+1}-q_j). \tag{5.1.12}$$

Putting everything together and re-exponentiating the Taylor expansion, we obtain

$$\langle q_{j+1}(\tilde{t}_{j+1})|q_j(\tilde{t}_j)\rangle = \int_{-\infty}^{+\infty} \frac{\mathrm{d}p_j}{2\pi\hbar}\, \exp\left[\frac{i}{\hbar}\Big(p_j(q_{j+1}-q_j) - \delta\tilde{t}H(p_j,q_j)\Big)\right]. \tag{5.1.13}$$

The integration over p_j is ill-defined. However, making the analytic continuation $\tilde{t} = i\tau$ and $p_j = -i\bar{p}_j$ — the *Wick rotation* — this integral may be recast in the Gaussian form

$$\frac{i}{2\pi\hbar}\int_{-\infty}^{+\infty} \mathrm{d}\bar{p}_j\, \exp(-a\bar{p}_j^2 + b\bar{p}_j + c) = \frac{i}{2\pi\hbar}\left(\frac{\pi}{a}\right)^{1/2} \exp\left(\frac{b^2}{4a} + c\right), \tag{5.1.14}$$

where

$$a = \frac{\delta\tau}{2\hbar m}, \quad b = \frac{q_{j+1}-q_j}{\hbar}, \quad c = \frac{\delta\tau}{2\hbar}m\omega^2 q_j^2. \tag{5.1.15}$$

Thus, we find

$$\langle q_{j+1}(i\tau_{j+1})|q_j(i\tau_j)\rangle = \mathcal{N}_j \exp\left\{-\frac{\delta\tau}{\hbar}\left[\frac{m}{2}\left(\frac{q_{j+1}-q_j}{\delta\tau}\right)^2 + \frac{1}{2}m\omega^2 q_j^2\right]\right\}, \tag{5.1.16}$$

where we have hidden the coefficients in the normalisation $\mathcal{N}_j$. Hence, we may write

$$\langle q_f(i\tau_f)|q_i(i\tau_i)\rangle = \mathcal{N}\int\cdots\int\prod_{j=1}^{N-1}\mathrm{d}q_j\,\exp\left\{-\frac{\delta\tau}{\hbar}\left[\frac{m}{2}\left(\frac{q_{j+1}-q_j}{\delta\tau}\right)^2+\frac{1}{2}m\omega^2 q_j^2\right]\right\}. \tag{5.1.17}$$

Taking the continuum limit, $N\to\infty$, we recognise that

$$\frac{q_{j+1}-q_j}{\delta\tau}=\dot{q}_j=\frac{\mathrm{d}q_j}{\mathrm{d}\tau}. \tag{5.1.18}$$

The summation in the exponent is the Riemann sum for the integral

$$\bar{S}(\tau_f,\tau_i)=\int_{\tau_i}^{\tau_f}\mathrm{d}\tau\,\frac{1}{2}\Big(m\dot{q}^2+m\omega^2q^2\Big), \tag{5.1.19}$$

which is the *Euclidean* or *imaginary-time action*. We then arrive at the *Euclidean path integral*

$$\langle q_f(i\tau_f)|q_i(i\tau_i)\rangle=\mathcal{N}\int[\mathrm{d}q]\,\exp\left[-\frac{1}{\hbar}S_{\mathrm{E}}(\tau_f,\tau_i)\right]. \tag{5.1.20}$$

Making the analytic continuation $\tau=-i\tilde{t}$, we obtain the familiar action and the *Minkowski* or *real-time path integral*

$$\langle q_f(\tilde{t}_f)|q_i(\tilde{t}_i)\rangle=\mathcal{N}\int[\mathrm{d}q]\,\exp\left[\frac{i}{\hbar}S(\tilde{t}_f,\tilde{t}_i)\right]. \tag{5.1.21}$$

This is the path integral representation of the probability amplitude for the propagation of a *signal* from position q_i at a time $\tilde{t}_i$ to a position q_f at time $\tilde{t}_f$. The probability amplitude for the *transition between states* is obtained by convoluting with the initial wavefunction $\psi(q_i,\tilde{t}_i)$, cf. (5.1.3).

We have derived this result assuming an explicit, quadratic form for the potential. However, the same arguments follow for any potential $V(\hat{q})$ that is a function only of $\hat{q}$.

5.2 The Generating Functional

Suppose now that we want to perturb the oscillator from its ground state, the vacuum, and watch how it relaxes back to that ground state over some perceivably-infinite length of time. This corresponds to a driven oscillator, whose evolution is described by the inhomogeneous differential equation

$$m\ddot{q}(\tilde{t}) + m\omega^2 q(\tilde{t}) = \hbar j(\tilde{t}), \tag{5.2.1}$$

where $\hbar j(\tilde{t})$ is some driving force. This equation of motion is equivalent to adding to the action a term

$$\int_{-\infty}^{+\infty} \mathrm{d}\tilde{t}\, \hbar j(\tilde{t}) q(\tilde{t}). \tag{5.2.2}$$

The solution of the inhomogeneous equation (5.2.1) may be written as

$$q(\tilde{t}) = q_0(\tilde{t}) + \hbar \int_{-\infty}^{+\infty} \mathrm{d}\tilde{t}'\, G(\tilde{t} - \tilde{t}') j(\tilde{t}'), \tag{5.2.3}$$

where $q_0(\tilde{t})$ is the solution of the homogeneous equation

$$m\ddot{q}_0(\tilde{t}) + m\omega^2 q_0(\tilde{t}) = 0. \tag{5.2.4}$$

The Green's function $G(\tilde{t} - \tilde{t}')$ must satisfy

$$m\left[\frac{\mathrm{d}^2}{\mathrm{d}\tilde{t}^2} + \omega^2\right] G(\tilde{t} - \tilde{t}') = \delta(\tilde{t} - \tilde{t}'), \tag{5.2.5}$$

the solution of which may be found subject to suitably-imposed boundary conditions. This equation defines an operator

$$G^{-1}(\tilde{t} - \tilde{t}') = m\left[\frac{\mathrm{d}^2}{\mathrm{d}\tilde{t}^2} + \omega^2\right]. \tag{5.2.6}$$

In order to generalise this problem to our path-integral description, we define

the *generating functional*

$$\mathcal{Z}[j] = \langle 0(+\infty)|0(-\infty)\rangle_j = \langle 0(-\infty)|\mathrm{T}\left[\exp\left(\frac{i}{\hbar}\int_{-\infty}^{+\infty}\mathrm{d}\tilde{t}\,\hbar j(\tilde{t})\hat{q}(\tilde{t})\right)\right]|0(+\infty)\rangle\,, \tag{5.2.7}$$

which is the vacuum-to-vacuum transition amplitude in the presence of an external source j. The explicit time-dependence of the vacuum states is a consequence of the presence of this external source. For now, we will refrain from commenting on the behaviour of this source in the infinitely-distant past and future. Decomposing the vacuum state in the basis of position eigenstates, we may proceed as we did in the previous section to derive a path-integral representation of this generating functional. We find

$$\mathcal{Z}[j] = \mathcal{N}\int[\mathrm{d}q]\,\exp\left[\frac{i}{\hbar}\int_{-\infty}^{+\infty}\mathrm{d}\tilde{t}\,\Big(L(\dot{q},q)+\hbar j(\tilde{t})q(\tilde{t})\Big)\right], \tag{5.2.8}$$

where L is the Lagrangian

$$L(\dot{q},q) = \frac{1}{2}m\dot{q}^2(\tilde{t}) - \frac{1}{2}m\omega^2 q^2(\tilde{t}). \tag{5.2.9}$$

Integrating by parts and assuming that $\dot{q}(\tilde{t})$ vanishes at the boundaries of integration, we may write the exponent in the form

$$\frac{i}{\hbar}\int_{-\infty}^{+\infty}\mathrm{d}\tilde{t}\left[-\frac{1}{2}q(\tilde{t})\Big(m\frac{\mathrm{d}^2}{\mathrm{d}\tilde{t}^2}+m\omega^2\Big)q(\tilde{t})+\hbar j(\tilde{t})q(\tilde{t})\right]. \tag{5.2.10}$$

Recognising the contents of the parenthesis as the operator defined in (5.2.6), this exponent may be rewritten as

$$\frac{i}{\hbar}\int_{-\infty}^{+\infty}\mathrm{d}\tilde{t}\left[-\frac{1}{2}q(\tilde{t})G^{-1}(\tilde{t}-\tilde{t}')q(\tilde{t})+\hbar j(\tilde{t})q(\tilde{t})\right]. \tag{5.2.11}$$

Using the general form of the solution of the inhomogeneous equation in (5.2.3), we may complete the square in this exponent and write the generating functional in the

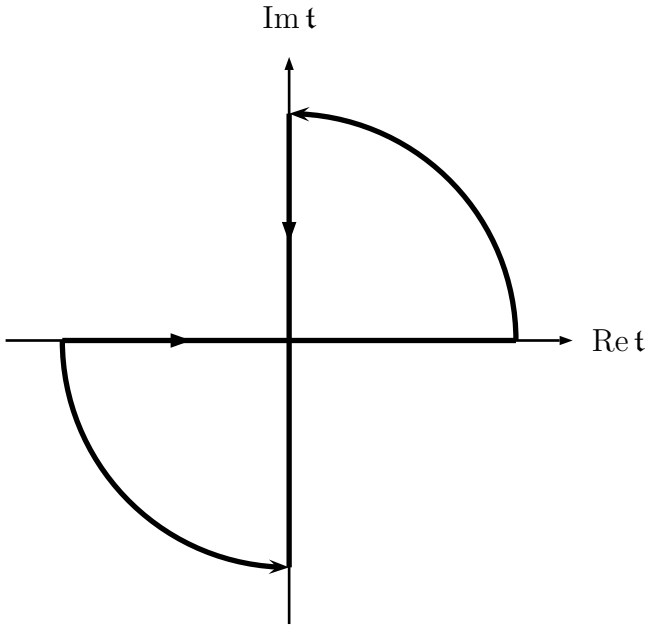


Figure 5.1: A sketch of the complex-time plane $\mathfrak{t} = \tilde{t} - i\tau \in \mathbb{C}$*, showing the closed contour used to perform the Wick rotation between Euclidean and Minkowski space-time path integrals.*

form

$$\mathcal{Z}[j] = \mathcal{Z}[0] \exp\left[\frac{i\hbar}{2} \iint_{-\infty}^{+\infty} \mathrm{d}\tilde{t}\, \mathrm{d}\tilde{t}'\, j(\tilde{t}) G(\tilde{t} - \tilde{t}') j(\tilde{t}')\right], \tag{5.2.12}$$

where $\mathcal{Z}[0]$ is the generating functional in the absence of external sources.

At this point, we recall that the path integral was defined subject to our ability to perform the Wick rotation between real and imaginary times. This analytic continuation relies on our ability to close an integration contour in the complex-time plane that contains sections which run parallel and coincident with the real axis and anti-parallel and coincident with the imaginary axis. This contour is shown in Figure 5.1. We denote the complex time by the Gothic character $\mathfrak{t} = \tilde{t} - i\tau \in \mathbb{C}$. The contribution from the curved sections that arc over the upper-right and the lower-left quadrants must therefore vanish in order for this analytic continuation to hold. This yields the following constraints on the analytic continuation of the

Green's function to complex times:

$$\lim_{\tau\to+\infty} G(\tilde{t}-i\tau)=0, \quad \tilde{t}<0, \tag{5.2.13a}$$

$$\lim_{\tau\to-\infty} G(\tilde{t}-i\tau)=0, \quad \tilde{t}>0. \tag{5.2.13b}$$

where we have taken $\mathfrak{t}'=0$ for convenience.

5.3 The Propagator

In this section, we will proceed to solve the Cauchy problem in 5.2.5 explicitly and derive the form of the Green's function $G(\tilde{t}-\tilde{t}')$. We first introduce the functions $G^{\gtrless}(\tilde{t}-\tilde{t}')$, writing

$$G(\tilde{t}-\tilde{t}')=\theta(\tilde{t}-\tilde{t}')G^{>}(\tilde{t}-\tilde{t}')+\theta(\tilde{t}'-\tilde{t})G^{<}(\tilde{t}-\tilde{t}'). \tag{5.3.1}$$

The unit step function $\theta(\tilde{t}-\tilde{t}')$ may be written in the contour-integral representation

$$\theta(\tilde{t})=i\int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega'}{2\pi\hbar}\,\frac{e^{-i\omega'\tilde{t}}}{\omega'+i\epsilon}=\begin{cases}1, & \tilde{t}>0,\\ \frac{1}{2}, & \tilde{t}=0,\\ 0, & \tilde{t}<0,\end{cases} \tag{5.3.2}$$

where $\epsilon=0^{+}$. Given that $G^{\gtrless}$ are the solutions of a second-order, linear differential equation , we make the Ansätze

$$G^{\gtrless}(\tilde{t}-\tilde{t}')=A^{\gtrless}e^{-i\omega(\tilde{t}-\tilde{t}')}+B^{\gtrless}e^{i\omega(\tilde{t}-\tilde{t}')}, \tag{5.3.3}$$

subject to the following boundary conditions: the Dirichlet continuity condition

$$G^{>}(0)=G^{<}(0); \tag{5.3.4}$$

and the Neumann discontinuity condition

$$\lim_{\epsilon\to 0^+}\left[m\frac{\mathrm{d}}{\mathrm{d}\tilde{t}}G^{>}(\tilde{t}-\tilde{t}')\Big|_{\tilde{t}=\tilde{t}'+\epsilon}-m\frac{\mathrm{d}}{\mathrm{d}\tilde{t}}G^{<}(\tilde{t}-\tilde{t}')\Big|_{\tilde{t}=\tilde{t}'-\epsilon}\right]=1. \tag{5.3.5}$$

The validity of the Wick rotation led to the constraints in (5.2.13), which immediately restricts $B^{>}=A^{<}=0$. Subsequently, (5.3.4) and (5.3.5) yield the system

$$A^{>}e^{-i\omega\tilde{t}'}-B^{<}e^{i\omega\tilde{t}'}=0, \tag{5.3.6a}$$

$$A^{>}e^{-i\omega\tilde{t}'}+B^{<}e^{i\omega\tilde{t}'}=\frac{i}{m\omega}, \tag{5.3.6b}$$

from which we obtain the results

$$G^{>}(\tilde{t}-\tilde{t}')=\frac{i}{2m\omega}e^{-i\omega(\tilde{t}-\tilde{t}')}; \tag{5.3.7a}$$

$$G^{<}(\tilde{t}-\tilde{t}')=\frac{i}{2m\omega}e^{i\omega(\tilde{t}-\tilde{t}')}. \tag{5.3.7b}$$

Using the Fourier representation of the unit step function, we find the contour-integral representation of the Green's function

$$G(\tilde{t}-\tilde{t})=-\frac{1}{m}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega'}{2\pi\hbar}\,\frac{e^{-i\omega'(\tilde{t}-\tilde{t}')}}{\omega'^2-\omega^2+i\epsilon}. \tag{5.3.8}$$

It follows that the validity of the Wick rotation, and the convergence of the path integral, requires us to subtract from ω^2 a small imaginary part, i.e., $\omega^2\to\omega^2-i\epsilon$, $\epsilon\to 0^+$. This is the so-called *Feynman prescription*, which allows us to avoid the poles in the Fourier transform of the Green's function. This is however, not the only possible prescription: one may make the analytic continuations $\omega^2\to\omega^2+i\epsilon$, the so-called *Dyson prescription*; or the sign-dependent prescriptions $\omega^2\to\omega^2+i\omega\epsilon$ and $\omega^2\to\omega^2-i\omega\epsilon$. Each leads to a Green's function with slightly different analytic structure. The Dyson prescription leads to the interchange of $G^{>}$ and $G^{<}$, whereas the sign-dependent prescriptions yield Green's functions that vanish for $\tilde{t}>\tilde{t}'$ and $\tilde{t}<\tilde{t}'$, respectively. These prescriptions lead then to *retarded* and *advanced* Green's functions. For a more comprehensive discussion, the reader is directed to the texts

by S. Pokorski [71] and W. Greiner & J. Reinhardt [73]. However, we make note of this issue in preparation for our treatment of the corresponding Green's functions of out-of-equilibrium systems.

We consider now the *vacuum expectation value* (VEV) of the time-ordered product of position operators — the time-ordered two-point *correlation function* —

$$i\Delta_{\mathrm{F}}(\tilde{t}-\tilde{t}') = \langle 0|\mathrm{T}\big[\hat{q}(\tilde{t})\hat{q}(\tilde{t}')\big]|0\rangle\,. \tag{5.3.9}$$

This object is the *Feynman propagator*. For $\tilde{t} > \tilde{t}'$, we may insert complete sets of position eigenstates as before to derive the path-integral representation

$$\langle 0|\hat{q}(t)\hat{q}(t')|0\rangle = \mathcal{N}\int[\mathrm{d}q]\, q(\tilde{t})q(\tilde{t}')e^{\frac{i}{\hbar}S}. \tag{5.3.10}$$

For $\tilde{t} < \tilde{t}'$, we would obtain

$$\langle 0|\hat{q}(\tilde{t}')\hat{q}(\tilde{t})|0\rangle = \mathcal{N}\int[\mathrm{d}q]\, q(\tilde{t}')q(\tilde{t})e^{\frac{i}{\hbar}S}. \tag{5.3.11}$$

Comparing with the definition of the generating functional, it follows that

$$i\Delta_{\mathrm{F}}(\tilde{t}-\tilde{t}') = \langle 0|\mathrm{T}[q(\tilde{t})q(\tilde{t}')]|0\rangle = \Big(\frac{1}{i}\Big)^2\frac{1}{Z[0]}\frac{\delta^2\mathcal{Z}[j]}{\delta j(\tilde{t})\delta j(\tilde{t}')}\Big|_{j=0}, \tag{5.3.12}$$

in which case

$$i\Delta_{\mathrm{F}}(\tilde{t}-\tilde{t}') = -i\hbar G(\tilde{t}-\tilde{t}') = \frac{i}{m}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega'}{2\pi}\,\frac{e^{-i\omega'(\tilde{t}-\tilde{t}')}}{\omega'^2-\omega^2+i\epsilon}. \tag{5.3.13}$$

We may then write the generating functional in the form

$$\mathcal{Z}[j] = \mathcal{Z}[0]\exp\left[-\frac{1}{2}\iint_{-\infty}^{+\infty}\mathrm{d}\tilde{t}\,\mathrm{d}\tilde{t}'\, j(\tilde{t})i\Delta_{\mathrm{F}}(\tilde{t}-\tilde{t}')j(\tilde{t}')\right]. \tag{5.3.14}$$

The Feynman propagator can be decomposed in the form

$$i\Delta_{\mathrm{F}}(\tilde{t}-\tilde{t}') = \theta(\tilde{t}-\tilde{t}')i\Delta^{>}(\tilde{t}-\tilde{t}') + \theta(\tilde{t}'-\tilde{t})i\Delta^{<}(\tilde{t}-\tilde{t}'), \tag{5.3.15}$$

where we have introduced the Wightman propagators

$$i\Delta^{>}(\tilde{t}-\tilde{t}') = \langle 0|\hat{q}(\tilde{t})\hat{q}(\tilde{t}')|0\rangle\,, \tag{5.3.16a}$$

$$i\Delta^{<}(\tilde{t}'-\tilde{t}) = \langle 0|\hat{q}(\tilde{t})\hat{q}(\tilde{t}')|0\rangle\,. \tag{5.3.16b}$$

Using the time-dependent position operator in (4.5.33b) and the algebra of the creation and annihilation operators explicitly, we can verify that

$$i\Delta^{>}(\tilde{t}-\tilde{t}') = \frac{\hbar}{2m\omega}e^{-i\omega(\tilde{t}-\tilde{t}')}, \tag{5.3.17a}$$

$$i\Delta^{<}(\tilde{t}-\tilde{t}') = \frac{\hbar}{2m\omega}e^{i\omega(\tilde{t}-\tilde{t}')} \tag{5.3.17b}$$

consistent with (5.3.7).

Later, we will introduce a plethora of propagators, which will include those corresponding to the Dyson, retarded and advanced prescriptions highlighted above. However, these introductions are deliberately delayed until those propagators are of specific use.

6 Imaginary Time Formalism

The aim of this next chapter is to apply the path-integral, Green's function approach to the quantum harmonic oscillator in the context of quantum statistical mechanics. This will lead us to the *imaginary-time formalism* due to Matsubara [22]. Combined with the second quantisation of the chapter that then follows, we will have succeeded in introducing all the prerequisites necessary to the formulation of our approach to non-equilibrium quantum dynamics.

A full and exhaustive introduction to the imaginary-time and real-time formalisms of thermal field theory is beyond the scope of thesis. However, comprehensive introductions are provided in [74–82].

6.1 The Bloch Equation

In the previous chapter, we obtained the canonical density operator of a quantum mechanical subsystem in thermodynamic equilibrium at a temperature T:

$$\hat{\rho} = e^{-\beta \hat{H}}, \tag{6.1.1}$$

where we emphasise that we have separated the density operator from its normalisation, for reasons that will now become apparent.

It is clear that this density operator satisfies the following first-order differential

equation:

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}\beta} = -\hat{H}\hat{\rho}. \tag{6.1.2}$$

— the *Bloch equation*. Writing the density operator in the form

$$\hat{\rho}(\beta) = e^{-\hat{H}(\beta-0)} \tag{6.1.3}$$

and comparing with (4.1.20), this looks very much like the Schrödinger-picture evolution operator in imaginary time, subject to the boundary condition

$$\hat{\rho}(0) = \mathbb{I}. \tag{6.1.4}$$

This suggests that we may introduce the evolution operator of a *modified* interaction picture

$$\hat{U}(\beta) = e^{\beta\hat{H}^0}e^{-\beta\hat{H}}, \tag{6.1.5}$$

which satisfies

$$\frac{\mathrm{d}\hat{U}(\beta)}{\mathrm{d}\beta} = -\hat{H}^{\mathrm{int}}_{\mathrm{I}'}(\beta)\hat{U}(\beta), \tag{6.1.6}$$

where the interaction of the Hamiltonian has become temperature-dependent. This picture is *modified* in the sense that it is the distribution of temperature dependence amongst operators and states that is of interest, not the distribution of real-time dependence. Thus, we have denoted this modified interaction picture by a subscript I' to differentiate it from that introduced previously. With respect to the real-time dependence, this result could be in any picture. The solution to this equation may be obtained in analogy to the real-time interaction-picture evolution operator, except that we must introduce a time-ordering in an imaginary-time variable τ, which we denote by the operator T_τ:

$$\mathrm{T}_\tau\big[\hat{O}(\tau_1)\hat{O}(\tau_2)\cdots\hat{O}(\tau_n)\big] = \hat{O}(\tau_1)\hat{O}(\tau_2)\cdots\hat{O}(\tau_n), \tau_1 > \tau_2 > \cdots > \tau_n. \tag{6.1.7}$$

Hence, we find

$$\hat{U}(\beta) = \mathrm{T}_\tau\left[\exp\left(-\int_0^\beta \mathrm{d}\tau\, \hat{H}^{\mathrm{int}}_{\mathrm{I}'}(\tau)\right)\right]. \tag{6.1.8}$$

This is just the Wick rotation $\tilde{t} = i\tau$ to imaginary time of the real-time evolution operator with the restriction of the range of integration to be over the interval $[0, \beta]$.

Returning to the full canonical density operator, it follows that an operator $\hat{O}(\tilde{t}_i)$ evolves in this imaginary-time direction subject to

$$\hat{O}(\tilde{t}_i + i\beta) = \hat{\rho}(\beta)\hat{O}(\tilde{t}_i)\hat{\rho}^{-1}(\beta), \tag{6.1.9}$$

where we emphasise that this is true for all pictures with respect to the real time. This interpretation of the canonical density operator as an evolution operator in imaginary time is the basis of an approach to quantum statistical mechanics due to Matsubara, known unimaginatively as the *imaginary-time formalism*. The introduction of the key concepts of this approach to equilibrium statistical mechanics is the subject of this chapter.

6.2 The KMS Relation

Having interpreted the canonical density operator as an evolution operator in imaginary time, we now consider the EEV of the time-ordered product of interaction-picture operators

$$\langle \mathrm{T}\big[\hat{O}_{\mathrm{I}}(\tilde{t})\hat{O}_{\mathrm{I}}(\tilde{t}')\big]\rangle_{\beta} = \frac{1}{Z}\mathrm{tr}\,\hat{\rho}_{\mathrm{I}}(\beta)\mathrm{T}\big[\hat{O}_{\mathrm{I}}(\tilde{t})\hat{O}_{\mathrm{I}}(\tilde{t}')\big]. \tag{6.2.1}$$

We note that it has been necessary to specify a picture explicitly, since, for times $\tilde{t} \neq \tilde{t}'$, this object is picture-dependent. We may freely move the density operator inside the time-ordering and we insert between the operators the product

$$\hat{\rho}^{-1}(\beta)\hat{\rho(\beta)} = \hat{\rho(\beta)}\hat{\rho}(-\beta) = \mathbb{I}. \tag{6.2.2}$$

From (6.1.9), it follows that

$$\mathrm{tr}\,\hat{\rho}_{\mathrm{I}}(\beta)\mathrm{T}\big[\hat{O}_{\mathrm{I}}(t)\hat{O}_{\mathrm{I}}(t')\big] = \mathrm{tr}\,\mathrm{T}\big[\hat{O}_{\mathrm{I}}(t+i\beta)\hat{\rho}_{\mathrm{I}}(\beta)\hat{O}_{\mathrm{I}}(t')\big]. \tag{6.2.3}$$

Using the cyclicity of the trace and the fact that we are free to reorder the operators inside the time-ordering, we obtain the *Kubo-Martin-Schwinger* (KMS) *relation*

$$\langle \mathrm{T}\big[\hat{O}_{\mathrm{I}}(\tilde{t})\hat{O}_{\mathrm{I}}(\tilde{t}')\big]\rangle_\beta = \langle \mathrm{T}\big[\hat{O}_{\mathrm{I}}(\tilde{t}+i\beta)\hat{O}_{\mathrm{I}}(\tilde{t}')\big]\rangle_\beta = \langle \mathrm{T}\big[\hat{O}_{\mathrm{I}}(\tilde{t})\hat{O}_{\mathrm{I}}(\tilde{t}'-i\beta)\big]\rangle_\beta . \tag{6.2.4}$$

6.3 Thermal Propagators

In this final section, we generalise the vacuum expectation values of products of operators to quantum statistical mechanics, introducing the *thermal propagator*, the ensemble expectation value of products of operators. Hereafter, these thermal propagators will be referred to simply as the propagators. Indeed, this seems reasonable since we anticipate that in the zero-temperature limit, we should obtain the vacuum expectation values with which we started.

The thermal Wightman propagators are defined via

$$i\Delta^{>}(\tilde{t}-\tilde{t}') = \frac{1}{Z}\mathrm{tr}\,\hat{\rho}(\beta)\hat{q}(\tilde{t})\hat{q}(\tilde{t}'), \tag{6.3.1a}$$

$$i\Delta^{<}(\tilde{t}-\tilde{t}') = \frac{1}{Z}\mathrm{tr}\,\hat{\rho}(\beta)\hat{q}(\tilde{t}')\hat{q}(\tilde{t}). \tag{6.3.1b}$$

Evaluating the trace of the former in the basis of energy eigenstates, we obtain

$$i\Delta^{>}(\tilde{t}-\tilde{t}') = Z^{-1}\sum_{n,m=0}^{\infty} e^{-\beta E_n}e^{i(E_n-E_m)(\tilde{t}-\tilde{t}')}|\langle n|\hat{q}|m\rangle|^2. \tag{6.3.2}$$

In the limit that $T \to 0$ ($\beta \to \infty$), we see that only the lowest energy state survives due to the Boltzmann suppression. This lowest energy state is precisely the vacuum and we see that we recover the familiar zero-temperature propagator. Analytically continuing $\tilde{t} \to \mathfrak{t} = \tilde{t} - i\tau \in \mathbb{C}$ and $\tilde{t}' \to \mathfrak{t}' = \tilde{t}' - i\tau \in \mathbb{C}$, we see also that the propagator is convergent only for $-\beta \leq \mathrm{Im}(\mathfrak{t}-\mathfrak{t}') \leq 0$. As a result, we interpret the KMS relation (6.2.4) as the requirement that the imaginary time τ must be periodic on $(0,\beta]$. We note that this periodicity requirement supersedes the constraints in (5.2.13), ensurinng the validity of the Wick rotation. In fact, this requirement is

entirely equivalent to those constraints since in the zero-temperature limit $\beta \to \infty$.

Using the algebra of the creation and annihilation operators and performing the summations we obtain

$$i\Delta^{>}(\tilde{t}-\tilde{t}') = \frac{1}{2m\omega}\{[1+f_{\mathrm{B}}(\omega)]e^{-i\omega(\tilde{t}-\tilde{t}')} + f_{\mathrm{B}}(\omega)e^{i\omega(\tilde{t}-\tilde{t}')}\}, \tag{6.3.3a}$$

$$i\Delta^{<}(\tilde{t}-\tilde{t}') = \frac{1}{2m\omega}\{f_{\mathrm{B}}(\omega)e^{-i\omega(\tilde{t}-\tilde{t}')} + [1+f_{\mathrm{B}}(\omega)]e^{i\omega(\tilde{t}-\tilde{t}')}\}. \tag{6.3.3b}$$

It follows then that the Feynman propagator takes the form

$$i\Delta_{\mathrm{F}}(\tilde{t}-\tilde{t}') = \frac{1}{m}\int\frac{\mathrm{d}\omega'}{2\pi}\,e^{-i\omega'(\tilde{t}-\tilde{t})}\left[\frac{i}{\omega'^2-\omega^2+i\epsilon} + 2\pi f_{\mathrm{B}}(|\omega'|)\delta(\omega'^2-\omega^2)\right]. \tag{6.3.4}$$

The thermal Wightman propagators satisfy the KMS relation

$$i\Delta^{>}(\tilde{t}-\tilde{t}') = i\Delta^{<}(\tilde{t}-\tilde{t}'-i\beta), \tag{6.3.5}$$

and equivalently in frequency space

$$i\Delta^{>}(\omega') = e^{\beta\omega'}i\Delta^{<}(\omega'), \tag{6.3.6}$$

where

$$i\Delta^{>}(\omega') = 2\pi\varepsilon(\omega')[1+f_{\mathrm{B}}(\omega')]\delta(\omega'^2-\omega^2), \tag{6.3.7a}$$

$$i\Delta^{<}(\omega') = 2\pi\varepsilon(\omega')f_{\mathrm{B}}(\omega')\delta(\omega'^2-\omega^2), \tag{6.3.7b}$$

and ε is the signum function, which may be written in terms of the unit step function as

$$\varepsilon(\omega') = \theta(\omega') - \theta(-\omega'). \tag{6.3.8}$$

We can quickly convince ourselves of the consistency of these results with the relation

$$e^{\beta\omega'}f_{\mathrm{B}}(\beta\omega') = 1 + f_{\mathrm{B}}(\omega'). \tag{6.3.9}$$

6.4 The Matsubara Propagator

If our interest is in the ensemble expectation value of thermodynamic observables, the real-time dependence of the thermal propagators is seemingly redundant. In which case, we may work entirely in terms of the imaginary-time dependence.

Hence, we wish to calculate Green's functions in imaginary-time. Wick-rotating the generating functional in (5.2.8) to negative imaginary-time $\tilde{t} = -i\tau$ and compactifying the imaginary-time direction on $(0, \beta]$, we obtain the generating functional of the imaginary-time formalism of the quantum harmonic oscillator

$$\mathcal{Z}[j] = \mathcal{N} \int \big[\mathrm{d}q\big] \, \exp\left[- \int_0^\beta \mathrm{d}\tau \, \Big(\bar{L}(\dot{q}, q) - j(\tau) q(\tau) \Big) \right], \tag{6.4.1}$$

where $\bar{L}$ is the Euclidean or imaginary-time Lagrangian

$$\bar{L}(\dot{q}, q) = \frac{1}{2} \Big[m\dot{q}^2 + m\omega^2 q^2 \Big]. \tag{6.4.2}$$

The derivative

$$\dot{q} = \frac{\mathrm{d}q}{\mathrm{d}\tau} \tag{6.4.3}$$

is taken with respect to the imaginary time τ. We may then introduce the imaginary-time propagator

$$\bar{\Delta}(\tau - \tau') = \big\langle \mathrm{T}_\tau \big[\hat{q}(\tau) \hat{q}(\tau') \big] \big\rangle_\beta = \frac{1}{\mathcal{Z}[0]} \frac{\delta^2 \mathcal{Z}[j]}{\delta j(\tau) \delta j(\tau')} \bigg|_{j=0}. \tag{6.4.4}$$

Completing the square in the exponent as before, we may write the imaginary-time generating functional in the form,

$$\mathcal{Z}[j] = \mathcal{Z}[0] \int \big[\mathrm{d}q\big] \, \exp\left[\frac{1}{2} \iint_0^\beta \mathrm{d}\tau \, \mathrm{d}\tau' \, j(\tau) \bar{\Delta}(\tau - \tau') j(\tau') \right], \tag{6.4.5}$$

where we have written

$$q(\tau) = q_0(\tau) + \int_0^\beta \mathrm{d}\tau\, \bar{\Delta}(\tau - \tau') j(\tau'). \tag{6.4.6}$$

The imaginary-time propagator must satisfy

$$m\Big[-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + \omega^2 \Big] \bar{\Delta}(\tau - \tau') = \delta(\tau - \tau'). \tag{6.4.7}$$

In the limit $j = 0$, the imaginary-time generating functional is precisely the partition function.

The imaginary-time propagator, as argued above in the derivation of the KMS relation, must be periodic on $(0, \beta]$, in which case,

$$\bar{\Delta}(\tau) = \bar{\Delta}(\tau + \beta). \tag{6.4.8}$$

Fourier transforming, it follows that

$$\int \mathrm{d}\tau\, e^{i\omega'\tau} \bar{\Delta}(\tau) = \int \mathrm{d}\tau\, e^{i\omega'\tau} \bar{\Delta}(\tau + \beta). \tag{6.4.9}$$

Making the change of variables $\tau' = \tau + \beta$ on the right-hand side, this equality requires that the frequencies ω' are discrete:

$$\omega' \to \omega_n = \frac{2\pi n}{\beta}. \tag{6.4.10}$$

These are the so-called *Matsubara frequencies*. The inverse Fourier transform is then replaced by the discrete form

$$\bar{\Delta}(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{+\infty} e^{-i\omega_n \tau} \bar{\Delta}(i\omega_n), \tag{6.4.11}$$

where $\bar{\Delta}(i\omega_n)$ is the *Matsubara propagator*. Substituting this result into (6.4.7), we find

$$\bar{\Delta}(i\omega_n) = \frac{1}{\omega_n^2 + \omega^2}. \tag{6.4.12}$$

We have suggested that, when working with equilibrium systems, the real-time dependence is not of interest. This is of course not entirely true. For instance, we might wish to calculate the decay rate of a particle in a heat bath. Here, it is clear that we want to work in real time, in which case we want to continue results back to real time. However, this analytic continuation is a subtle issue and for the sake of clarity, we will postpone its discussion for now. Suffice to say, it is not merely a question of performing the inverse Wick rotation $-i\tau = \tilde{t}$ and replacing the discrete Matsubara frequencies by their continuous counterparts.

The ITF, for which there is a wealth of literature, will not be discussed in a great deal more detail in this thesis, except to establish the correspondence with the forthcoming approach in the thermodynamic equilibrium limit. This is for the reason that the ITF is, in essence, a mathematical convenience — albeit a useful one — for calculations in thermodynamic equilibrium, in which the density operator is of the canonical form. It is therefore inapplicable to the non-equilibrium systems in which we are interested.

7 The Scalar Field

In our discussions of the quantum harmonic oscillator, all modes had the same frequency ω. The natural generalisation then is to sum over contributions from oscillators of all possible frequencies. We move then to quantum field theory, in which the position operator $\hat{q}(\tilde{t})$ is superseded by some *field operator* $\hat{\phi}(\tilde{t}, \mathbf{x})$, which is a function of both space and time and acts to create and destroy the quanta of energy that we interpret as *particles*.

In this chapter, we review the quantisation of a massive, scalar quantum field theory. This toy theory will be our playground for the development of an approach to the non-equilibrium dynamics of these fields.

7.1 Canonical Quantisation

In this section, we introduce the scalar field theory with which we will develop the discussions of Part II. We consider a self-interacting theory with mass M, described by the bare, interaction-picture Lagrangian density

$$\mathcal{L}(x) = \tfrac{1}{2}\partial_\mu \Phi(x)\partial^\mu \Phi(x) - \tfrac{1}{2}M^2\Phi^2(x) - \tfrac{1}{3!}g\Phi^3(x) - \tfrac{1}{4!}\lambda\Phi^4(x), \tag{7.1.1}$$

where g and λ are dimensionful and dimensionless couplings respectively. The shorthand $x \equiv x^\mu = (x^0, \mathbf{x})$ denotes the four-dimensional space-time arguments of field operators. The Minkowski space-time metric is taken to have the signature $(+,-,-,-)$. For a more detailed introduction to the scalar field with reference to

Lorentz-invariance and representations of the Poincaré, see for instance [83].

It will prove constructive to set out again from the Schrödinger picture introduced in Chapter 4, in which we recall that state vectors are *time-dependent* and basis vectors and operators are, in the absence of external sources, *time-independent*. The *time-independent* Schrödinger-picture field operator, denoted by a subscript S, may be written in the familiar, plane-wave decomposition

$$\Phi_{\mathrm{S}}(\mathbf{x};\tilde{t}_i) = \int \mathrm{d}\Pi_{\mathbf{p}} \left[a_{\mathrm{S}}(\mathbf{p};\tilde{t}_i)e^{i\mathbf{p}\cdot\mathbf{x}} + a^{\dagger}_{\mathrm{S}}(\mathbf{p};\tilde{t}_i)e^{-i\mathbf{p}\cdot\mathbf{x}} \right], \tag{7.1.2}$$

where we have introduced the short-hand

$$\int \mathrm{d}\Pi_{\mathbf{p}} \equiv \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3} \frac{1}{2E(\mathbf{p})} = \int \frac{\mathrm{d}^4 p}{(2\pi)^4}\, 2\pi\theta(p_0)\delta(p^2 - M^2) \tag{7.1.3}$$

for the Lorentz-invariant phase-space (LIPS). $E(\mathbf{p}) = \sqrt{\mathbf{p}^2 + M^2}$ is the energy of the single-particle mode with three-momentum $\mathbf{p}$ and θ is the unit step function, defined in (5.3.2).

As this point, we emphasise that we have defined the interaction-, Heisenberg- and Schrödinger-pictures to be coincident at the finite, microscopic boundary time $\tilde{t}_i$, such that

$$\Phi_{\mathrm{S}}(\mathbf{x};\tilde{t}_i) = \Phi_{\mathrm{I}}(\tilde{t}_i,\mathbf{x}) = \Phi_{\mathrm{H}}(\tilde{t}_i,\mathbf{x}), \tag{7.1.4}$$

where implicit dependence upon the boundary time $\tilde{t}_i$ is marked by separation from explicit arguments by a semi-colon.

The *time-independent*, Schrödinger-picture operators $a^{\dagger}_{\mathrm{S}}(\mathbf{p};\tilde{t}_i)$ and $a_{\mathrm{S}}(\mathbf{p};\tilde{t}_i)$ are the well-known creation and annihilation operators, superseding those introduced in Chapter 4 for the quantum harmonic oscillator, which act on the stationary vacuum $|0\rangle$, respectively creating and destroying *time-independent*, single-particle

momentum eigenstates, according to

$$a_{\mathrm{S}}^{\dagger}(\mathbf{p};\tilde{t}_i)|0\rangle = |\mathbf{p};\tilde{t}_i\rangle, \tag{7.1.5a}$$

$$a_{\mathrm{S}}(\mathbf{p};\tilde{t}_i)|\mathbf{p}';\tilde{t}_i\rangle = (2\pi)^3 2E(\mathbf{p})\delta^{(3)}(\mathbf{p}-\mathbf{p}')|0\rangle, \tag{7.1.5b}$$

$$a_{\mathrm{S}}(\mathbf{p};\tilde{t}_i)|0\rangle = 0. \tag{7.1.5c}$$

The momentum eigenstates $|\mathbf{p};\tilde{t}_i\rangle$ respect the orthonormality condition

$$\langle\mathbf{p}';\tilde{t}_i|\mathbf{p};\tilde{t}_i\rangle = (2\pi)^3 2E(\mathbf{p})\delta^{(3)}(\mathbf{p}-\mathbf{p}'). \tag{7.1.6}$$

In analogy to the discussion in Section 4.2, we define the *time-dependent*, interaction-picture field operator via

$$\Phi_{\mathrm{I}}(x) = e^{iH_{\mathrm{S}}^0(x_0-\tilde{t}_i)}\Phi_{\mathrm{S}}(\mathbf{x};\tilde{t}_i)e^{-iH_{\mathrm{S}}^0(x_0-\tilde{t}_i)}, \tag{7.1.7}$$

where H_{S}^0 is the free-part of the Hamiltonian in the Schrödinger picture. Using the commutators

$$\left[H_{\mathrm{S}}^0, a_{\mathrm{S}}(\mathbf{p};\tilde{t}_i)\right] = -E(\mathbf{p})a_{\mathrm{S}}(\mathbf{p};\tilde{t}_i), \tag{7.1.8a}$$

$$\left[H_{\mathrm{S}}^0, a_{\mathrm{S}}^{\dagger}(\mathbf{p};\tilde{t}_i)\right] = +E(\mathbf{p})a_{\mathrm{S}}^{\dagger}(\mathbf{p};\tilde{t}_i), \tag{7.1.8b}$$

the interaction-picture field operator may be written

$$\Phi_{\mathrm{I}}(x) = \int \mathrm{d}\Pi_{\mathbf{p}} \left[a_{\mathrm{S}}(\mathbf{p};\tilde{t}_i)e^{-iE(\mathbf{p})(x_0-\tilde{t}_i)}e^{i\mathbf{p}\cdot\mathbf{x}} + a_{\mathrm{S}}^{\dagger}(\mathbf{p};\tilde{t}_i)e^{iE(\mathbf{p})(x_0-\tilde{t}_i)}e^{-i\mathbf{p}\cdot\mathbf{x}} \right], \tag{7.1.9}$$

or, equivalently, in terms of interaction-picture operators only,

$$\Phi_{\mathrm{I}}(x) = \int \mathrm{d}\Pi_{\mathbf{p}} \left[a_{\mathrm{I}}(\mathbf{p},0)e^{-iE(\mathbf{p})x_0}e^{i\mathbf{p}\cdot\mathbf{x}} + a_{\mathrm{I}}^{\dagger}(\mathbf{p},0)e^{iE(\mathbf{p})x_0}e^{-i\mathbf{p}\cdot\mathbf{x}} \right], \tag{7.1.10}$$

where it should be stressed that the *time-dependent*, interaction-picture creation and annihilation operators are evaluated at the microscopic time 0. Hereafter, we will omit the subscript I on interaction-picture operators for convenience. We may write

the four-dimensional Fourier transform of the interaction-picture field operator as

$$\Phi(p) = \int \mathrm{d}^4x\, e^{ip.x}\Phi(x) = 2\pi\delta(p^2 - M^2)\big[\,\theta(p_0)a(\mathbf{p},0) + \theta(-p_0)a^\dagger(-\mathbf{p},0)\big]. \quad (7.1.11)$$

In the case that the interactions are switched off adiabatically at time $\tilde{t}_i$, we may define the asymptotic *in* creation and annihilation operators via

$$a_{\mathrm{in}}^{(\dagger)}(\mathbf{p}) \equiv Z^{-1/2} \lim_{\tilde{t}_i \to -\infty} a_{\mathrm{S}}^{(\dagger)}(\mathbf{p};\tilde{t}_i)e^{+(-)iE(\mathbf{p})\tilde{t}_i}, \quad (7.1.12)$$

where $Z = 1 + \mathcal{O}(\hbar)$ is the wavefunction renormalisation. We then recover the more familiar form of the interaction-picture scalar field operator. Herein, we see the importance of keeping track of the finite boundary time $\tilde{t}_i$: it is necessary to ensure that our forthcoming generalisations are consistent with asymptotic field theory [84] in the limit $\tilde{t}_i \to -\infty$.

We choose to begin our quantisation by defining the commutator of interaction-picture fields

$$\big[\Phi(x), \Phi(y)\big] = i\Delta^0(x, y; M^2), \quad (7.1.13)$$

where $i\Delta^0(x, y; M^2)$ is the *tree-level* or *free* Pauli-Jordan propagator. Herein, we denote free propagators by a superscript 0. The condition of micro-causality requires that the interaction-picture fields commute for space-like separations $(x - y)^2 < 0$. This restricts $i\Delta^0(x, y; M^2)$ to be invariant under spatial translations, having the Poincaré-invariant form

$$i\Delta^0(x, y; M^2) = \int \mathrm{d}\Pi_{\mathbf{p}} \Big[e^{-iE(\mathbf{p})(x^0-y^0)}e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} - \big(x \longleftrightarrow y\big)\Big]. \quad (7.1.14)$$

This is simply the difference of two counter-propagating packets of plane waves, as we should expect. It is the Poincaré-invariant form of (7.1.14) that we wish to maintain once thermal background effects are included. Pre-empting the forthcoming analysis,

we introduce the *double* Fourier transform

$$i\Delta^0(p,p';M^2) = \iint \mathrm{d}^4x\,\mathrm{d}^4y\, e^{ip\cdot x}e^{-ip'\cdot y}\, i\Delta^0(x,y;M^2) \tag{7.1.15a}$$

$$= 2\pi\varepsilon(p_0)\delta(p^2-M^2)(2\pi)^4\delta^{(4)}(p-p'), \tag{7.1.15b}$$

where ε is the signum function in (6.3.8). Note that we have defined the Fourier transforms such that four-momentum p flows *away from* the point x and four-momentum p' flows *towards* the point y.

From (7.1.13) and (7.1.14), we may derive the familiar equal-time commutation relations

$$i\Delta^0(x,y)\big|_{x^0=y^0=\tilde{t}} = \big[\Phi(\tilde{t},\mathbf{x}),\Phi(\tilde{t},\mathbf{y})\big] = 0, \tag{7.1.16a}$$

$$\partial_{x_0} i\Delta^0(x,y)\big|_{x^0=y^0=\tilde{t}} = \big[\pi(\tilde{t},\mathbf{x}),\Phi(\tilde{t},\mathbf{y})\big] = -i\delta^{(3)}(\mathbf{x}-\mathbf{y}), \tag{7.1.16b}$$

$$\partial_{x_0}\partial_{y_0} i\Delta^0(x,y)\big|_{x^0=y^0=\tilde{t}} = \big[\pi(\tilde{t},\mathbf{x}),\pi(\tilde{t},\mathbf{y})\big] = 0, \tag{7.1.16c}$$

where $\pi(x) = \partial_{x_0}\Phi(x)$ is the conjugate momentum operator, cf. (4.1.7). In order to satisfy the constraints of (7.1.13), the creation and annihilation operators must respect the commutation relation

$$\big[a(\mathbf{p},\tilde{t}\,),a^\dagger(\mathbf{p}',\tilde{t}\,)\big] = \big(2\pi\big)^3 2E(\mathbf{p})\delta^{(3)}(\mathbf{p}-\mathbf{p}'), \tag{7.1.17}$$

with all other commutators vanishing.

The vacuum expectation of the commutator of Heisenberg-picture field operators may be expressed as a superposition of interaction-picture field commutators by means of the Källén-Lehmann spectral representation [85, 86]:

$$\langle 0|\big[\Phi_{\mathrm{H}}(x),\Phi_{\mathrm{H}}(y)\big]|0\rangle = i\Delta(x,y) = \int_0^\infty \mathrm{d}s\,\sigma(s) i\Delta^0(x,y;s), \tag{7.1.18}$$

where $i\Delta^0(x,y;s)$ is the free Pauli-Jordan propagator in (7.1.14) with M^2 replaced by s and $i\Delta(x,y)$ is the *dressed* or *resummed* propagator. The positive spectral density $\sigma(s)$ contains all information about the spectrum of single- and multi-particle

states produced by the Heisenberg-picture field operators. Note that for the homogeneous, stationary vacuum $|0\rangle$, $\sigma(s)$ is independent of the space-time coordinates and the resummed Pauli-Jordan propagator maintains its translational invariance. If $\sigma(s)$ is normalised such that

$$\int_0^\infty \mathrm{d}s\, \sigma(s) = 1, \tag{7.1.19}$$

the equal-time commutation relations of Heisenberg-picture operators maintain exactly the form in (7.1.16). In this case, the spectral function cannot depend upon any fluctuations in the background. It is clear then that for non-trivial 'vacua', i.e., thermal backgrounds, the spectral density becomes a function also of the coordinates. The spectral structure of the resummed propagators will then obtain non-trivial space-time dependence. In this case, the convenient factorisation of the Källén-Lehmann representation breaks down and the equal-time commutation relations of Heisenberg-picture field operators do not maintain their canonical form.

We define the retarded and advanced, causal propagators

$$i\Delta_{\mathrm{R}}(x,y) \equiv \theta(x_0 - y_0) i\Delta(x,y), \tag{7.1.20a}$$

$$i\Delta_{\mathrm{A}}(x,y) \equiv -\theta(y_0 - x_0) i\Delta(x,y). \tag{7.1.20b}$$

Using the Fourier representation of the unit step function in (5.3.2), we introduce a convenient representation of these causal propagators in terms of the convolution

$$i\Delta_{\mathrm{R(A)}}(p,p') = i\int \frac{\mathrm{d}k_0}{2\pi} \frac{i\Delta(p_0 - k_0, p_0' - k_0; \mathbf{p}, \mathbf{p}')}{k_0 + (-)i\epsilon}. \tag{7.1.21}$$

After substituting for the free Pauli-Jordan propagator in (7.1.15a), we find the Fourier transform of the free causal propagators

$$i\Delta^0_{\mathrm{R(A)}}(p,p') = \frac{i}{\big(p_0 + (-)i\epsilon\big)^2 - \mathbf{p}^2 - M^2}(2\pi)^4 \delta^{(4)}(p - p'), \tag{7.1.22}$$

where we draw attention to the sign-dependent pole prescription discussed in Chap-

ter 5.

The absolutely-ordered, Wightman propagators are defined as

$$i\Delta_{>}(x,y) \equiv \langle \Phi(x)\Phi(y)\rangle, \tag{7.1.23a}$$

$$i\Delta_{<}(x,y) \equiv \langle \Phi(y)\Phi(x)\rangle. \tag{7.1.23b}$$

We may then write the *causality relation*

$$\Delta(x,y) = \Delta_{>}(x,y) - \Delta_{<}(x,y) = \Delta_{\mathrm{R}}(x,y) - \Delta_{\mathrm{A}}(x,y). \tag{7.1.24}$$

We also define the non-causal Hadamard propagator, which is the expectation of the field anti-commutator

$$i\Delta_{1}(x,y) \equiv \langle \big\{ \Phi(x), \Phi(y) \big\} \rangle. \tag{7.1.25}$$

The time-ordered, Feynman and anti-time-ordered, Dyson propagators are respectively

$$i\Delta_{\mathrm{F}}(x,y) \equiv \langle \mathrm{T}[\Phi(x)\Phi(y)]\rangle, \tag{7.1.26a}$$

$$i\Delta_{\mathrm{D}}(x,y) \equiv \langle \bar{\mathrm{T}}[\Phi(x)\Phi(y)]\rangle, \tag{7.1.26b}$$

where T and $\bar{\mathrm{T}}$ are the time- and anti-time-ordering operators. Explicitly,

$$\Delta_{\mathrm{F}}(x,y) = \theta(x_0 - y_0)\Delta_{>}(x,y) + \theta(y_0 - x_0)\Delta_{<}(x,y), \tag{7.1.27a}$$

$$\Delta_{\mathrm{D}}(x,y) = \theta(x_0 - y_0)\Delta_{<}(x,y) + \theta(y_0 - x_0)\Delta_{>}(x,y). \tag{7.1.27b}$$

We may then write the *unitarity relation*

$$\Delta_{1}(x,y) = \Delta_{\mathrm{F}}(x,y) + \Delta_{\mathrm{D}}(x,y) = \Delta_{>}(x,y) + \Delta_{<}(x,y) = 2i\mathrm{Im}\,\Delta_{\mathrm{F}}(x,y). \tag{7.1.28}$$

Finally, we define the principal-part propagator

$$\Delta_{\mathcal{P}}(x,y) = \frac{1}{2}\big[\Delta_{\mathrm{R}}(x,y) + \Delta_{\mathrm{A}}(x,y)\big] = \mathrm{Re}\,\Delta_{\mathrm{F}}(x,y), \tag{7.1.29}$$

where we are reminded that, in general,

$$\mathrm{Re}\big(\mathrm{Im}\big)F(x,y) \neq \iint \frac{\mathrm{d}^4p}{(2\pi)^4}\frac{\mathrm{d}^4p'}{(2\pi)^4}\, e^{-ip\cdot x}e^{ip'\cdot y}\,\mathrm{Re}\big(\mathrm{Im}\big)F(p,p'), \tag{7.1.30}$$

except when $F(p,p') = F(-p,-p')$.

The definitions and the relations discussed above are valid for both free and resummed propagators. In Appendix A, we list the properties of these propagators in both coordinate and momentum representations as well as a number of useful identities, which we will refer to throughout the forthcoming discussions. These considerations and the analysis of the following sections are generalised to the complex scalar field in Chapter 13. A comprehensive introduction to these propagators and their contour-integral representations is provided in [73].

Part II

Non-equilibrium Mechanics

8 Introduction to Part II

The aim of Part I was to cover those topics prerequisite to our development of a quantum field-theoretic description of non-equilibrium statistical mechanics. In Part II, we embark upon the formulation of this description.

We begin in Chapter 9 by introducing the Schwinger-Keldysh CTP formalism, a means for calculating equal-time expectation values of products of field operators. Proceeding then to generalise the EEVs introduced previously to arbitrary density operators, we derive in Chapter 10 the most general form of the various propagators defined in 7 in the presence of non-homogeneous backgrounds. By means of the CJT effective action, we derive a perturbation theory based upon these non-homogeneous propagators. In Chapter 11, we show that the results from these chapters are entirely consistent with established approaches in the thermodynamic equilibrium. With reference to these equilibrium results, we argue in Chapter 12 that the perturbation series derived in Chapter 10 is free of the pinching singularities thought to spoil perturbative approaches to non-equilibrium thermal field theory. In Chapter 13 and in preparation for the toy model discussed in Chapter 17, we outline the generalisation of these ideas, including those from equilibrium thermal field theory, to the complex scalar field. In Chapter 14, we introduce an unambiguous definition of the number density of particles based upon the conserved Noether charge. This then permits the derivation of perturbative time-evolution equations as outlined in Chapter 15 and in which we establish the consistency of this approach with those of the Boltzmann equation and gradient-expanded Kadanoff-Baym equations in the classical (or at least, semi-classical) limit. Chapter 16 provides a detailed technical discussion

of the calculation of loop integrals built out of our non-homogeneous propagators. This is performed in a manner as close as is feasible to the more familiar results from zero-temperature quantum field theory.

Finally, in Chapter 17, we apply the formalism to the thermalisation of a simple toy model, comprising a massive real scalar field and a less massive complex scalar field. Within this chapter, we derive the time-dependent width of the massive scalar and show that it exhibits oscillations with time-dependent frequencies. These non-Markovian oscillations are interpreted as a signal of memory effects. We show that, as result of the microscopic violation of energy conservation due to systematic inclusion of finite-time effects, the particle width obtains contributions from processes that would normally be kinematically forbidden. These evanescent contributions are shown to be significant to the early-time evolution of these non-equilibrium systems.

For more general introductions to existing approaches to non-equilibrium thermal field theory, see [87–89]

9 The CTP Formalism

It will prove illustrative to discuss the formalisms that we will subsequently apply to theories with non-trivial vacua firstly in the context of the zero-temperature quantum field theory with which we are well acquainted. In the following section, we will motivate and outline the use of the so-called *in-in* or closed-time path (CTP)9.1 formalism due to Schwinger and Keldysh [23, 24]. Subsequently, we will justify the introduction of a 2×2 matrix propagator, restricting the form of its elements subject to the familiar constraints of causality and unitarity, outlined above in (7.1.24) and (7.1.28).

In the calculation of scattering-matrix elements, we are concerned with the transition amplitude between *in* and *out* asymptotic states, single-particle states defined respectively in the infinitely-distant past and future. On the other hand, in quantum statistical mechanics, we are interested in the calculation of EEVs of operators at defined times. In order to calculate such objects in a field-theoretic framework, we require an approach that allows us to determine the transition amplitude between states of the *same time*. This approach is the Schwinger-Keldysh CTP formalism.

Let us consider for illustration the following observable in the Schrödinger picture:

$$\int[\mathrm{d}\Phi]\ {}_{\mathrm{S}}\langle\Phi(\mathbf{z}),\tilde{t}_f|\Phi_{\mathrm{S}}(\mathbf{x};\tilde{t}_i)\Phi_{\mathrm{S}}(\mathbf{y};\tilde{t}_i)|\Phi(\mathbf{z}),\tilde{t}_f\rangle_{\mathrm{S}}, \tag{9.0.1}$$

where $|\Phi(\mathbf{z}),\tilde{t}_f\rangle_{\mathrm{S}}$ is a *time-dependent* eigenstate of the *time-independent*, Schrödinger-picture field operator $\Phi_{\mathrm{S}}(\mathbf{x};\tilde{t}_i)$ with eigenvalue $\Phi(\mathbf{z})$. $[\mathrm{d}\Phi]$ represents the functional

integral over field configurations $\Phi(\mathbf{z})$ and we recall that implicit dependence upon the boundary time $\tilde{t}_i$ is marked by a semi-colon.

As an aside, we see that there are seven explicit degrees of freedom: the microscopic time $\tilde{t}_f$ and the two spatial coordinates $\mathbf{x}$ and $\mathbf{y}$; and one implicit degree of freedom, the boundary time $\tilde{t}_i$. Pre-empting the forthcoming discussions, we note that this is the number of degrees of freedom required to construct meaningful statistical observables that depend simultaneously on macroscopic space-time coordinates and three-momenta, without violating Heisenberg's uncertainty principle. These degrees of freedom will turn out to be the macroscopic, central space-time coordinate ($t = \tilde{t}_f - \tilde{t}_i$, $\mathbf{X} = (\mathbf{x} + \mathbf{y})/2$) and the three-momentum $\mathbf{p}$, conjugate to the relative coordinate $\mathbf{R} = \mathbf{x} - \mathbf{y}$.

In the interaction picture, the same observable is

$$\int [\mathrm{d}\Phi]\ {}_{\mathrm{I}}\langle \Phi(\mathbf{z}), \tilde{t}_f | \Phi_{\mathrm{I}}(\tilde{t}_f, \mathbf{x}) \Phi_{\mathrm{I}}(\tilde{t}_f, \mathbf{y}) | \Phi(\mathbf{z}), \tilde{t}_f \rangle_{\mathrm{I}}; \tag{9.0.2}$$

and in the Heisenberg picture,

$$\int [\mathrm{d}\Phi]\ {}_{\mathrm{H}}\langle \Phi(\mathbf{z}); \tilde{t}_i | \Phi_{\mathrm{H}}(\tilde{t}_f, \mathbf{x}) \Phi_{\mathrm{H}}(\tilde{t}_f, \mathbf{y}) | \Phi(\mathbf{z}); \tilde{t}_i \rangle_{\mathrm{H}}. \tag{9.0.3}$$

We see then that in the interaction and Heisenberg pictures, the physical observables must be constructed from time-dependent vectors and operators that are evaluated at *equal times*. Any observable built out of time-dependent vectors and operators that are evaluated at different times would be *picture dependent* and therefore unphysical.

9.1 The CTP Contour

In order to generate equal-time observables of the form in (9.0.3), we first introduce the *in* vacuum state $|0_{\mathrm{in}}; \tilde{t}_i\rangle$, which is at time $\tilde{t}_i$ a time-independent eigenstate of the Heisenberg field operator $\Phi_{\mathrm{H}}(x)$ with zero eigenvalue (see [34, 35]). We then require

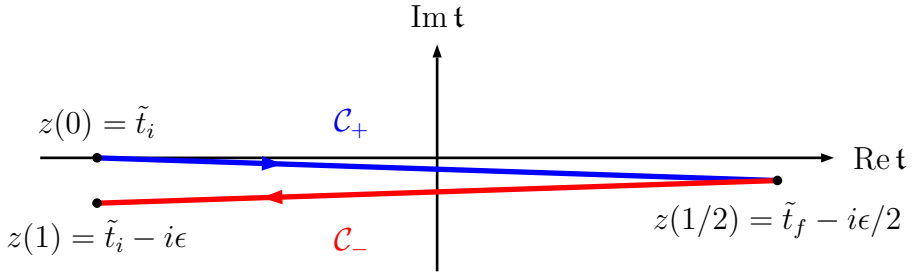


Figure 9.1: The closed-time path, $\mathcal{C} = \mathcal{C}_+ \cup \mathcal{C}_-$, running first along $\mathcal{C}_+$ from $\tilde{t}_i$ to $\tilde{t}_f - i\epsilon/2$, before returning along $\mathcal{C}_-$ from $\tilde{t}_f - i\epsilon/2$ to $\tilde{t}_i - i\epsilon$.

a means of driving the amplitude $\langle 0_{\rm in}, \tilde{t}_i | 0_{\rm in}, \tilde{t}_i \rangle$ by the appropriate introduction of external sources.

We proceed as follows: we imagine evolving our *in* state at time $\tilde{t}_i$ forwards in time under the influence of a source $J_+(x)$ to some *out* state at time $\tilde{t}_f$ in the future, which will be an incoherent sum over all possible future states. We then evolve this superposition of states backwards again under the influence of a second source $J_-(x)$, returning to the same initial time $\tilde{t}_i$ and the original *in* state. The sources $J_\pm(x)$ are assumed to vanish adiabatically at the bounds of the interval $[\tilde{t}_i,\ \tilde{t}_f]$. We may interpret the path of this evolution as defining a closed contour $\mathcal{C} = \mathcal{C}_+ \cup \mathcal{C}_-$ in the complex-time plane (t-plane, $\mathfrak{t} \in \mathbb{C}$), which is the union of two anti-parallel branches: $\mathcal{C}_+$, running from $\tilde{t}_i$ to $\tilde{t}_f - i\epsilon/2$; and $\mathcal{C}_-$, running from $\tilde{t}_f - i\epsilon/2$ back to $\tilde{t}_i - i\epsilon$, which we shall refer to respectively as the positive, time-ordered and negative, anti-time-ordered branches (see Figure 9.1). The small imaginary part $\epsilon = 0^+$ has been added to allow us to distinguish the two, essentially coincident, branches. We parametrise the distance along the contour, starting from $\tilde{t}_i$, by the real variable $u \in [0, 1]$, which increases monotonically along $\mathcal{C}$. We may then define the contour by a path $\tilde{z}(u) = \tilde{t}(u) - i\tilde{\tau}(u) \in \mathfrak{t}$, where $\tilde{t}(0) = \tilde{t}(1) = \tilde{t}_i$ and $\tilde{t}(1/2) = \tilde{t}_f$. Explicitly,

$$\tilde{z}(u) = \theta(\tfrac{1}{2} - u)\big[\tilde{t}_i + 2u\big(\tilde{t}_f - \tilde{t}_i\big)\big] + \theta(u - \tfrac{1}{2})\big[\tilde{t}_i + 2\big(1 - u\big)\big(\tilde{t}_f - \tilde{t}_i\big)\big] - i\epsilon u, \quad (9.1.1)$$

where we recall from (5.3.2) that $\theta(0) = 1/2$.

The state $|\Phi(\mathbf{x}); \tilde{t}_f\rangle_{\rm H}$ is an eigenstate of the Heisenberg field operator, satisfying

the eigenvalue equation

$$\Phi_{\rm H}(x)|\Phi(\mathbf{x});\tilde{t}_f\rangle_{\rm H} = \Phi(\mathbf{x})|\Phi(\mathbf{x});\tilde{t}_f\rangle_{\rm H} \tag{9.1.2}$$

and forming a complete orthonormal basis, respecting the orthonormality condition

$$\int[{\rm d}\Phi]\ |\Phi(\mathbf{x});\tilde{t}_f\rangle_{\rm H\,H}\langle\Phi(\mathbf{x});\tilde{t}_f| = \mathbb{I}, \tag{9.1.3}$$

where we recall that $[{\rm d}\Phi]$ represents the functional integral over field configurations. We may then write our *in-in* generating functional as

$$\begin{aligned}\mathcal{Z}[J_\pm] &= \int[{\rm d}\Phi]\,\langle 0_{\rm in},\tilde{t}_i|\Phi(\mathbf{x}),\tilde{t}_f\rangle_{J_-}\langle\Phi(\mathbf{x}),\tilde{t}_f|0_{\rm in},\tilde{t}_i\rangle_{J_+}\\ &= \int[{\rm d}\Phi]\,\langle 0_{\rm in},\tilde{t}_i|\bar{\rm T}e^{-i\int_{\tilde{t}_i}^{\tilde{t}_f}{\rm d}^4x\,\Phi_{\rm H}(x)J_-(x)}|\Phi(\mathbf{x}),\tilde{t}_f\rangle\\ &\qquad\times\langle\Phi(\mathbf{x}),\tilde{t}_f|{\rm T}e^{i\int_{\tilde{t}_i}^{\tilde{t}_f}{\rm d}^4x\,\Phi_{\rm H}(x)J_+(x)}|0_{\rm in},\tilde{t}_i\rangle.\end{aligned} \tag{9.1.4}$$

We emphasise that the x_0 integrations run from $\tilde{t}_i$ to $\tilde{t}_f$ and that the 'latest' time (with $u = 1$) appears to the left. We note also that, due to the presence of the external sources $J_\pm$, the time dependence of the eigenstates of the Heisenberg field operator are now explicit.

We denote by $\Phi_\pm(x) \equiv \Phi(x^0 \in \mathcal{C}_\pm, \mathbf{x})$ fields with real-time variable x^0 confined to the positive and negative branches of the contour, respectively. We then define the doublets [34, 35]

$$\Phi^a(x) = \begin{pmatrix}\Phi_+(x)\\ \Phi_-(x)\end{pmatrix}, \quad \Phi_a(x) = \eta_{ab}\Phi^b(x) = \begin{pmatrix}\Phi_+(x) & -\Phi_-(x)\end{pmatrix}, \tag{9.1.5}$$

where $a, b = 1, 2$ and the $\mathbb{SO}(1,1)$ 'metric' $\eta_{ab} = {\rm diag}(1,-1)$. Inserting into (9.1.4) complete sets of eigenstates of the Heisenberg field operator at intermediate times, we may derive a path-integral representation of the *in-in* generating functional:

$$\mathcal{Z}[J_a] = \int[{\rm d}\Phi^a]\,\exp\left[i\left(S[\Phi^a] + \int_{\tilde{t}_i}^{\tilde{t}_f}{\rm d}^4x\,J_a(x)\Phi^a(x)\right)\right], \tag{9.1.6}$$

with action,

$$S[\Phi^a,\tilde{t}_i,\tilde{t}_f]=\int_{\tilde{t}_i}^{\tilde{t}_f}\mathrm{d}^4x\,\Big[\tfrac{1}{2}\eta_{ab}\partial_\mu\Phi^a(x)\partial^\mu\Phi^b(x)-\tfrac{1}{2}\big(M^2\eta_{ab}-i\epsilon\mathbb{I}_{ab}\big)\Phi^a(x)\Phi^b(x)$$
$$-\tfrac{1}{3!}g\eta_{abc}\Phi^a(x)\Phi^b(x)\Phi^c(x)-\tfrac{1}{4!}\lambda\eta_{abcd}\Phi^a(x)\Phi^b(x)\Phi^c(x)\Phi^d(x)\Big],\quad(9.1.7)$$

where $\eta_{abc\ldots}$ is $+1$ for $a=b=c=\cdots=1$ and -1 for $a=b=c=\cdots=2$. The $\epsilon=0^+$ gives the familiar Feynman prescription, ensuring convergence of the *in-in* path-integral. We note that the damping term is proportional to the identity matrix $\mathbb{I}_{ab}$ and not the 'metric' η_{ab}. This prescription requires the addition of a contour-dependent damping term, proportional to $\varepsilon(\frac{1}{2}-u)$, which has the same sign on both the positive and negative branches of the contour.

In order to preserve the correspondence with scattering-matrix theory in the asymptotic limit $\tilde{t}_i\to-\infty$, we choose $\tilde{t}_f=-\tilde{t}_i$. This choice is made to ensure that the action is *manifestly CPT* invariant (invariant under charge-, parity- and time-reversal transformations), even when time-translation invariance, as will be the case for out-of-equilibrium thermal backgrounds. As a result, the natural origin for the macroscopic time t is the boundary time $\tilde{t}_i$, that is the time at which all pictures are coincident and there is no ambiguity in the specification of the boundary conditions. The time $\tilde{t}_i$ is the point at which the interactions are switched on and the macroscopic time $t=\tilde{t}_f-\tilde{t}_i=2\tilde{t}_f$ is then simply the time over which the system has been permitted to evolve.

The more familiar time- and anti-time-ordering operators, see (4.2.24) and (4.2.29), are superseded by a path-ordering operator $\mathrm{T}_{\mathcal{C}}$. In order to quantify this path-ordering, we introduce the contour-dependent step function

$$\theta_{\mathcal{C}}(x^0-y^0)\equiv\theta(u_x-u_y),\quad(9.1.8)$$

where $x^0=\mathrm{Re}\,\tilde{z}(u_x)$ and $y^0=\mathrm{Re}\,\tilde{z}(u_y)$. This subsequently yields a contour-

dependent delta function

$$\delta_{\mathcal{C}}(x^0 - y^0) = \frac{\delta(u_x - u_y)}{\left|\frac{\mathrm{d}\tilde{z}}{\mathrm{d}u}\right|} = \frac{\delta(u_x - u_y)}{2|\tilde{t}_f - \tilde{t}_i|} = \frac{\delta(u_x - u_y)}{2t}. \tag{9.1.9}$$

We may then introduce the path-ordered propagator

$$i\Delta_{\mathcal{C}}(x, y) \equiv \langle \mathrm{T}_{\mathcal{C}}[\Phi(x)\Phi(y)]\rangle. \tag{9.1.10}$$

For x^0 and y^0 on the positive branch, the path-ordering is equivalent to the familiar time-ordering and we obtain the time-ordered, Feynman propagator $i\Delta_{\mathrm{F}}$. On the other hand, for x^0 and y^0 on the negative branch, the path-ordering is equivalent to anti-time-ordering and we obtain the anti-time-ordered, Dyson propagator $i\Delta_{\mathrm{D}}$. For x^0 on the positive branch and y^0 on the negative branch, x^0 is always 'earlier' than y^0 and we obtain the absolutely-ordered, negative-frequency Wightman propagator $i\Delta_{>}$. Conversely, for y^0 on the positive branch and x^0 on the negative branch the opposite is true and we obtain the positive-frequency Wightman propagator $i\Delta_{<}$. In the $\mathbb{SO}(1,1)$ notation, we write the CTP propagator as the 2×2 matrix

$$i\Delta^{ab}(x, y) \equiv \langle \mathrm{T}_{\mathcal{C}}[\Phi^a(x)\Phi^b(y)]\rangle = i\begin{bmatrix} \Delta_{\mathrm{F}}(x, y) & \Delta_{<}(x, y) \\ \Delta_{>}(x, y) & \Delta_{\mathrm{D}}(x, y) \end{bmatrix}. \tag{9.1.11}$$

We may then write the *in-in* generating functional in the form

$$\begin{aligned} \mathcal{Z}[J_a] = \exp\left[i\int_{\Omega_t} \mathrm{d}^4x\, V\left(\frac{1}{i}\frac{\delta}{\delta J_a}\right)\right] \\ \times \int [\mathrm{d}\Phi^a]\, \exp\left[-\frac{i}{2}\iint_{\Omega_t} \mathrm{d}^4x\, \mathrm{d}^4y\, J_a(x)\Delta^{0,\,ab}(x, y)J_b(y)\right], \end{aligned} \tag{9.1.12}$$

where Ω_t is the Minkowski space-time volume bounded by hypersurfaces $x_0 = \pm t/2$ and $i\Delta^{0,\,ab}(x, y)$ is the free CTP propagator. We may then express the resummed

CTP propagator as follows:

$$i\Delta^{ab}(x,y) = \frac{1}{i}\frac{\delta}{\delta J_a(x)}\frac{1}{i}\frac{\delta}{\delta J_b(y)}\mathcal{Z}[J_a]\bigg|_{J_{1,2}=0}, \tag{9.1.13}$$

where the functional derivatives satisfy

$$\frac{\delta}{\delta J_a(x)}\int_{\Omega_t}\mathrm{d}^4y\, J^b(y) = \eta^{ab}\delta^{(4)}(x-y). \tag{9.1.14}$$

In our forthcoming analysis, it will prove useful to rotate the CTP propagator into the so-called Keldysh basis [30] by the orthogonal transformation

$$\tilde{\Delta}^{ab}(x,y) \equiv O^a{}_c O^b{}_d \Delta^{cd}(x,y) = \begin{bmatrix} 0 & \Delta_{\mathrm{A}}(x,y) \\ \Delta_{\mathrm{R}}(x,y) & \Delta_1(x,y) \end{bmatrix}, \quad O^{ab} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{9.1.15}$$

In Chapter 10, we will generalise these discussions to macroscopic ensembles by incorporating background effects in terms of physical sources. In this case, the surface integral $\oint_{\partial\Omega_t}\mathrm{d}s_\mu\Phi^a(x)\partial^\mu\Phi^b(x)$ may not in general vanish on the boundary hypersurface $\partial\Omega_t$ of the volume Ω_t. However, by requiring that the '+'- and '−'-type fields satisfy

$$\Phi_+(x)\partial^\mu\Phi_+(x)\big|_{x^\mu\in\partial\Omega_t} = \Phi_-(x)\partial^\mu\Phi_-(x)\big|_{x^\mu\in\partial\Omega_t}, \tag{9.1.16}$$

we can ensure that surface terms cancel between the positive and negative branches and the free part of the action may be rewritten in the form

$$S_0[\Phi^a,t] = \iint_{\Omega_t}\mathrm{d}^4x\,\mathrm{d}^4y\,\tfrac{1}{2}\Phi^a(x)\Delta^{0,-1}_{ab}(x,y)\Phi^b(y), \tag{9.1.17}$$

defining the free inverse CTP propagator

$$\Delta^{0,-1}_{ab}(x,y) = \big[-\big(\Box_x^2 + M^2\big)\eta_{ab} + i\epsilon\mathbb{I}_{ab}\big]\delta^{(4)}(x-y), \tag{9.1.18}$$

where $\Box_x^2 \equiv \frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x_\mu}$ is the d'Alembertian operator and $\Box_x^2 + M^2$ is the familiar Klein-Gordon operator. Note that the variational principle remains well-defined irrespective of (9.1.16), since we are always free to choose the variation of the field

$\delta\Phi^a(x)$ to vanish for x^μ on $\partial\Omega_t$.

In the absence of interactions, eigenstates of the free Hamiltonian will propagate uninterrupted from times infinitely distant in the past to times infinitely far in the future and, as such, we may safely extend the limits of integration in the free part of the action to positive and negative infinity, since

$$\big(\Box_x^2 + M^2\big)\Phi^a(x)\big|_{x_0\notin[-t/2,\ t/2]} = 0. \tag{9.1.19}$$

The free CTP propagator is then obtained by inverting (9.1.18) subject to the inverse relation

$$\int \mathrm{d}^4 z\, \Delta^{0,\,-1}_{ab}(x,z)\Delta^{0,\,bc}(z,y) = \eta_a{}^c\delta^{(4)}(x-y), \tag{9.1.20}$$

where the domain of integration over z_0 is infinite. We expect to recover the familiar propagators of the *in-out* formalism of asymptotic field theory, which we relate to scattering-matrix elements by means of reduction techniques, such as that due to Lehmann, Symanzik and Zimmermann [90]; and unitarity cutting rules [91–94] via the optical theorem. It follows that the free Feynman (Dyson) propagators satisfy the inhomogeneous Klein-Gordon equation

$$-\big(\Box_x^2 + M^2\big)i\Delta^0_{\mathrm{F(D)}}(x,y) = (-)i\delta^{(4)}(x-y); \tag{9.1.21}$$

and the free Wightman propagators satisfy the homogeneous equation

$$-\big(\Box_x^2 + M^2\big)i\Delta^0_{>(<)}(x,y) = 0. \tag{9.1.22}$$

In the double momentum representation, the free part of the action is

$$S_0[\Phi^a, t\to\infty] = \iint \frac{\mathrm{d}^4p}{\big(2\pi\big)^4}\frac{\mathrm{d}^4p'}{\big(2\pi\big)^4}\,\frac{1}{2}\Phi^a(p)\Delta^{0,\,-1}_{ab}(p,p')\Phi^b(-p'), \tag{9.1.23}$$

where

$$\Delta_{ab}^{0,\,-1}(p,p') = \begin{bmatrix} p^2 - m^2 + i\epsilon & 0 \\ 0 & -\big(p^2 - m^2 - i\epsilon\big) \end{bmatrix} \big(2\pi\big)^4 \delta^{(4)}(p-p') \tag{9.1.24}$$

is the Fourier transform of the free inverse CTP propagator, satisfying the inverse relation

$$\int \frac{\mathrm{d}^4 q}{(2\pi)^4}\, \Delta_{ab}^{0,\,-1}(p,q)\Delta^{0,\,bc}(q,p') = \eta_a{}^c (2\pi)^4 \delta^{(4)}(p-p'). \tag{9.1.25}$$

Given that the free inverse CTP propagator is proportional to a four-dimensional delta function of the two momenta, it may be written more conveniently in the familiar *single* Fourier representation as

$$\Delta_{ab}^{0,\,-1}(p) = \begin{bmatrix} p^2 - m^2 + i\epsilon & 0 \\ 0 & -\big(p^2 - m^2 - i\epsilon\big) \end{bmatrix}, \tag{9.1.26}$$

satisfying the inverse relation

$$\Delta_{ab}^{0,\,-1}(p)\Delta^{0,bc}(p) = \eta_a{}^c. \tag{9.1.27}$$

9.2 The Free CTP Propagator

We proceed now to make the following Ansatz for the most general form of the free CTP propagator, without evaluating the correlation functions directly:

$$\Delta^{0,ab}(p) = \begin{bmatrix} \big[p^2 - M^2 + i\epsilon\big]^{-1} + \tilde{c}_1(p)\delta(p^2 - M^2) & \tilde{c}_3(p)\delta(p^2 - M^2) \\ \tilde{c}_2(p)\delta(p^2 - M^2) & -\big[p^2 - M^2 - i\epsilon\big]^{-1} + \tilde{c}_4(p)\delta(p^2 - M^2) \end{bmatrix}. \tag{9.2.1}$$

The $\tilde{c}_i(p) \equiv \theta(p_0)c_i(p) + \theta(-p_0)c_i'(p)$ are as yet undetermined, analytic functions of the four-momentum p, which may in general be complex. The elements of the leading diagonal are the Fourier transforms of the most general translationally-invariant solutions to the inhomogeneous Klein-Gordon equation (9.1.21) and the off-diagonal

elements, the most general translationally-invariant solutions to the homogeneous Klein-Gordon equation (9.1.22). The form of the elements is determined by the following constraints:

(i) ***CPT*** The scalar field is even under CPT transformations, yielding the parity relations in (A.4). As such, we require that

$$\tilde{c}_{1(4)}(p) = \tilde{c}_{1(4)}(-p), \quad \tilde{c}_2(p) = \tilde{c}_3(-p). \tag{9.2.2}$$

(ii) **Hermiticity** The Hermiticity relations outlined in (A.4) require

$$\tilde{c}_4(p) = -\tilde{c}_1^*(p), \quad \tilde{c}_2(p) = -\tilde{c}_3^*(-p). \tag{9.2.3}$$

We see then that $\tilde{c}_2(p)$ and $\tilde{c}_3(p)$ must be purely imaginary.

(iii) **Causality** The causality relation in (7.1.24) may be written in terms of the elements of the CTP propagator as

$$\Delta(x,y) = \Delta_>(x,y) - \Delta_<(x,y) = \varepsilon(x_0 - y_0)[\Delta_{\mathrm{F}}(x,y) - \Delta_{\mathrm{D}}(x,y)]. \tag{9.2.4}$$

Given (A.3), we see that the Pauli-Jordan propagator is proportional only to the real, dispersive part of the Feynman propagator. We can convince ourselves that an even-parity, on-shell dispersive part will contribute to the free Pauli-Jordan propagator terms which are non-vanishing for space-like separations, violating the micro-causality condition outlined in Section 7.1. It follows then that $\tilde{c}_1(p)$ and $\tilde{c}_4(p)$ are also purely imaginary-valued functions. We shall therefore replace the $\tilde{c}_i(p)$ by the real-valued functions $\tilde{f}_i(p)$ through $\tilde{c}_i(p) \equiv -2\pi i \tilde{f}_i(p)$, where the minus sign and factor of 2π have been included for later convenience. The explicit form of the free Pauli-Jordan propagator in (7.1.15a) then yields the constraint

$$\tilde{f}_2(p) - \tilde{f}_3(p) = \varepsilon(p_0). \tag{9.2.5}$$

(iv) **Unitarity** The unitarity relation in (7.1.28) requires

$$\tilde{f}_2(p) + \tilde{f}_3(p) = 1 + \tilde{f}_1(p) + \tilde{f}_4(p). \tag{9.2.6}$$

Solving this system for the $\tilde{f}_i(p)$, we obtain the result

$$\Delta^{0,ab}(p) = \begin{bmatrix} \frac{1}{p^2-M^2+i\epsilon} - 2\pi i\tilde{f}(p)\delta(p^2-M^2) & -2\pi i\big[\theta(-p_0)+\tilde{f}(p)\big]\delta(p^2-M^2) \\ -2\pi i\big[\theta(p_0)+\tilde{f}(p)\big]\delta(p^2-M^2) & \frac{-1}{p^2-M^2-i\epsilon} - 2\pi i\tilde{f}(p)\delta(p^2-M^2) \end{bmatrix}, \tag{9.2.7}$$

where all elements contain terms dependent upon the same function

$$\tilde{f}(p) \equiv \tilde{f}_1(p) = \theta(p_0)f(p) + \theta(-p_0)f(-p). \tag{9.2.8}$$

These terms correspond to the VEV of the normal-ordered product of fields $\langle{:}\Phi(x)\Phi(y){:}\rangle$, which is vanishing for the trivial vacuum $|0\rangle$. Therefore, we must conclude that $\tilde{f}(p)$ is also vanishing in this case. We then obtain the set of propagators familiar from the unitarity cutting rules of absorptive part theory (cf. [91, 92]):

$$\Delta^{0,ab}(p) = \begin{bmatrix} \big[p^2-M^2+i\epsilon\big]^{-1} & -2\pi i\theta(-p_0)\delta(p^2-M^2) \\ -2\pi i\theta(p_0)\delta(p^2-M^2) & -\big[p^2-M^2-i\epsilon\big]^{-1} \end{bmatrix}. \tag{9.2.9}$$

We may arrive at the same result by considering the CTP propagator in the Keldysh representation (9.1.15). The constraints outlined above permit us to add to the free Hadamard propagator any purely imaginary, even function of p proportional to $\delta(p^2-M^2)$, that is

$$\tilde{\Delta}^{0,ab}(p) = \begin{bmatrix} 0 & [(p_0-i\epsilon)^2-\mathbf{p}^2-M^2]^{-1} \\ [(p_0+i\epsilon)^2-\mathbf{p}^2-M^2]^{-1} & -2\pi i\delta(p^2-M^2) \end{bmatrix} - 2\pi i 2\tilde{f}(p)\delta(p^2-M^2)\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}. \tag{9.2.10}$$

We note that there is no such freedom to add terms to the retarded and advanced propagators as a result of the constraints on the form of the free Pauli-Jordan

propagator. Given that

$$\mathbf{O}^{\mathsf{T}}\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}\mathbf{O} = \frac{1}{2}\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}, \tag{9.2.11}$$

we immediately arrive at (9.2.7).

9.3 The Resummed CTP Propagator

In the case of the resummed CTP propagator, we must invert on the restricted domain $[-t/2, t/2]$ subject to the inverse relation

$$\int_{\Omega_t} \mathrm{d}^4 z\, \Delta^{-1}_{ab}(x,z)\Delta^{bc}(z,y) = \eta_a{}^c \delta^{(4)}(x-y). \tag{9.3.1}$$

The momentum representation of this inverse relation takes the form

$$\iint \frac{\mathrm{d}^4 q}{\big(2\pi\big)^4}\frac{\mathrm{d}^4 q'}{\big(2\pi\big)^4}\, \Delta^{-1}_{ab}(p,q)(2\pi)^4\delta^{(4)}_t(q-q')\Delta^{bc}(q',p') = \eta_a{}^c(2\pi)^4\delta^{(4)}_t(p-p'), \tag{9.3.2}$$

where we have defined

$$\delta^{(4)}_t(p-p') = \delta_t(p_0-p'_0)\delta^{(3)}(\mathbf{p}-\mathbf{p}') = \frac{1}{(2\pi)^4}\iint_{\Omega_t}\mathrm{d}^4x\,\mathrm{d}^4y\, e^{ip\cdot x}e^{-ip'\cdot y}\,\delta^{(4)}(x-y). \tag{9.3.3}$$

The restriction of the domain of integration has lead to the introduction of the analytic weight function

$$\delta_t(p_0-p'_0) = \frac{t}{2\pi}\,\mathrm{sinc}\Big[\Big(\frac{p_0-p'_0}{2}\Big)t\Big], \tag{9.3.4}$$

which has replaced the energy-conserving delta function that we would otherwise anticipate. Using the fact that

$$\lim_{t\to\infty}\delta_t(p_0-p'_0) = \delta(p_0-p'_0), \tag{9.3.5}$$

we can however quickly recover the more familiar, asymptotic form when the boundary time $\tilde{t}_i = -t/2$ is taken to be in the distant past. The weight function satisfies

the convolution

$$\int \mathrm{d}q_0\, \delta_t(p_0 - q_0)\delta_t(q_0 - p_0') = \delta_t(p_0 - p_0'). \tag{9.3.6}$$

The emergence of the function δ_t is a consequence of the assertion that the time-evolution and the mapping between quantum-mechanical pictures are governed by the familiar, interaction-picture evolution operator

$$U(\tilde{t}_f, \tilde{t}_i) = \mathrm{T}\exp\left[i\int_{\tilde{t}_i}^{\tilde{t}_f} \mathrm{d}\tilde{t}\, H^{\mathrm{int}}(\tilde{t}\,)\right], \tag{9.3.7}$$

where the limits of integration are *finite*. This evolution is defined for times greater than the boundary time $\tilde{t}_i$. We recall that this boundary time is the point at which the three pictures are coincident. It is at this point that we may be confident of the unambiguous specification of boundary conditions. We stress then that δ_t is neither a prescription nor is it an *a priori* regularisation of the delta function.

We shall see later that the oscillatory behaviour of the sinc function is fundamentally important to the dynamical behaviour of the system. Before proceeding therefore, let us convince ourselves that these oscillations persist if we smear the switching on of the interactions, that is we impose the adiabatic switching of the interaction Hamiltonian for microscopic times outside the interval $[-t/2, t/2]$. We proceed then to introduce to the interaction Hamiltonian the Gaussian function

$$A_t(\tilde{t}) = \exp\Big(-\frac{\tilde{t}^2}{2t^2}\Big), \tag{9.3.8}$$

such that the evolution operator takes the form

$$U(\tilde{t}_f, \tilde{t}_i) = \mathrm{T}\exp\left[i\int_{\tilde{t}_i}^{\tilde{t}_f} \mathrm{d}\tilde{t}\, A_t(\tilde{t}) H^{\mathrm{int}}(\tilde{t})\right]. \tag{9.3.9}$$

Clearly, for $\tilde{t} \gg t$, the interaction vanishes. In the free part of the action, where we recall that we take the limit $t \to \infty$, we see that $A_t(\tilde{t}) \to 1$ as required. With this

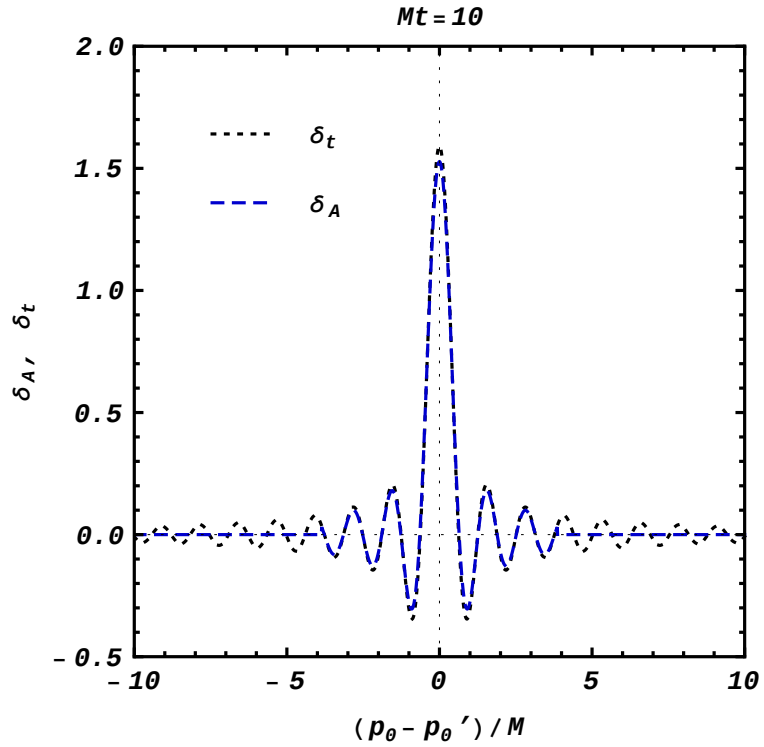


Figure 9.2: Comparison of $\delta_t(p_0 - p_0')$ (black dotted) and $\delta_A(p_0 - p_0')$ (blue dashed). We have introduced a mass parameter M so that all axes are dimensionless.

in place, it is clear that we must make the following replacement:

$$\delta_t(p_0 - p_0') \to \delta_A(p_0 - p_0') \equiv \frac{1}{2\pi}\int_{-t/2}^{t/2} \mathrm{d}\tilde{t}\, e^{-i(p_0-p_0')\tilde{t}} A_t(\tilde{t})$$
$$= \frac{t}{2\sqrt{2\pi}} e^{-\frac{1}{2}(p_0-p_0')^2 t^2}\left[\mathrm{erf}\left(\frac{1-2i(p_0-p_0)'t}{2\sqrt{2}}\right) + \mathrm{erf}\left(\frac{1+2i(p_0-p_0)'t}{2\sqrt{2}}\right)\right], \quad (9.3.10)$$

in which the oscillatory behaviour persists due to the error functions of complex arguments. The behaviour of both of these functions is shown in Figure 9.2, in which we see that the Gaussian function has little effect on the central region of the sinc function as would expect.

10 Non-Homogeneous Backgrounds

Until now, we have considered the vacuum to be an 'empty' state with all quantum numbers zero. In the following section, we replace that 'empty' vacuum state with some macroscopic background, which may in general be inhomogeneous and incoherent. This non-trivial 'vacuum' is described by the density operator ρ. The density operator is necessarily Hermitian and, for a closed system, evolves in the interaction picture according to the von Neumann or quantum Liouville equation

$$\frac{\mathrm{d}\rho(\tilde{t})}{\mathrm{d}\tilde{t}} = -i\big[H^{\mathrm{int}}(\tilde{t}), \rho(\tilde{t})\,\big], \tag{10.0.1}$$

where $H^{\mathrm{int}}(\tilde{t})$ is the interaction part of the Hamiltonian in the interaction picture. Developing the usual Neumann series, we find that $\rho(\tilde{t}) = U^{-1}(\tilde{t}, \tilde{t}_i)\rho(\tilde{t}_i)U^{-1}(\tilde{t}, \tilde{t}_i)$, where U is the evolution operator in (9.3.7). In the absence of external sources, the partition function $\mathcal{Z} = \mathrm{tr}\,\rho$ is time-independent. In corollary, in the presence of external sources, the partition function is in general time-dependent. We recall that the field operators of the interaction picture evolve under the free part of the Hamiltonian. We are interested in evaluating at the microscopic time $\tilde{t}_f = t/2$ the time-dependent ensemble expectation values (EEVs) of field operators $\langle\bullet\rangle_t$, where the *bra-ket* now denotes the weighted expectation

$$\langle\bullet\rangle_t = \frac{\mathrm{tr}\,\rho(\frac{t}{2})\,\bullet}{\mathrm{tr}\,\rho(\frac{t}{2})}. \tag{10.0.2}$$

As discussed in Chapter 9, the physical observables in the interaction-picture are of the form

$$\langle\Phi(\tfrac{t}{2},\mathbf{x})\Phi(\tfrac{t}{2},\mathbf{y})\rangle_t = \frac{\mathrm{tr}\,\rho(\frac{t}{2})\Phi(\frac{t}{2},\mathbf{x})\Phi(\frac{t}{2},\mathbf{y})}{\mathrm{tr}\,\rho(\frac{t}{2})}, \tag{10.0.3}$$

i.e., equal-time.

In the presence of this non-trivial background, the *out* state is replaced by the density operator at the time $\tilde{t}_f = \frac{t}{2}$ and as such, the *in-in* generating functional becomes

$$\mathcal{Z}[\rho, J_\pm, t] = \mathrm{tr}\left[\bar{\mathrm{T}}e^{-i\int_{\Omega_t}\mathrm{d}^4x\, J_-(x)\Phi_{\mathrm{H}}(x)}\right]\rho_{\mathrm{H}}(t/2)\left[\mathrm{T}e^{i\int_{\Omega_t}\mathrm{d}^4x\, J_+(x)\Phi_{\mathrm{H}}(x)}\right]. \tag{10.0.4}$$

We note that within the generating functional, the Heisenberg-picture density operator has explicit time dependence due to the presence of the external sources $J_\pm$.

10.1 The Schwinger-Dyson Equation in the CTP Formalism

Proceeding by inserting complete sets of eigenstates of the Heisenberg field operator at intermediate times, we obtain the path-integral representation

$$\mathcal{Z}[\rho, J_a, t] = \int[\mathrm{d}\Phi^a]\ {}_{\mathrm{H}}\langle\Phi_-(\mathbf{x}), t/2|\rho_{\mathrm{H}}(t/2)|\Phi_+(\mathbf{x}), t/2\rangle_{\mathrm{H}} \times \exp\left[i\left(S[\Phi^a, t\to\infty] + \int_{\Omega_t}\mathrm{d}^4x\, J_a(x)\Phi^a(x)\right)\right]. \tag{10.1.1}$$

As before, we have extended the limits of integration to infinity in the free part of the action. Following [35], we write the kernel ${}_{\mathrm{H}}\langle\Phi_-(\mathbf{x}), t/2|\rho_{\mathrm{H}}(t/2)|\Phi_+(\mathbf{x}), t/2\rangle_{\mathrm{H}}$ as an infinite series of poly-local sources:

$${}_{\mathrm{H}}\langle\Phi_-(\mathbf{x}), t/2|\rho_{\mathrm{H}}(t/2)|\Phi_+(\mathbf{x}), t/2\rangle_{\mathrm{H}} = \exp\big(iK[\Phi^a, t]\big), \tag{10.1.2}$$

where

$$K[\Phi^a,t]=K+\int_{\Omega_t}\mathrm{d}^4x\,K_a(x,t)\Phi^a(x)+\frac{1}{2}\iint_{\Omega_t}\mathrm{d}^4x\,\mathrm{d}^4x'\,K_{ab}(x,x',t)\Phi^a(x)\Phi^b(x')+\cdots. \tag{10.1.3}$$

Hereafter, all space-time integrals are assumed to run over the hypervolume Ω_t. We absorb K into the overall normalisation and K_a into a redefinition of the source J_a, such that the *in-in* generating functional may be written

$$\begin{aligned}\mathcal{Z}[J_a,K_{ab},\cdots,t]=\int[\mathrm{d}\Phi^a]\exp\Bigg[i\Bigg(&S[\Phi^a]+\int\mathrm{d}^4x\,J_a(x)\Phi^a(x)\\&+\frac{1}{2}\iint\mathrm{d}^4x\,\mathrm{d}^4y\,K_{ab}(x,x')\Phi^a(x)\Phi^b(x')\\&+\frac{1}{6}\iiint\mathrm{d}^4x\,\mathrm{d}^4x'\,\mathrm{d}^4x''\,K_{abc}(x,x',x'')\Phi^a(x)\Phi^b(x')\Phi^c(x'')+\cdots\Bigg)\Bigg],\end{aligned} \tag{10.1.4}$$

where we have omitted the explicit t dependence of the sources for convenience.

The Cornwall-Jackiw-Tomboulis (CJT) effective action [33] is given by the Legendre transform

$$\begin{aligned}\Gamma[\hat\Phi^a,\mathcal{G}^{ab},\mathcal{G}^{abc},\cdots]=\mathcal{W}[J_a,K_{ab},K_{abc}]&-\int\mathrm{d}^4x\,J_a(x)\hat\Phi^a(x)\\&-\frac{1}{2}\iint\mathrm{d}^4x\,\mathrm{d}^4x'\,K_{ab}(x,x')\left[\hat\Phi^a(x)\hat\Phi^b(x')+i\hbar\mathcal{G}^{ab}(x,x')\right]\\&-\frac{1}{6}\iiint\mathrm{d}^4x\,\mathrm{d}^4x'\,\mathrm{d}^4x''\,K_{abc}(x,x',x'')\Big[\hat\Phi^a(x)\hat\Phi^b(x')\hat\Phi^c(x'')\\&+3i\hbar\mathcal{G}^{(ab}(x,x')\hat\Phi^{c)}(x'')-\hbar^2\mathcal{G}^{abc}(x,x',x'')\Big]+\cdots,\end{aligned} \tag{10.1.5}$$

where $\mathcal{W}[J_a,K_{ab},K_{abc},\cdots]=-i\hbar\ln\mathcal{Z}[J_a,K_{ab},K_{abc},\cdots]$ is the generating functional of connected ensemble Green's functions. We obtain the infinite systems

$$\hat\Phi^a(x)=\frac{\delta\mathcal{W}}{\delta J_a(x)}=\langle\Phi^a(x)\rangle, \tag{10.1.6a}$$

$$i\hbar\mathcal{G}^{ab}(x,x') = 2\frac{\delta\mathcal{W}}{\delta K_{ab}(x,x')} - \hat{\Phi}^a(x)\hat{\Phi}^b(x')$$
$$= -i\hbar\frac{\delta^2\mathcal{W}}{\delta J_a(x)\delta J_b(x')} = \langle \mathrm{T}_{\mathcal{C}}\big[\Phi^a(x)\Phi^b(x')\big]\rangle - \langle\Phi^a(x)\rangle\langle\Phi^b(x')\rangle, \tag{10.1.6b}$$

$$-\hbar^2\mathcal{G}^{abc}(x,x',x'') = 6\frac{\delta\mathcal{W}}{\delta K_{abc}(x,x',x'')} - 3i\hbar\mathcal{G}^{(ab}(x,x')\hat{\Phi}^{c)}(x'') - \hat{\Phi}^a(x)\hat{\Phi}^b(x')\hat{\Phi}^c(x'')$$
$$= -\hbar^2\frac{\delta^3\mathcal{W}}{\delta J_a(x)\delta J_b(x')\delta J_c(x'')}, \tag{10.1.6c}$$

and

$$\frac{\delta\Gamma}{\delta\hat{\Phi}^a(x)} = -J_a(x) - \int \mathrm{d}^4x'\, K_{ab}(x,x')\hat{\Phi}^b(x')$$
$$- \frac{1}{2}\iint \mathrm{d}^4x'\,\mathrm{d}^4x''\, K_{abc}(x,x',x'')$$
$$\times\Big[\hat{\Phi}^b(x')\hat{\Phi}^c(x'') + i\hbar\mathcal{G}^{bc}(x',x'')\Big] - \cdots, \tag{10.1.7a}$$

$$\frac{\delta\Gamma}{\delta\mathcal{G}^{ab}(x,x')} = -\frac{i\hbar}{2}K_{ab}(x,x') - \frac{i\hbar}{2}\int \mathrm{d}^4x''\, K_{abc}(x,x',x'')\hat{\Phi}^c(x'') - \cdots, \tag{10.1.7b}$$

$$\frac{\delta\Gamma}{\delta\mathcal{G}^{abc}(x,x',x'')} = -\frac{i\hbar}{6}K_{abc}(x,x',x'') - \cdots, \tag{10.1.7c}$$

where the parentheses (abc) denote cyclic permutation of the indices a, b, c.

We may simplify this infinite system by assuming that the initial conditions do not contain any three-point or higher correlations. We may then take the tri-local and higher kernels (K_{abc}, K_{abcd}, $\cdots$) to be vanishing. We eliminate the three-point and higher connected Green's functions ($\mathcal{G}^{abc}$, $\mathcal{G}^{abcd}$, $\cdots$) as dynamical variables by performing a second Legendre transform

$$\Gamma[\hat{\Phi}^a,\mathcal{G}^{ab}] \equiv \Gamma[\hat{\Phi}^a,\mathcal{G}^{ab},\tilde{\mathcal{G}}^{abc},\cdots], \tag{10.1.8}$$

where the $\tilde{\mathcal{G}}$'s are functionals of $\hat{\Phi}^a$ and $\mathcal{G}^{ab}$ given by

$$\frac{\delta\Gamma}{\delta\mathcal{G}^{abc\ldots}}[\hat{\Phi}^a,\mathcal{G}^{ab},\tilde{\mathcal{G}}^{abc},\cdots] = 0. \tag{10.1.9}$$

The effective action is evaluated by expanding around the constant background

field $\Phi_0^a(x) = \Phi^a(x) - \hbar^{1/2}\phi^a(x)$, defined at the saddle-point

$$\frac{\delta S[\Phi^a]}{\delta \Phi^a(x)}\Big|_{\Phi=\Phi_0} + J_a(x) + \int \mathrm{d}^4x'\, K_{ab}(x,x')\Phi_0^b(x') = 0. \tag{10.1.10}$$

The result of this expansion is well known (see [32, 33]) and we obtain the two-particle-irreducible (2PI) CJT effective action

$$\begin{aligned}\Gamma[\hat{\Phi}^a, \mathcal{G}^{ab}] &= S[\hat{\Phi}^a] \\ &+ \frac{i\hbar}{2}\,\mathrm{tr}_x\left[\ln_x\,\det_{ab}\,\mathcal{G}^{-1}_{ac} * G^{0,cb} + \frac{\delta^2 S[\hat{\Phi}^a]}{\delta\hat{\Phi}^a\delta\hat{\Phi}^b} * \mathcal{G}^{ab} - \eta_a{}^a\right] + \hbar^2\Gamma_2[\hat{\Phi}^a, \mathcal{G}^{ab}],\end{aligned} \tag{10.1.11}$$

where we have used a subscript x and the $*$'s to remind us that the trace, logarithm and products are intended in the functional sense. The overall normalisation has been chosen such that the conventional effective action (see [95])

$$\Gamma[\hat{\Phi}^a] \equiv \Gamma[\hat{\Phi}^a, \tilde{\mathcal{G}}^{ab}] = S[\hat{\Phi}^a] + \frac{i\hbar}{2}\mathrm{tr}_x\,\ln_x\,\det_{ab}\,G^{-1}_{ac} * G^{0,cb} + \mathcal{O}(\hbar^2) \tag{10.1.12}$$

is recovered in the limit $K_{ab} \to 0$, where $\tilde{\mathcal{G}}^{ab}$ satisfies

$$\frac{\delta\Gamma}{\delta\tilde{\mathcal{G}}^{ab}}[\hat{\Phi}^a, \tilde{\mathcal{G}}^{ab}] = 0. \tag{10.1.13}$$

$G^{0,ab}$ is defined in relation to the functional operator

$$\begin{aligned}G^{-1}_{ab}(\hat{\Phi}^a; x, x') &= \frac{\delta^2 S[\hat{\Phi}^a]}{\delta\hat{\Phi}^a(x)\delta\hat{\Phi}^b(x')} + K_{ab}(x,x') \\ &= G^{0,-1}_{ab}(x,x') + \frac{\delta^2 S^{\mathrm{int}}[\hat{\Phi}^a]}{\delta\hat{\Phi}^a(x)\delta\hat{\Phi}^b(x')} + K_{ab}(x,x')\end{aligned} \tag{10.1.14}$$

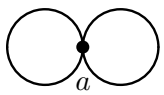
and $S^{\mathrm{int}}[\hat{\Phi}^a]$ is the interaction part of the action. It is clear then that all Green's functions depend upon the state of the system at the macroscopic time t through the bi-local source K_{ab}.

For the Lagrangian in (7.1.1),

$$
\begin{aligned}
&G^{-1}_{ab}(\hat{\Phi}^a; x, x') \\
&= -\Big[\big(\Box_x + M^2\big)\eta_{ab} + g\eta_{abc}\hat{\Phi}^c(x) + \frac{1}{2}\lambda\eta_{abcd}\hat{\Phi}^c(x)\hat{\Phi}^d(x)\Big]\delta^{(4)}(x-x') + K_{ab}(x,x'),
\end{aligned}
\tag{10.1.15}
$$

where the delta function arises from the locality of the Lagrangian. $\Gamma_2[\hat{\Phi}^a, \mathcal{G}^{ab}]$ is the sum of all 2PI vacuum graphs

$$
\Gamma_2[\hat{\Phi}^a, \mathcal{G}^{ab}] = -i\sum_{a,b}\Bigg[\frac{1}{8}\;\delta_{ab} + \frac{1}{12}\;
\begin{array}{c}
\\
a \bullet\!\!-\!\!-\!\!\bullet b
\end{array}
\Bigg],
\tag{10.1.16}
$$



where combinatorial factors have been written explicitly and we associate with each n-point vertex a factor of

$$
iS^{(n)}_a(\hat{\Phi}^a; x) = i\frac{\delta^n S[\hat{\Phi}^a]}{\delta\big[\hat{\Phi}^a(x)\big]^n}
\tag{10.1.17}
$$

and each line a factor of $i\mathcal{G}^{ab}(\hat{\Phi}^a; x, y)$. The three- and four-point vertices are

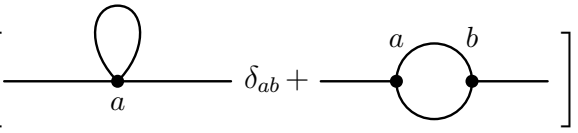
$$
iS^{(3)}_a(\hat{\Phi}^a; x) = -ig\eta_{aaa} - i\lambda\eta_{aaaa}\hat{\Phi}^a(x), \quad iS^{(4)}_a(\hat{\Phi}^a; x) = -i\lambda\eta_{aaaa}.
\tag{10.1.18}
$$

Functionally differentiating the effective action with respect to $\mathcal{G}^{ab}(x,y)$, using Jacobi's formula to evaluate the variation of the determinant over the CTP indices, we obtain the Schwinger-Dyson (SD) equation

$$
\mathcal{G}^{-1}_{ab}(\hat{\Phi}^a; x, y) = G^{-1}_{ab}(\hat{\Phi}^a; x, y) + \Pi_{ab}(\hat{\Phi}^a; x, y),
\tag{10.1.19}
$$

where

$$\Pi_{ab}(\hat{\Phi}^a;x,y) = -2i\hbar\frac{\delta\Gamma_2[\hat{\Phi}^a,\mathcal{G}^{ab}]}{\delta\mathcal{G}^{ab}(x,y)} = -i\hbar\Bigg[$$



$$\Bigg] \tag{10.1.20}$$

is the proper, truncated 1PI self-energy and a combinatorial factor of $\frac{1}{2}$ has been absorbed into the diagrammatics.

The CTP self-energy may be written in matrix form as

$$\Pi_{ab}(x,y) = \begin{bmatrix} \Pi(x,y) & -\Pi_<(x,y) \\ -\Pi_>(x,y) & -\Pi^*(x,y) \end{bmatrix}, \tag{10.1.21}$$

where $\Pi(x,y)$ and $-\Pi^*(x,y)$ are the time- and anti-time-ordered self-energies; and $\Pi_>(x,y)$ and $\Pi_<(x,y)$ are the positive- and negative-frequency, absolutely-ordered self-energies respectively. In analogy to the propagator definitions discussed earlier, we also define

$$\Pi_1(x,y) = \Pi_>(x,y) + \Pi_<(x,y) = \Pi(x,y) - \Pi^*(x,y) = 2i\mathrm{Im}\,\Pi(x,y), \tag{10.1.22a}$$

$$\Pi_{\mathcal{P}}(x,y) = \frac{1}{2}\big[\Pi_{\mathrm{R}}(x,y) + \Pi_{\mathrm{A}}(x,y)\big] = \mathrm{Re}\,\Pi(x,y), \tag{10.1.22b}$$

$$\mathit{\Gamma}(x,y) = \Pi_>(x,y) - \Pi_<(x,y) = \Pi_{\mathrm{R}}(x,y) - \Pi_{\mathrm{A}}(x,y), \tag{10.1.22c}$$

satisfying relations analogous to those described in Appendix A. We show in Chapter 11 that $\mathit{\Gamma}(x,y)$ is related to the familiar Breit-Wigner width in the zero-temperature limit. In the Keldysh representation [30], the CTP self-energy is

$$\tilde{\Pi}_{ab}(x,y) = \begin{bmatrix} \Pi_1(x,y) & \Pi_{\mathrm{R}}(x,y) \\ \Pi_{\mathrm{A}}(x,y) & 0 \end{bmatrix}. \tag{10.1.23}$$

In the limit $\hat{\Phi}^a(x) \to 0$, the SD equation reduces to

$$\Delta^{-1}_{ab}(x,y,t) = \Delta^{0,-1}_{ab}(x,y) + K_{ab}(x,y,t) + \Pi_{ab}(x,y,t), \tag{10.1.24}$$

where $\Delta^{0,-1}_{ab}(x,y)$ is the free inverse CTP propagator defined in (9.1.18) and we

have re-introduced the explicit t dependence for clarity. In the double momentum representation, this becomes

$$\Delta^{-1}_{ab}(p,p',t) = \Delta^{0,-1}_{ab}(p,p') + K_{ab}(p,p',t) + \Pi_{ab}(p,p',t). \tag{10.1.25}$$

In order to interpret Δ^{ab} as the expectation value of products of field operators, as we shall see in Sections 10.3 and 11, that is to make connection with the canonical operator approach in Section 7.1, we must account for the fact that the interaction picture creation and annihilation operators of the Fourier representation of the field operator are defined at time 0, not the time $t/2$ of the density operator. We make a redefinition of the field eigenvalues in the exponent of the generating functional

$$\Phi(p) = e^{ip_0 t/2}\Phi'(p). \tag{10.1.26}$$

This amounts to multiplying through (10.1.25) by a phase $e^{i(p_0-p'_0)t/2}$, which we absorb into the definitions of the propagators, bi-local source and self-energy.

Convoluting from the right and left with the weight function δ_t and the resummed and free CTP propagators respectively, we obtain the Feynman-Dyson (FD) series

$$\begin{aligned}\Delta^{ab}(p,p',t) = \Delta^{0,ab}(p,p',t) - \int\cdots\int \frac{\mathrm{d}^4q}{(2\pi)^4}\frac{\mathrm{d}^4q'}{(2\pi)^4}\frac{\mathrm{d}^4q''}{(2\pi)^4}\frac{\mathrm{d}^4q'''}{(2\pi)^4}\,\Delta^{0,ac}(p,q)\\ \times(2\pi)^4\delta^{(4)}_t(q-q')\Big[K_{cd}(q',q'',t)+\Pi_{cd}(q',q'',t)\Big](2\pi)^4\delta^{(4)}_t(q''-q''')\Delta^{db}(q''',p',t),\end{aligned} \tag{10.1.27}$$

Given the form of δ_t in (9.3.3), we see that this series does not collapse to the resummation familiar from zero-temperature field theory and as such we cannot write the form of the resummed propagator directly in this double momentum representation.

We shall see in Chapter 11 that, beyond the tree-level, we may safely ignore the contribution to the FD series of the bi-local source. In this case and given that δ_t satisfies the convolution in (9.3.6), we absorb the weight functions into the self-

energy, attaching them to the vertices, see Chapter 17. The FD series may then be written in the more concise form

$$\Delta^{ab}(p,p',t) = \Delta^{0,ab}(p,p',t) - \iint \frac{\mathrm{d}^4q}{(2\pi)^4}\frac{\mathrm{d}^4q'}{(2\pi)^4}\,\Delta^{0,ac}(p,q,t)\Pi_{cd}(q,q',t)\Delta^{db}(q',p',t). \tag{10.1.28}$$

For t finite, $\delta_t(p_0 - p_0')$ is analytic in the limit $p_0 = p_0'$ and, as we shall see in Chapter 12, the systematic incorporation of these finite-time effects will ensure that the perturbation expansion is free of pinch singularities [96, 97].

10.2 Applicability of the Gradient Expansion

It will prove instructive to consider further the possibility of resumming the CTP propagator to a closed analytic form by working in a mixed representation of momentum and space-time coordinates: the Wigner representation. Defining the relative and central coordinates

$$R^\mu_{xy} = x^\mu - y^\mu, \qquad X^\mu_{xy} = \frac{x^\mu + y^\mu}{2}, \tag{10.2.1}$$

such that

$$x^\mu = X^\mu_{xy} + \frac{1}{2}R^\mu_{xy}, \quad y^\mu = X^\mu_{xy} - \frac{1}{2}R^\mu_{xy}, \tag{10.2.2}$$

we introduce the Wigner transform: the Fourier transform with respect to the relative coordinate only. Explicitly, the Wigner transform of a function $F(R,X)$ is

$$F(p,X) = \int \mathrm{d}^4R\, e^{ip\cdot R}F(R,X). \tag{10.2.3}$$

We recall that the resummed propagator satisfies the inverse relation

$$\int_{\Omega_t} \mathrm{d}^4z\, \Delta^{-1}_{ab}(x,z)\Delta^{bc}(z,y) = \delta^{(4)}(x-y), \tag{10.2.4}$$

where we have omitted the t dependence of the propagators for convenience. We

emphasise that the domain of integration is restricted in z_0 to be in the range $[-t/2, t/2]$. The Wigner transform of the inverse relation takes the form

$$\int_{\Omega_t} \mathrm{d}^4 z \iint \frac{\mathrm{d}^4 p}{(2\pi)^4} \frac{\mathrm{d}^4 p'}{(2\pi)^4}\, e^{-ip\cdot R_{xz}} e^{-ip'\cdot R_{zy}}\, \Delta^{-1}_{ab}(p, X_{xz}) \Delta^{bc}(p', X_{zy}) \\ = \iint \frac{\mathrm{d}^4 p}{(2\pi)^4} \frac{\mathrm{d}^4 p'}{(2\pi)^4}\, e^{-ip\cdot x} e^{ip'\cdot y}\, \eta_a{}^c (2\pi)^4 \delta^{(4)}(p - p'). \quad (10.2.5)$$

In the case where deviations from homogeneity are small, i.e., when the characteristic scale of macroscopic variations in the background is large in comparison to the microscopic single-particle excitations, we may perform a gradient expansion of the inverse relation in terms of the soft derivative $\partial^\mu_{X_{xy}} \equiv \partial/\partial X_{xy,\mu}$, writing $X_{xz} = X_{xy} + R_{zy}/2$ and $X_{zy} = X_{xy} - R_{xz}/2$. After integrating by parts, we then obtain

$$\iint \frac{\mathrm{d}^4 p}{(2\pi)^4} \frac{\mathrm{d}^4 p'}{(2\pi)^4}\, e^{-ip\cdot x} e^{ip'\cdot y}\, (2\pi)^4 \delta^{(4)}_t(p - p') \\ \times \Delta^{-1}_{ab}(p, X) \exp\Big[-\frac{i}{2}\big(\overleftarrow{\partial_p} \cdot \overrightarrow{\partial_X} - \overleftarrow{\partial_X} \cdot \overrightarrow{\partial_{p'}}\big)\Big] \Delta^{bc}(p', X) \\ = \iint \frac{\mathrm{d}^4 p}{(2\pi)^4} \frac{\mathrm{d}^4 p'}{(2\pi)^4}\, e^{-ip\cdot x} e^{ip'\cdot y}\, \eta_a{}^c (2\pi)^4 \delta^{(4)}(p - p'). \quad (10.2.6)$$

We now define the central and relative momenta

$$q^\mu = \frac{p^\mu + p'^\mu}{2}, \qquad Q^\mu = p^\mu - p'^\mu, \quad (10.2.7)$$

conjugate to the relative and central coordinates, respectively. It follows that

$$p^\mu = q^\mu + \frac{1}{2} Q^\mu, \quad p'^\mu = q^\mu - \frac{1}{2} Q^\mu, \quad (10.2.8)$$

allowing us to rewrite (10.2.6) in the form

$$\int \frac{\mathrm{d}^4 Q}{(2\pi)^4}\, e^{-iQ\cdot X}\, (2\pi)^4 \delta^{(4)}_t(Q) \\ \times \exp\big[-i(\diamondsuit^-_{q,X} + 2\diamondsuit^+_{Q,X})\big] \{\Delta^{-1}_{ab}(q + Q/2, X)\} \{\Delta^{bc}(q - Q/2, X)\} \\ = \int \frac{\mathrm{d}^4 Q}{(2\pi)^4}\, e^{-iQ\cdot X}\, \eta_a{}^c (2\pi)^4 \delta^{(4)}_t(Q), \quad (10.2.9)$$

where, following [36, 37], we have introduced the diamond operator

$$\diamondsuit^{\pm}_{p,X}\{A\}\{B\} = \frac{1}{2}\{A,B\}^{\pm}_{p,X} \tag{10.2.10}$$

and $\{A,B\}^{\pm}_{p,X}$ denote the symmetric and anti-symmetric Poisson brackets

$$\{A,B\}^{\pm}_{p,X} \equiv \frac{\partial A}{\partial p^{\mu}}\frac{\partial B}{\partial X_{\mu}} \pm \frac{\partial A}{\partial X^{\mu}}\frac{\partial B}{\partial p_{\mu}}. \tag{10.2.11}$$

For $t > 0$, we may perform the integral on the right-hand side, yielding

$$\begin{aligned}&\int\frac{\mathrm{d}^4Q}{(2\pi)^4}\,e^{-iQ\cdot X}\,(2\pi)^4\delta^{(4)}_t(Q)\\ &\times\exp\big[-i(\diamondsuit^{-}_{q}+2\diamondsuit^{+}_{Q})\big]\{\Delta^{-1}_{ab}(q+Q/2,X)\}\{\Delta^{bc}(q-Q/2,X)\} = \eta_a{}^c\theta(t-2|X_0|),\end{aligned} \tag{10.2.12}$$

For late times, $t\to\infty$, this result reduces to

$$e^{-i\diamondsuit^{-}_{q,X}}\{\Delta^{-1}_{ab}(q,X)\}\{\Delta^{bc}(q,X)\} = \eta_a{}^c, \tag{10.2.13}$$

It is then clear that we may only evaluate the familiar closed form of the resummed CTP propagator if we truncate the gradient expansion to *zeroth* order. However, this is valid only for a static and spatially homogeneous system.

10.3 Non-Homogeneous Free Propagators

Herein, we relax any assumptions about the form of the density operator, taking it to be in general non-diagonal but symmetric in both Hilbert and Fock spaces. We may write the most general interaction-picture density matrix at the microscopic

time $\tilde{t}_f = t/2$ as

$$\rho(\tfrac{t}{2}) = C\exp\Bigg[-\int \mathrm{d}\Pi_{\mathbf{k}_1}\, W_{10}(\mathbf{k}_1;0)a^\dagger(\mathbf{k}_1,\tfrac{t}{2}) - \int \mathrm{d}\Pi_{\mathbf{k}'_1}\, W_{01}(0;\mathbf{k}'_1)a(\mathbf{k}'_1,\tfrac{t}{2}) \\ - \iint \mathrm{d}\Pi_{\mathbf{k}_1}\,\mathrm{d}\Pi_{\mathbf{k}'_1} W_{11}(\mathbf{k}_1;\mathbf{k}'_1)a^\dagger(\mathbf{k}_1,\tfrac{t}{2})a(\mathbf{k}'_1,\tfrac{t}{2}) - \cdots \\ - \frac{1}{n!}\frac{1}{m!}\int\cdots\int \Big[\prod_{i=1}^{n}\mathrm{d}\Pi_{\mathbf{k}_i}\Big]\Big[\prod_{j=1}^{m}\mathrm{d}\Pi_{\mathbf{k}'_j}\Big] W_{nm}(\{\mathbf{k}_i\};\{\mathbf{k}'_j\})\prod_{i=1}^{n}a^\dagger(\mathbf{k}_i,\tfrac{t}{2})\prod_{j=1}^{m}a(\mathbf{k}'_j,\tfrac{t}{2})\Bigg], \tag{10.3.1}$$

where we shall set the constant C to unity without loss of generality. The real-valued weights $W_{nm}(\{\mathbf{k}\}_n;\{\mathbf{k}'\}_m)$ depend on the state of the system at time $t/2$ and satisfy

$$W_{nm}(\{\mathbf{k}\}_n;\{\mathbf{k}'\}_m) = W_{mn}(\{\mathbf{k}'\}_m,\{\mathbf{k}\}_n). \tag{10.3.2}$$

The density operator may be written in the basis of momentum eigenstates by multiplying the exponential form above by the completeness relation of the basis of Fock states at time $t/2$:

$$\mathbf{I} = |0\rangle\langle 0| + \sum_{\ell=1}^{\infty}\frac{1}{\ell!}\Bigg[\prod_{k=1}^{\ell}\int \mathrm{d}\Pi_{\mathbf{p}_k}\Bigg]|\{\mathbf{p}\}_\ell;t/2\rangle\langle\{\mathbf{p}\}_\ell;t/2|\,, \tag{10.3.3}$$

where $|\{\mathbf{p}\}_\ell;t/2\rangle$ is the multi-mode Fock state $|\mathbf{p}_1;t/2\rangle\otimes|\mathbf{p}_2;t/2\rangle\otimes\cdots\otimes|\mathbf{p}_\ell;t/2\rangle$. This will yield an intractable infinite series of n-to-m-particle initial correlations. Taking all $W_{nm}(\{\mathbf{k}\}_n;\{\mathbf{k}\}_m)$ to be zero if $n+m>2$, i.e. taking a Gaussian-like initial density operator, it is still possible to generate all possible n-to-m-particle initial correlations. In Appendix B, we include the expansion of the general Gaussian-like density operator explicitly, where we include only sufficient terms to visualise the form of the expansion.

By exploiting the remaining freedom in the commutation relations in (7.1.17), we may hide our ignorance of the series expansion of the density operator by writing the EEVs of two-point products of interaction-picture creation and annihilation

operators as

$$\langle a^\dagger(\mathbf{p}',0)a(\mathbf{p},0)\rangle_t = 2\,\mathscr{E}(\mathbf{p},\mathbf{p}')f(\mathbf{p},\mathbf{p}',t)e^{i[E(\mathbf{p})-E(\mathbf{p}')]t/2}, \tag{10.3.4}$$

$$\langle a(\mathbf{p}',0)a(\mathbf{p},0)\rangle_t = 2\,\mathscr{E}(\mathbf{p},\mathbf{p}')g(\mathbf{p},\mathbf{p}',t)e^{i[E(\mathbf{p})+E(\mathbf{p}')]t/2}, \tag{10.3.5}$$

consistent with (7.1.13) and (7.1.16). The energy factor $2\mathscr{E}(\mathbf{p},\mathbf{p}')$, having dimensions E^1, arises from the fact that the 'number operator' $a^\dagger(\mathbf{p})a(\mathbf{p})$ of quantum field theory has dimensions E^{-2}, i.e., it does *not* have the dimensions of a number. The statistical distribution functions f and g have dimensions E^3 and, in particular, the function $f(\mathbf{p},\mathbf{p}',t)$ is related to the particle number density. The remaining two-point products follow from the algebra of the creation and annihilation operators in (7.1.17), yielding the constraints

$$f(\mathbf{p},\mathbf{p}',t) = f(\mathbf{p}',\mathbf{p},t), \quad g(\mathbf{p},\mathbf{p}',t) = g(\mathbf{p}',\mathbf{p},t), \tag{10.3.6}$$

with the added requirement that the energy factor is symmetric in $\mathbf{p}$ and $\mathbf{p}'$. Taking note that the density operator is constructed from on-shell Fock states, the natural Ansatz for this energy factor is

$$\mathscr{E}(\mathbf{p},\mathbf{p}') = \sqrt{E(\mathbf{p})E(\mathbf{p}')}. \tag{10.3.7}$$

This Ansatz constitutes a redefinition of the creation and annihilation operators such that the LIPS measure of the plane-wave expansion of the field operator is replaced by the non-covariant measure

$$\int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3}\frac{1}{\sqrt{2E(\mathbf{p})}}, \tag{10.3.8}$$

which we immediately recognise from relativistic quantum mechanics.

In order that we may treat connected Green's functions, it is in general neces-

sary to consider the EEVs of single creation or annihilation operators

$$\langle a(\mathbf{p},0)\rangle_t = 2\sqrt{E(\mathbf{p})}w(\mathbf{p},t)e^{iE(\mathbf{p})t/2}. \tag{10.3.9}$$

We define the connected distribution functions

$$f_{\rm con}(\mathbf{p},\mathbf{p}',t) \equiv f(\mathbf{p},\mathbf{p}',t) - w(\mathbf{p},t)w(\mathbf{p}',t), \tag{10.3.10a}$$

$$g_{\rm con}(\mathbf{p},\mathbf{p}',t) \equiv g(\mathbf{p},\mathbf{p}',t) - w(\mathbf{p},t)w(\mathbf{p}',t), \tag{10.3.10b}$$

consistent with (10.3.6).

We are now in a position to derive the most general form of the Fourier transform of the free CTP propagator, satisfying the inverse relation

$$\int\frac{\mathrm{d}^4q}{(2\pi)^4}\,\Delta^{0,-1}_{ac}(p,q,t)\Delta^{0,cb}(q,p',t) = \eta_a{}^b(2\pi)^4\delta^{(4)}(p-p'). \tag{10.3.11}$$

It is worth clarifying that this propagator is 'free' in the spectral sense, i.e., it corresponds to the free part of the action, see Chapter 9.

Proceeding as in Section 9.2, we make the following Ansatz:

$$\begin{aligned}\Delta^{0,ab}(p,p',t) = {}& \begin{bmatrix} [p^2-M^2+i\epsilon]^{-1} & -i2\pi\theta(-p_0)\delta(p^2-M^2) \\ -i2\pi\theta(p_0)\delta(p^2-M^2) & -\big[p^2-M^2-i\epsilon\big]^{-1}\end{bmatrix}(2\pi)^4\delta^{(4)}(p-p') \\ - i\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}&2\pi|2p_0|^{1/2}\delta(p^2-M^2)\tilde f(p,p',t)e^{i(p_0-p'_0)t/2}2\pi|2p'_0|^{1/2}\delta(p'^2-M^2),\end{aligned} \tag{10.3.12}$$

which we confirm by evaluating the EEVs directly, using the algebra above. The form of the function $\tilde f(p,p',t)$ is

$$\tilde f(p,p',t) = \sum_{s=\pm1}\Big[\theta(sp_0)\theta(sp'_0)f(s\mathbf{p},s\mathbf{p}',t) + \theta(sp_0)\theta(-sp'_0)g(s\mathbf{p},-s\mathbf{p}',t)\Big], \tag{10.3.13}$$

satisfying $\tilde f(p,p',t) = \tilde f^\dagger(-p',-p,t) = \tilde f(-p,-p',t)$ and containing all information about the state of the ensemble at time t. Hereafter, we shall assume that the density operators under discussion are diagonal in particle number, so that we may

set the g functions to zero for simplicity.

We stress that, in this most general case, the free phases have not cancelled and appear explicitly in the free CTP propagator. The appearance of this phase is a result of our choice to work in the interaction picture, where the density matrix transforms under the interaction part of the Hamiltonian and the fields by the free part.

The retarded and advanced propagators take the form

$$\Delta^0_{\mathrm{R(A)}}(p,p') = \frac{1}{(p_0+(-)i\epsilon)^2-\mathbf{p}^2-M^2}(2\pi)^4\delta^{(4)}(p-p'); \tag{10.3.14}$$

and the Pauli-Jordan, Hadamard and principal-part propagators become

$$\Delta^0(p,p',t) = -i2\pi\varepsilon(p_0)\delta(p^2-M^2)(2\pi)^4\delta^{(4)}(p-p'), \tag{10.3.15a}$$

$$\begin{aligned}\Delta^0_1(p,p',t) =& -i2\pi\delta(p^2-M^2)(2\pi)^4\delta^{(4)}(p-p') \\ & -i2\pi|2p_0|^{1/2}\delta(p^2-M^2)2\tilde{f}(p,p',t)e^{i(p_0-p'_0)t/2}2\pi|2p'_0|^{1/2}\delta(p'^2-M^2),\end{aligned} \tag{10.3.15b}$$

$$\Delta^0_{\mathcal{P}}(p,p',t) = \mathcal{P}\frac{1}{p^2-M^2}(2\pi)^4\delta^{(4)}(p-p'). \tag{10.3.15c}$$

Having obtained a closed form for the free CTP propagators, we need then to make connection with the bi-local source of the path-integral representation. Replacing the exponent of the *in-in* generating functional in (10.1.4) with its Fourier transform, keeping only sources up to and including K_{ab} in the expansion of the density operator, we complete the square in the exponent by making a shift in the field:

$$\Phi^a(p) = \Phi'^a(p) - \hat{\Delta}^a_{0,b}(p)J^b(-p), \tag{10.3.16}$$

where

$$\hat{\Delta}^{0,\,ab}(p) = \begin{bmatrix} \frac{1}{p^2-M^2+i\epsilon} & -2\pi i\theta(-p_0)\delta(p^2-M^2) \\ -2\pi i\theta(p_0)\delta(p^2-M^2) & -\frac{1}{p^2-M^2-i\epsilon}\end{bmatrix} \tag{10.3.17}$$

Figure 10.1: The Feynman-diagrammatic interpretation of the free non-homogeneous scalar propagator, where the double line represents momentum-violating coupling to the thermal background through the bi-local source.

is the inverse of the CTP propagator with $\tilde{f}$ set to zero, cf. (10.3.12). The boundary conditions on the normal-ordered product of fields are contained within the poly-local sources and hence do not appear in $\hat{\Delta}^0$. It is worth noting that

$$\hat{\Delta}^0_{\rm F}(p) = {\rm Re}\,\Delta^0_{\rm R}(p) + i\varepsilon(p_0){\rm Im}\,\Delta^0_{\rm R}(p), \tag{10.3.18}$$

cf. the Feynman representation of the 2×2 matrix propagator as discussed in [30]. This object has no physical interpretation. The *in-in* generating functional subsequently takes the form

$$\begin{aligned}\mathcal{Z}[J,K] = \mathcal{Z}[0,K]\exp\Bigg[\frac{i}{2}\iint\frac{{\rm d}^4p}{(2\pi)^4}\frac{{\rm d}^4p'}{(2\pi)^4}\\ \Big[J^a(p)\hat{\Delta}_{0,a}{}^c(p)K_{cb}(p,p')\Phi^{b'}(p') + \Phi^{a'}(p)K_{ac}(p,p')\hat{\Delta}^c_{0,b}(p')J^b(p')\\ - J^a(p)\Big(\hat{\Delta}_{0,ab}(p)(2\pi)^4\delta^{(4)}(p-p') - \hat{\Delta}_{0,a}{}^c(p)K_{cd}(p,p')\hat{\Delta}^d_{0,b}(p')\Big)J^b(p')\Big]\Bigg].\end{aligned} \tag{10.3.19}$$

The remaining linear terms yield contributions to the free propagator proportional to K^2, which we shall see in Chapter 11 may be neglected. Keeping then the term bi-linear in the source J, by (9.1.13), we find the free CTP propagator

$$i\Delta^{ab}_0(p,p') = i\hat{\Delta}^{ab}_0(p)(2\pi)^4\delta^{(4)}(p-p') + i\hat{\Delta}^{ac}_0(p)iK_{cd}(p,p')i\hat{\Delta}^{db}_0(p'). \tag{10.3.20}$$

Interpreting this result diagrammatically, we assign to the CTP propagator of our real scalar field Feynman diagram in Figure 10.1.

11 The Thermodynamic Equilibrium Limit

For clarity, in the following section, we discuss the correspondence of the discussions thus far with the familiar equilibrium results. The purpose is firstly to emphasise the consistency of the generalised formulation described in the previous sections and to derive relations between the elements of the equilibrium CTP propagator in preparation for Chapter 12, in which we argue that our approach is free of pinching singularities.

In the equilibrium limit, the density operator is diagonal in particle number and, as such, we must set all amplitudes except W_{11} to zero in (10.3.1). The general density operator, cf. (B.1), then reduces to the series

$$\begin{aligned}\rho = |0\rangle\langle 0| &+ \iint \mathrm{d}\Pi_{\mathbf{k}_1}\,\mathrm{d}\Pi_{\mathbf{k}'_1}\,\Big[(2\pi)^3 2E(\mathbf{k}_1)\delta^{(3)}(\mathbf{k}_1-\mathbf{k}'_1) - W_{11}(\mathbf{k}_1;\mathbf{k}'_1) \\ &\quad + \frac{1}{2}\int \mathrm{d}\Pi_{\mathbf{q}_1}\, W_{11}(\mathbf{k}_1;\mathbf{q}_1)W_{11}(\mathbf{q}_1;\mathbf{k}'_1) + \cdots\Big]|\mathbf{k}_1\rangle\langle\mathbf{k}'_1| \\ &+ \frac{1}{2}\int\cdots\int \mathrm{d}\Pi_{\mathbf{k}_1}\,\mathrm{d}\Pi_{\mathbf{k}_2}\,\mathrm{d}\Pi_{\mathbf{k}'_1}\,\mathrm{d}\Pi_{\mathbf{k}'_2}\,\Big[(2\pi)^3 2E(\mathbf{k}_1)\delta^{(3)}(\mathbf{k}_1-\mathbf{k}'_1) - W_{11}(\mathbf{k}_1;\mathbf{k}'_1) \\ &\quad + \frac{1}{2}\int \mathrm{d}\Pi_{\mathbf{q}_1}\, W_{11}(\mathbf{k}_1;\mathbf{q}_1)W_{11}(\mathbf{q}_1;\mathbf{k}'_1) + \cdots\Big]\Big[(2\pi)^3 2E(\mathbf{k}_2)\delta^{(3)}(\mathbf{k}_2-\mathbf{k}'_2) \\ &\quad - W_{11}(\mathbf{k}_2;\mathbf{k}'_2) + \frac{1}{2}\int \mathrm{d}\Pi_{\mathbf{q}_2}\, W_{11}(\mathbf{k}_2;\mathbf{q}_2)W_{11}(\mathbf{q}_2;\mathbf{k}'_2) + \cdots\Big]|\mathbf{k}_1,\mathbf{k}_2\rangle\langle\mathbf{k}'_1,\mathbf{k}'_2| + \cdots,\end{aligned} \tag{11.0.1}$$

where we have omitted time arguments for convenience. In this case, the g function

is trivially zero and the f function takes the form of the series

$$f(\mathbf{p},\mathbf{p}',t) = (2\pi)^3 2E(\mathbf{p})\delta^{(3)}(\mathbf{p}-\mathbf{p}') - W_{11}(\mathbf{p};\mathbf{p}') + \frac{1}{2}\int \mathrm{d}\Pi_{\mathbf{q}}\, W_{11}(\mathbf{p};\mathbf{q})W_{11}(\mathbf{q};\mathbf{p}') + \cdots$$
$$+ \int \mathrm{d}\Pi_{\mathbf{q}} \Big[(2\pi)^3 2E(\mathbf{p})\delta^{(3)}(\mathbf{p}-\mathbf{q}) - W_{11}(\mathbf{p};\mathbf{q}) + \cdots\Big]$$
$$\times \Big[(2\pi)^3 2E(\mathbf{q})\delta^{(3)}(\mathbf{q}-\mathbf{p}') - W_{11}(\mathbf{q};\mathbf{p}') + \cdots\Big] + \cdots, \quad (11.0.2)$$

where disconnected parts have been cancelled order-by-order in the expansion by the normalisation $\mathrm{tr}\,\rho$ in (10.0.2).

The equilibrium density operator must also be diagonal in momenta and is thus obtained by taking

$$W_{11}(\mathbf{k};\mathbf{k}') \to \beta E(\mathbf{k})(2\pi)^3\delta^{(3)}(\mathbf{k}-\mathbf{k}'), \quad (11.0.3)$$

where $\beta = 1/T$ is the inverse, thermodynamic temperature, consistent with familiar Gaussian form

$$\rho = \exp\Big[-\beta\int \mathrm{d}\Pi_{\mathbf{k}}\, E(\mathbf{k})a^\dagger(\mathbf{k})a(\mathbf{k})\Big] \quad (11.0.4)$$

and corresponding to the expected canonical, Boltzmann form,

$$\rho = e^{-\beta H}. \quad (11.0.5)$$

By convention, we have chosen not to include the partition function in the definition of the density matrix. After substituting for the equilibrium W_{11}, we obtain

$$\rho = |0\rangle\langle 0| + \sum_{n=1}^{\infty}\frac{1}{n!}\int\cdots\int\prod_{i=1}^{n}\Big[\mathrm{d}\Pi_{\mathbf{k}_i}\, f_\beta(\mathbf{k}_i)\Big]\bigotimes_{i=1}^{n}|\mathbf{k}_i\rangle\bigotimes_{i=1}^{n}\langle\mathbf{k}_i|\,, \quad (11.0.6)$$

where the amplitudes are the Boltzmann factors $f_\beta(\mathbf{k}) = e^{-\beta E(\mathbf{k})}$. The normalisation in (10.0.2) is then the canonical partition function $\mathcal{Z}(\beta) = \mathrm{tr}\, e^{-\beta H}$.

Substituting the limit (11.0.3) into the series expansion of the f function in

(11.0.2) and using the summations

$$\sum_{n=0}^{\infty} \frac{(-x)^n}{n!} = e^{-x}, \qquad \sum_{n=1}^{\infty} x^n = \frac{x}{1-x}, \tag{11.0.7}$$

we find the correspondence

$$f(\mathbf{p}, \mathbf{p}', t) \underset{\text{eq.}}{\longrightarrow} (2\pi)^3 \delta^{(3)}(\mathbf{p} - \mathbf{p}') f_{\text{B}}\big(E(\mathbf{p})\big), \tag{11.0.8a}$$

$$g(\mathbf{p}, \mathbf{p}', t) \underset{\text{eq.}}{\longrightarrow} 0, \tag{11.0.8b}$$

independent of time. These summations in (11.0.7) are precisely those that were used to derive the Bose-Einstein distribution in Chapter 4. We again stress that these expressions contain an implicit division by a phase-space volume. The dependence upon only the magnitude of the three-momentum $\mathbf{p}$ is a consequence of the homogeneity and isotropy implied by thermodynamic equilibrium. We note that thermodynamic equilibrium implies homogeneity but the converse is not true: homogeneity does not imply thermodynamic equilibrium. The presence of the three-dimensional delta function necessarily restores translational invariance.

It is known that the pinch singularities present in perturbative expansions cancel in the equilibrium limit (see Chapter 12) and we can safely take the limit $t \to \infty$ throughout the *in-in* generating functional, as we should expect for a system with static macroscopic properties. Working then in the single-momentum representation, we obtain the familiar free equilibrium, CTP propagators

$$i\Delta_{\text{F}}^0(p) = i\big[p^2 - M^2 + i\varepsilon\big]^{-1} + 2\pi f_{\text{B}}(|p_0|)\delta(p^2 - M^2), \tag{11.0.9a}$$

$$\begin{aligned} i\Delta_{>}^0(p) &= 2\pi\big[\theta(p_0) + f_{\text{B}}(|p_0|)\big]\delta(p^2 - M^2) \\ &\equiv 2\pi\varepsilon(p_0)\big[1 + f_{\text{B}}(p_0)\big]\delta(p^2 - M^2), \end{aligned} \tag{11.0.9b}$$

$$\begin{aligned} i\Delta_{<}^0(p) &= 2\pi\big[\theta(-p_0) + f_{\text{B}}(|p_0|)\big]\delta(p^2 - M^2) \\ &\equiv 2\pi\varepsilon(p_0) f_{\text{B}}(p_0)\delta(p^2 - M^2). \end{aligned} \tag{11.0.9c}$$

These are to be compared with those derived for the quantum harmonic oscillator

in Chapter 6. The form of the Wightman propagators written in terms of the signum function are of particular convenience in the calculation of loop diagrams (see Section 11.1), although we must take care when taking the zero-temperature limit, as is clear in (11.0.9c) for $p_0 < 0$.

Returning to (10.3.19), it follows from the results above that in equilibrium the bi-local source must be proportional to a four-dimensional delta function of the momenta, i.e.,

$$K_{ab}(p,p') \underset{\text{eq.}}{\longrightarrow} (2\pi)^4\delta^{(4)}(p-p')K_{ab}(p), \tag{11.0.10}$$

where $K_{ab}(p)$ must satisfy

$$\hat{\Delta}^{ac}(p)K_{cd}(p)\hat{\Delta}^{db}(p) = 2\pi i\delta(p^2-M^2)f_{\text{B}}\big(E(\mathbf{p})\big)\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}. \tag{11.0.11}$$

Solving the resulting system of equations, keeping terms to leading order in ϵ, and noting that the bi-local source should be written in terms of the three-momentum only, we find

$$K_{ab}(p) = 2i\epsilon f_{\text{B}}\big(E(\mathbf{p})\big)\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}. \tag{11.0.12}$$

By virtue of the limit representation of the delta function

$$\delta(x) = \lim_{\epsilon\to 0}\frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2}, \tag{11.0.13}$$

we can quickly convince ourselves that we do indeed obtain the correct free CTP propagator. We see also that the terms linear in J remaining in (10.3.19) may safely be taken to zero, since they will on functional differentiation yield contributions to the free propagator proportional to $K^2 \sim \epsilon^2$.

Alternatively, interpreting the Boltzmann factor as an evolution operator in negative-imaginary time, as we did in Chapter 6, and using the cyclicity of the trace in the EEV, we find the KMS relation of the scalar Wightman propagators

$$\Delta_{>}(x^0-y^0;\mathbf{x}-\mathbf{y}) = \Delta_{<}(x^0-y^0+i\beta;\mathbf{x}-\mathbf{y}). \tag{11.0.14}$$

The momentum representation

$$\Delta_>(p) = e^{\beta p_0}\Delta_<(p) \tag{11.0.15}$$

yields the final constraint on $\tilde{f}(p)$ in (9.2.8):

$$\tilde{f}(p) = \theta(p_0)f_{\rm B}(p_0) + \theta(-p_0)f_{\rm B}(-p_0) = f_{\rm B}(|p_0|), \tag{11.0.16}$$

where $f_{\rm B}(p_0) = [e^{\beta p_0} - 1]^{-1}$ is the Bose-Einstein distribution function. Furthermore, the KMS relation also leads to the fluctuation-dissipation theorem

$$\Delta_1(p) = \big[1 + 2f_{\rm B}(p_0)\big]\Delta(p), \tag{11.0.17}$$

relating the causality and unitarity relations in (7.1.24) and (7.1.28). Subsequently, by means of (11.0.15), we may write all propagators in terms of the retarded propagator:

$$\mathrm{Re}\,\Delta_{\rm F}(p) = \mathrm{Re}\,\Delta_{\rm R}(p), \tag{11.0.18a}$$

$$\mathrm{Im}\,\Delta_{\rm F}(p) = \varepsilon(p_0)\mathrm{Im}\,\Delta_{\rm R}(p)\big[1 + 2f_{\rm B}(|p_0|)\big], \tag{11.0.18b}$$

$$\Delta_>(p) = 2i\varepsilon(p_0)\mathrm{Im}\,\Delta_{\rm R}(p)\big[\theta(p_0) + f_{\rm B}(|p_0|)\big], \tag{11.0.18c}$$

$$\Delta_<(p) = 2i\varepsilon(p_0)\mathrm{Im}\,\Delta_{\rm R}(p)\big[\theta(-p_0) + f_{\rm B}(|p_0|)\big]. \tag{11.0.18d}$$

The resummed CTP propagator is given by the homogeneous limit of the SD equation in (10.1.24)

$$\Delta^{-1}_{ab}(p) = \Delta^{0,-1}_{ab} + K_{ab}(p) + \Pi_{ab}(p), \tag{11.0.19}$$

where the CTP self-energy is

$$\Pi_{ab}(p) = \begin{bmatrix} \Pi(p) & -\Pi_<(p) \\ -\Pi_>(p) & -\Pi^*(p) \end{bmatrix}. \tag{11.0.20}$$

We note that the various self-energies satisfy identities analogous to those in Ap-

pendix A. In the free case, the self-energy is zero and the equilibrium CTP propagator is obtained by inverting with K_{ab} given by (11.0.12). Beyond the tree-level, however, the contribution from the bi-local source may safely be taken to zero, at which point it follows that the inverse, resummed propagator is explicitly

$$\Delta^{-1}_{ab}(p) = \begin{bmatrix} p^2 - M^2 + \Pi(p) & -\Pi_<(p) \\ -\Pi_>(p) & -p^2 + M^2 - \Pi^*(p) \end{bmatrix}. \tag{11.0.21}$$

This may be inverted exactly, yielding the resummed CTP propagator

$$\Delta^{ab}(p) = \frac{1}{\big[p^2 - M^2 + \mathrm{Re}\,\Pi_\mathrm{R}(p)\big]^2 + \big[\mathrm{Im}\,\Pi_\mathrm{R}(p)\big]^2} \times \begin{bmatrix} p^2 - M^2 + \Pi^*(p) & -\Pi_<(p) \\ -\Pi_>(p) & -p^2 + M^2 - \Pi(p) \end{bmatrix}. \tag{11.0.22}$$

The self-energies satisfy the unitarity and causality relations

$$\Pi_1(p) = \Pi_>(p) + \Pi_<(p) = \Pi(p) - \Pi^*(p) = 2i\mathrm{Im}\,\Pi(p), \tag{11.0.23a}$$

$$\mathit{\Gamma}(p) = 2iM\Gamma(p) = \Pi_>(p) - \Pi_<(p) = \Pi_\mathrm{R}(p) - \Pi_\mathrm{A}(p) = 2i\mathrm{Im}\,\Pi_\mathrm{R}(p), \tag{11.0.23b}$$

where $\Gamma(p)$ is the familiar Breit-Wigner width, relating the imaginary part of the retarded self-energy to physical reaction rates [98, 99]. The KMS relation leads also to the detailed balance condition

$$\Pi_>(p) = e^{\beta p_0}\Pi_<(p), \tag{11.0.24}$$

resulting from the implicit dependence of the self-energies on the boundary conditions via the bi-local source. In combination with (11.0.23), we find, consistent with

(11.0.18)

$$\mathrm{Re}\,\Pi(p) = \mathrm{Re}\,\Pi_{\mathrm{R}}(p), \tag{11.0.25a}$$

$$\mathrm{Im}\,\Pi(p) = \varepsilon(p_0)\mathrm{Im}\,\Pi_{\mathrm{R}}(p)\big[1 + 2f_{\mathrm{B}}(|p_0|)\big], \tag{11.0.25b}$$

$$\Pi_{>}(p) = 2i\varepsilon(p_0)\mathrm{Im}\,\Pi_{\mathrm{R}}(p)\big[\theta(p_0) + f_{\mathrm{B}}(|p_0|)\big], \tag{11.0.25c}$$

$$\Pi_{<}(p) = 2i\varepsilon(p_0)\mathrm{Im}\,\Pi_{\mathrm{R}}(p)\big[\theta(-p_0) + f_{\mathrm{B}}(|p_0|)\big]. \tag{11.0.25d}$$

In the limit $\mathrm{Im}\,\Pi(p) \to \epsilon = 0^+$, ignoring the dispersive parts of the self-energy, we expect to recover the free propagators in (11.0.9). This limit is equivalent to taking

$$\mathrm{Im}\,\Pi_{\mathrm{R}}(p) \to \epsilon_{\mathrm{R}} \equiv \varepsilon(p_0)\,\epsilon, \tag{11.0.26}$$

where $\epsilon = 0^+$. Rewriting the resummed CTP propagator in (11.0.22) in terms of the retarded self-energy, we can convince ourselves that we do indeed obtain consistent free propagators in this limit.

11.1 Imaginary-Time Correspondence

The equilibrium density operator in (11.0.5) permits a path-integral representation in negative imaginary-time equivalent to that described in Chapter 6 for the quantum harmonic oscillator. The imaginary-time generating functional of our real scalar theory is

$$\mathcal{Z}[J] = \int [\mathrm{d}\Phi]\, \exp\left[-\bar{S}[\Phi] + \int_0^\beta \mathrm{d}\tau_x \int \mathrm{d}^3\mathbf{x}\, J(\bar{x})\Phi(\bar{x})\right], \tag{11.1.1}$$

where

$$\bar{S}[\Phi] = \int_0^\beta \mathrm{d}\tau_x \int \mathrm{d}^3\mathbf{x}\, \left[\tfrac{1}{2}\partial_\mu\Phi(\bar{x})\partial_\mu\Phi(\bar{x}) + \tfrac{1}{2}M^2\Phi^2(\bar{x}) + \tfrac{1}{3!}g\Phi^3(\bar{x}) + \tfrac{1}{4!}\lambda\Phi^4(\bar{x})\right] \tag{11.1.2}$$

and $\tau_x \in (0, \beta]$. We recall that in the limit $\beta \to \infty$, this is precisely the familiar Wick rotation of the Minkowski-space generating functional with $x_0 \to -i\bar{x}_0$, where $\bar{S}$ is the Euclidean action and Euclidean coordinates are denoted by a horizontal

bar, i.e. $\bar{x}_\mu \equiv (\bar{x}_0, \mathbf{x})$.

The free, imaginary-time propagator is

$$\bar{\Delta}^0(\bar{x} - \bar{y}) = \frac{1}{\beta} \sum_{\ell=-\infty}^{+\infty} \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3}\, e^{i[\omega_\ell(\tau_x - \tau_y) + \mathbf{p}\cdot(\mathbf{x}-\mathbf{y})]} \bar{\Delta}_0(i\omega_\ell, \mathbf{p}), \tag{11.1.3}$$

where

$$\bar{\Delta}^0(i\omega_\ell, \mathbf{p}) = \frac{1}{\omega_\ell^2 + \mathbf{p}^2 + M^2} \tag{11.1.4}$$

is the Matsubara propagator with the discrete, Matsubara frequencies $\omega_\ell = 2\pi\ell/\beta$, $\ell \in \mathbb{Z}$. The resummed Matsubara propagator is given by the imaginary-time Schwinger-Dyson equation

$$\bar{\Delta}^{-1}(i\omega_\ell, \mathbf{p}) = \bar{\Delta}^{0,-1}(i\omega_\ell, \mathbf{p}) + \bar{\Pi}(i\omega_\ell, \mathbf{p}), \tag{11.1.5}$$

yielding

$$\bar{\Delta}(i\omega_\ell, \mathbf{p}) = \frac{1}{\omega_\ell^2 + \mathbf{p}^2 + M^2 + \bar{\Pi}(i\omega_\ell, \mathbf{p})}, \tag{11.1.6}$$

where $\bar{\Pi}(\omega_\ell, \mathbf{p})$ is the imaginary-time self-energy.

We may write the spectral representation of the free Matsubara propagator

$$\bar{\Delta}^0(i\omega_\ell, \mathbf{p}) = -i \int \frac{\mathrm{d}k_0}{2\pi} \frac{\Delta^0(k_0, \mathbf{p})}{i\omega_\ell - k_0}, \tag{11.1.7}$$

where

$$i\Delta^0(k_0, \mathbf{p}) = 2\pi\varepsilon(k_0)\delta(k_0^2 - \mathbf{p}^2 - M^2) \tag{11.1.8}$$

is the single-momentum representation of the free Pauli-Jordan function, consistent with (7.1.15a). Making the analytic continuation $i\omega_\ell \to p_0 + i\epsilon$ and comparing with the spectral representation of the retarded propagator in (7.1.21), we see that

$$\bar{\Delta}^0(i\omega_\ell \to p_0 + i\epsilon, \mathbf{p}) = -\Delta^0_{\mathrm{R}}(p). \tag{11.1.9}$$

This correspondence must also hold for the resummed Matsubara propagator. As

such, the analytic continuation of the imaginary-time self-energy

$$\bar{\Pi}(i\omega_\ell \to p_0 + i\epsilon, \mathbf{p}) = -\Pi_{\mathrm{R}}(p), \tag{11.1.10}$$

yields the equilibrium, retarded self-energy.

In order to convince ourselves of the relation between the imaginary-time self-energy and the real-time, retarded self-energy, we consider the bubble diagram of our toy scalar theory, described by the Lagrangian density in (7.1.1).

The one-loop, Wightman self-energy is given by

$$i\Pi^{(1)}_{>}(p) = \frac{(-ig)^2}{2}\int\frac{\mathrm{d}^4k}{(2\pi)^4}\, i\Delta^0_{>}(k) i\Delta^0_{>}(p-k). \tag{11.1.11}$$

Using the signum form of the positive, frequency Wightman propagator in equation (11.0.9b), we obtain

$$\begin{aligned}\Pi^{(1)}_{>}(p) &= i\pi g^2\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\int\mathrm{d}k_0\,\frac{1}{4E(\mathbf{k})E(\mathbf{p}-\mathbf{k})}\Big[1+f_{\mathrm{B}}(k_0)\Big]\Big[1+f_{\mathrm{B}}(p_0-k_0)\Big]\\ &\times\Big[\delta\big(k_0-E(\mathbf{k})\big)-\delta\big(k_0+E(\mathbf{k})\big)\Big]\Big[\delta\big(p_0-k_0-E(\mathbf{p}-\mathbf{k})\big)-\delta\big(p_0-k_0+E(\mathbf{p}-\mathbf{k})\big)\Big].\end{aligned} \tag{11.1.12}$$

We can show that the product of Bose-Einstein factors satisfies

$$f_{\mathrm{B}}(k_0)f_{\mathrm{B}}(p_0-k_0) = f_{\mathrm{B}}(p_0)\Big[1+f_{\mathrm{B}}(k_0)+f_{\mathrm{B}}(p_0-k_0)\Big]. \tag{11.1.13}$$

On integration over k_0, we then find

$$\begin{aligned}\Pi^{(1)}_{>}(p) &= i\pi g^2\Big[1+f_{\mathrm{B}}(p_0)\Big]\sum_{\alpha_1,\alpha_2=\pm1}\alpha_1\alpha_2\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\frac{1}{4E(\mathbf{k})E(\mathbf{p}-\mathbf{k})}\\ &\times\Big[1+f_{\mathrm{B}}\big(\alpha_1E(\mathbf{k})\big)+f_{\mathrm{B}}\big(\alpha_2E(\mathbf{p}-\mathbf{k})\big)\Big]\delta\big(p_0-\alpha_1E(\mathbf{k})-\alpha_2E(\mathbf{p}-\mathbf{k})\big).\end{aligned} \tag{11.1.14}$$

The identity in (11.0.25) then yields

$$\operatorname{Im}\Pi_{\mathrm{R}}^{(1)}(p) = \frac{\pi g^2}{2}\sum_{\alpha_1,\alpha_2=\pm 1}\alpha_1\alpha_2\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\frac{1}{4E(\mathbf{k})E(\mathbf{p}-\mathbf{k})}$$
$$\times\Big[1+f_{\mathrm{B}}\big(\alpha_1 E(\mathbf{k})\big)+f_{\mathrm{B}}\big(\alpha_2 E(\mathbf{p}-\mathbf{k})\big)\Big]\delta\big(p_0-\alpha_1E(\mathbf{k})-\alpha_2E(\mathbf{p}-\mathbf{k})\big). \quad (11.1.15)$$

The real part may be calculated from the time-ordered diagram directly and is given by

$$\operatorname{Re}\Pi_{\mathrm{R}}^{(1)}(p) = \operatorname{Re}\left[-i\frac{(-ig)^2}{2}\int\frac{\mathrm{d}^4k}{(2\pi)^4}\,i\Delta_{\mathrm{F}}^0(k)i\Delta_{\mathrm{F}}^0(p-k)\right]. \quad (11.1.16)$$

Explicitly,

$$\operatorname{Re}\Pi_{\mathrm{R}}^{(1)}(p) = -\frac{g^2}{2}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\frac{1}{4E(\mathbf{k})E(\mathbf{p}-\mathbf{k})}$$
$$\times\Bigg\{\int_{k_0^2\neq E^2(\mathbf{k})}\mathrm{d}k_0\left(\frac{1}{k^2-M^2}\Big[\frac{1}{2}+f_{\mathrm{B}}(p_0-k_0)\Big]\right.$$
$$\left.\times\Big[\delta\big(p_0-k_0-E(\mathbf{p}-\mathbf{k})\big)+\delta\big(p_0-k_0+E(\mathbf{p}-\mathbf{k})\big)\Big]\right)$$
$$+\int_{(p_0-k_0)^2\neq E^2(\mathbf{p}-\mathbf{k})}\mathrm{d}k_0\left(\frac{1}{(p-k)^2-M^2}\Big[\frac{1}{2}+f_{\mathrm{B}}(k_0)\Big]\Big[\delta\big(k_0-E(\mathbf{k})\big)+\delta\big(k_0+E(\mathbf{k})\big)\Big]\right)\Bigg\}, \quad (11.1.17)$$

where the integral subscripts remind us that the integration over the on-shell singularities are understood in the Cauchy principle-value sense. Integration over k_0 then yields the result

$$\operatorname{Re}\Pi_{\mathrm{R}}^{(1)}(p) = -\frac{g^2}{2}\sum_{\alpha_1,\alpha_2=\pm 1}\alpha_1\alpha_2\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\,\frac{1}{4E(\mathbf{k})E(\mathbf{p}-\mathbf{k})}$$
$$\times\frac{1+f_{\mathrm{B}}\big(\alpha_1E(\mathbf{k})\big)+f_{\mathrm{B}}\big(\alpha_2E(\mathbf{p}-\mathbf{k})\big)}{p_0-\alpha_1E(\mathbf{k})-\alpha_2E(\mathbf{p}-\mathbf{k})}. \quad (11.1.18)$$

In the imaginary-time formalism, the self-energy is given by

$$-\bar{\Pi}^{(1)}(i\omega_\ell, \mathbf{p}) = \frac{(-g)^2}{2\beta} \sum_{n=-\infty}^{+\infty} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \bar{\Delta}(i\omega_n, \mathbf{k}) \bar{\Delta}(i(\omega_\ell - \omega_n), \mathbf{p} - \mathbf{k}). \tag{11.1.19}$$

After performing the frequency summation over n (see for instance [82]), we obtain

$$\bar{\Pi}^{(1)}(i\omega_\ell, \mathbf{p}) = \frac{g^2}{2} \sum_{\alpha_1, \alpha_2 = \pm 1} \alpha_1 \alpha_2 \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{1}{4E(\mathbf{k})E(\mathbf{p}-\mathbf{k})} \times \frac{1 + f_{\mathrm{B}}\big(\alpha_1 E(\mathbf{k})\big) + f_{\mathrm{B}}\big(\alpha_2 E(\mathbf{p}-\mathbf{k})\big)}{i\omega_\ell - \alpha_1 E(\mathbf{k}) - \alpha_2 E(\mathbf{p}-\mathbf{k})}. \tag{11.1.20}$$

Making the analytic continuation $i\omega_\ell \to p_0 + i\epsilon$ and subsequently extracting the real and imaginary parts, we can convince ourselves that these results agree with the correspondence quoted in (11.1.10).

12 Pinching Singularities

Our aim is to provide a perturbative approach to non-equilibrium dynamics. As such, it is necessary that we first establish that perturbation theory is well-behaved applied in this context. In this chapter, we analyse the perturbative expansion of the CTP propagator, illustrating the origin of the pinching singularities thought to spoil such expansions out of equilibrium. We proceed then to describe how, with the systematic inclusion of finite-time effects, these pinching singularities do not in fact arise. The price that we pay for the absence of these pathologies is that our perturbative expansion does not fully encompass the dynamics of the system: the complete picture relies on the constraints provided by the inverse relation. However, this constraint will allow us to derive from this perturbation series equations of motion for the statistical distribution functions akin to those introduced by Kadanoff and Baym [45, 46], as we shall see in Chapter 15.

In order to proceed perturbatively, we truncate the FD series in (10.1.28) to leading order in the couplings, safely setting K_{ab} to zero, cf. (11.0.12). Explicitly,

$$\Delta^{(1),ab}(p_1,p_2,t) = \Delta^{0,ab}(p_1,p_2,t) - \iint \frac{\mathrm{d}^4q_1}{(2\pi)^4}\frac{\mathrm{d}^4q_2}{(2\pi)^4}\,\Delta^{0,ac}(p_1,q_1,t)\Pi^{(1)}_{cd}(q_1,q_2,t)\Delta^{0,db}(q_2,p_2,t). \quad (12.0.1)$$

It will prove convenient to work in a mixed CTP-physical basis by inserting between the external legs and self-energies the transformation outlined in (9.1.15). In this

case, we may write

$$\Delta^{(1),ab}(p_1,p_2,t) = \Delta^{0,ab}(p_1,p_2,t) - \frac{1}{2}\iint\frac{\mathrm{d}^4q_1}{(2\pi)^4}\frac{\mathrm{d}^4q_2}{(2\pi)^4}\,\Delta^{0,ac}_{\mathrm{ret}}(p_1,q_1,t)\Pi'^{(1)}_{cd}(q_1,q_2,t)\Delta^{0,db}_{\mathrm{adv}}(q_2,p_2,t), \quad (12.0.2)$$

where, making use of the relations in Appendix A and dropping the time arguments for convenience,

$$\begin{aligned}\Delta^{ac}_{\mathrm{ret}}(p_1,q_1) &= \begin{bmatrix}\Delta_{\mathrm{F}}(p_1,q_1) & \Delta_{<}(p_1,q_1)\\ \Delta_{>}(p_1,q_1) & -\Delta^{*}_{\mathrm{F}}(p_1,q_1)\end{bmatrix}\begin{bmatrix}1 & 1\\ -1 & 1\end{bmatrix}\\ &= \begin{bmatrix}\Delta_{\mathrm{R}}(p_1,q_1) & \Delta_{\mathrm{R}}(p_1,q_1)+2\Delta_{<}(p_1,q_1)\\ \Delta_{\mathrm{R}}(p_1,q_1) & -\Delta_{\mathrm{R}}(p_1,q_1)+2\Delta_{>}(p_1,q_1)\end{bmatrix}, \end{aligned} \quad (12.0.3)$$

and

$$\begin{aligned}\Delta^{ac}_{\mathrm{adv}}(p_1,q_1) &= \begin{bmatrix}1 & -1\\ 1 & 1\end{bmatrix}\begin{bmatrix}\Delta_{\mathrm{F}}(p_1,q_1) & \Delta_{<}(p_1,q_1)\\ \Delta_{>}(p_1,q_1) & -\Delta^{*}_{\mathrm{F}}(p_1,q_1)\end{bmatrix}\\ &= \begin{bmatrix}\Delta_{\mathrm{A}}(p_1,q_1) & \Delta_{\mathrm{A}}(p_1,q_1)\\ \Delta_{\mathrm{A}}(p_1,q_1)+2\Delta_{>}(p_1,q_1) & -\Delta_{\mathrm{A}}(p_1,q_1)+2\Delta_{<}(p_1,q_1)\end{bmatrix}. \end{aligned} \quad (12.0.4)$$

It follows then that the one-loop-inserted Feynman and positive-frequency Wightman propagators may be written in the form

$$\begin{aligned}\Delta^{(1)}_{\mathrm{F}}(p_1,p_2,t) &= \Delta^{0}_{\mathrm{F}}(p_1,p_2,t)\\ &\quad - \iint\frac{\mathrm{d}^4q_1}{(2\pi)^4}\frac{\mathrm{d}^4q_2}{(2\pi)^4}\Big[\Delta^{0}_{\mathrm{R}}(p_1,q_1,t)\Pi^{(1)}(p_1,q_1,t)\Delta^{0}_{\mathrm{A}}(q_2,p_2,t)\\ &+\Delta^{0}_{\mathrm{R}}(p_1,q_1,t)\Pi^{(1)}_{\mathrm{R}}(q_1,q_2,t)\Delta^{0}_{>}(q_2,p_2,t)+\Delta^{0}_{<}(p_1,q_1,t)\Pi^{(1)}_{\mathrm{A}}(q_1,q_2,t)\Delta^{0}_{\mathrm{A}}(q_2,p_2,t)\Big],\end{aligned} \quad (12.0.5)$$

and

$$\Delta^{(1)}_{>}(p_1,p_2,t) = \Delta^0_{\rm F}(p_1,p_2,t) \\ - \iint \frac{{\rm d}^4q_1}{(2\pi)^4}\frac{{\rm d}^4q_2}{(2\pi)^4}\Big[\Delta^0_{\rm R}(p_1,q_1,t)\Pi^{(1)}_{>}(p_1,q_1,t)\Delta^0_{\rm A}(q_2,p_2,t) \\ + \Delta^0_{\rm R}(p_1,q_1,t)\Pi^{(1)}_{\rm R}(q_1,q_2,t)\Delta^0_{>}(q_2,p_2,t) + \Delta^0_{>}(p_1,q_1,t)\Pi^{(1)}_{\rm A}(q_1,q_2,t)\Delta^0_{\rm A}(q_2,p_2,t)\Big], \tag{12.0.6}$$

where we have used the identities

$$\Pi_1 + \Pi_{\rm R} + \Pi_{\rm A} = 2\Pi, \tag{12.0.7a}$$

$$\Pi_1 + \Pi_{\rm R} - \Pi_{\rm A} = 2\Pi_{>}, \tag{12.0.7b}$$

cf. Appendix A.

In the equilibrium limit, where translational invariance is restored, these expansions can be rewritten as

$$\Delta^{(1)}_{\rm F}(p) = \Delta^0_{\rm F}(p) - \Big[\Delta^0_{\rm A}(p)\Pi^{(1)}(p)\Delta^0_{\rm R}(p) + \Delta^0_{>}(p)\Pi^{(1)}_{\rm R}(p)\Delta^0_{\rm R}(p) + \Delta^0_{\rm A}(p)\Pi^{(1)}_{\rm A}(p)\Delta^0_{<}(p)\Big], \tag{12.0.8}$$

and

$$\Delta^{(1)}_{>}(p) = \Delta^0_{>}(p) - \Big[\Delta^0_{\rm A}(p)\Pi^{(1)}_{>}(p)\Delta^0_{\rm R}(p) + \Delta^0_{>}(p)\Pi^{(1)}_{\rm R}(p)\Delta^0_{\rm R}(p) + \Delta^0_{\rm A}(p)\Pi^{(1)}_{\rm A}(p)\Delta^0_{>}(p)\Big], \tag{12.0.9}$$

where the single-momentum representations of the propagators and self-energies are those discussed in Chapter 11. Using the identities in (11.0.18) and (11.0.25), by virtue of the KMS relation, we can rewrite these expansions entirely in terms of the real and imaginary parts of the retarded functions. Following the algebra through, we can show that concerning terms involving $\delta^2(p^2 - M^2)$ — those terms containing pinching singularities — cancel. We are left with terms depending upon the product

$$\mathrm{Re}\,\Delta^0_{\rm R}(p)\mathrm{Im}\,\Delta^0_{\rm R}(p), \tag{12.0.10}$$

where

$$\mathrm{Re}\,\Delta^0_{\mathrm{R}}(p) = \mathcal{P}\frac{1}{p^2 - M^2}, \tag{12.0.11}$$

$\mathcal{P}$ denotes the principal value integral, and

$$\mathrm{Im}\,\Delta^0_{\mathrm{R}}(p) = -\pi\varepsilon(p_0)\delta(p^2 - M^2). \tag{12.0.12}$$

Considering the limit representation

$$\mathcal{P}\frac{1}{x} = \lim_{\epsilon\to 0}\frac{x}{x^2 + \epsilon^2}, \tag{12.0.13}$$

and that of the delta function in (11.0.13), we may show that

$$\mathrm{Re}\,\Delta^0_{\mathrm{R}}(p)\mathrm{Im}\,\Delta^0_{\mathrm{R}}(p) = \frac{\pi}{2}\varepsilon(p_0)\delta'(p^2 - M^2), \tag{12.0.14}$$

where $\delta'(x)$ is the derivative of the delta function, satisfying

$$\int_{-\infty}^{+\infty}\mathrm{d}x\ \delta'(x)y(x) = -y'(0). \tag{12.0.15}$$

This term then is also free of pinching singularities. In which case, we find the results,

$$\Delta^{(1)}_{\mathrm{F}}(p) = \frac{p^2 - M^2 + \Pi^{(1)}(p)}{\big(p^2 - M^2 + i\varepsilon\big)^2} + 2\pi i f_{\mathrm{B}}(|p_0|)\big[\delta(p^2 - M^2) + \hat{\Pi}^{*(1)}(p)\delta'(p^2 - M^2)\big], \tag{12.0.16a}$$

$$\Delta^{(1)}_{\gtrless}(p) = \frac{\Pi^{(1)}_{\gtrless}(p)}{\big(p^2 - M^2 + i\varepsilon\big)^2} + 2\pi i\big[\theta(\pm p_0) + f_{\mathrm{B}}(|p_0|)\big]\big[\delta(p^2 - M^2) + \hat{\Pi}^{*(1)}(p)\delta'(p^2 - M^2)\big], \tag{12.0.16b}$$

where we have introduced the self-energy function

$$\hat{\Pi}(p) = \mathrm{Re}\,\Pi_{\mathrm{R}}(p) + i\varepsilon(p_0)\mathrm{Im}\,\Pi_{\mathrm{R}}(p), \tag{12.0.17}$$

cf. (10.3.18), which we note has no physical interpretation. We have included the negative-frequency Wightman propagator for completeness. We may quickly convince ourselves that these results are consistent with the properties and relations in Appendix A and reduce to the expected form in the zero-temperature limit. In conclusion, we see that the perturbative expansion of the CTP propagator is indeed well-defined and free of pathologies in the thermodynamic equilibrium limit.

It is clear from the above analysis that the pinch singularities resulting from products of delta functions with identical arguments cancelled as a result of the KMS relation, valid only in thermodynamic equilibrium. As such, it would appear that the application of perturbation theory to non-equilibrium situations, in which the KMS relation does not hold, would be plagued by these pathologies.

However, we now realise the importance of our pedantic treatment of the finite boundary times. For finite t, the usual energy-conserving delta functions have been replaced by the time-dependent, sinc-like weight function δ_t. The systematic inclusion of this finite-time effect leads to microscopic violation of energy conservation at early times, as a result of Heisenberg's uncertainty principle. Therefore, for t finite, it is clear that these pinching singularities cannot occur, even for the most general distribution functions, since products of δ_t remain analytic. It is only when t is large that we might expect to encounter these pathologies.

We suspect then that these potential pathologies arise from terms like

$$\delta_t^2(p_0), \tag{12.0.18}$$

where $p_0 = \sum_i p_{i,0}$ is the sum over all energies flowing into the vertices. For t large, this term is dominated by the contribution from $p \to 0$. By l'Hôpitals rule and (9.3.5), we may show that these pathologies grow like

$$\delta_t^2(p_0) \underset{t \gg 1/M}{\longrightarrow} \frac{t}{4\pi}\delta(p_0). \tag{12.0.19}$$

Nevertheless, in taking the limit t to infinity, it is clear that our boundary

conditions are specified in the infinitely distant past and as such our system must have reached thermodynamic equilibrium. It follows therefore that in taking this limit we must also replace the t-dependent distribution functions by their equilibrium forms. Since the pinching singularities cancel in the equilibrium limit, the perturbative expansion remains free of pathologies.

The behaviour of the perturbative expansion can then be summarised as follows: for early times, the t-dependent vertices lead to microscopic violation of energy conservation, preventing the appearance of pinching singularities; for late times, the t-dependent distribution functions approach the equilibrium distributions and the growing pathologies begin to cancel, until, in the limit $t \to \infty$, we obtain the familiar equilibrium thermal field theory, known to be completely free of pathologies.

13 The Complex Scalar Field

In this chapter, we generalise our discussions to the complex scalar field χ. The global $U(1)$ symmetry of the Lagrangian leads to a non-vanishing conserved charge, which requires us to introduce the chemical potential. The complex scalar field is then described by the grand canonical distribution function.

13.1 Canonical Quantisation

We consider then the Lagrangian density

$$\mathcal{L}(x) = \partial_\mu \chi^\dagger(x) \partial^\mu \chi(x) - m^2 \chi^\dagger(x)\chi(x) - \tfrac{1}{4}\lambda\big[\chi^\dagger(x)\chi(x)\big]^2, \tag{13.1.1}$$

where the complex scalar field $\chi(x)$ may be written in the interaction picture in the familiar representation

$$\chi(x) = \int \mathrm{d}\Pi_{\mathbf{p}} \, \big[a(\mathbf{p},0)e^{-iE(\mathbf{p})x_0}e^{i\mathbf{p}\cdot\mathbf{x}} + b^\dagger(\mathbf{p},0)e^{iE(\mathbf{p})x}e^{-i\mathbf{p}\cdot\mathbf{x}}\big], \tag{13.1.2}$$

where $a^\dagger(\mathbf{p},0)$ and $a(\mathbf{p},0)$ ($b^\dagger(\mathbf{p},0)$ and $b(\mathbf{p},0)$) are the interaction-picture, particle (anti-particle) creation and annihilation operators, respectively. Under charge-conjugation, see (A.2a), the creation and annihilation operators satisfy

$$U_c^\dagger a(\mathbf{p},\tilde{t})U_c = \eta b(\mathbf{p},\tilde{t}), \tag{13.1.3a}$$

$$U_c^\dagger b^\dagger(\mathbf{p},\tilde{t})U_c s = \eta a^\dagger(\mathbf{p},\tilde{t}). \tag{13.1.3b}$$

Using (7.1.3), we may write the more convenient representations

$$\chi(x) = \int \frac{\mathrm{d}^4 p}{(2\pi)^4}\, e^{-ip\cdot x}\chi(p), \tag{13.1.4a}$$

$$\chi^\dagger(x) = \int \frac{\mathrm{d}^4 p}{(2\pi)^4}\, e^{-ip\cdot x}\chi^\dagger(-p), \tag{13.1.4b}$$

with the Fourier amplitude

$$\chi(p) = 2\pi\delta(p^2 - m^2)\big[\theta(p_0)a(\mathbf{p},0) + \theta(-p_0)b^\dagger(-\mathbf{p},0)\big]. \tag{13.1.5}$$

For the scalar field, the quantisation scheme depended only on the restriction placed upon the form of the field commutator. In the case of the complex scalar field, we have two degrees of freedom to fix. Thus, we begin with the following two field commutators:

$$\big[\chi(x), \chi(y)\big] = 0, \tag{13.1.6a}$$

$$\big[\chi(x), \chi^\dagger(y)\big] = i\Delta(x, y; m^2), \tag{13.1.6b}$$

where the Pauli-Jordan function has precisely the form in (7.1.14). As for the real scalar field, we may derive the equal-time commutation relations

$$i\Delta(x, y; m^2)\big|_{x^0=y^0=\tilde{t}} = \big[\chi(\tilde{t}, \mathbf{x}), \chi^\dagger(\tilde{t}, \mathbf{y})\big] = 0, \tag{13.1.7a}$$

$$\partial_{x_0} i\Delta(x, y; m^2)\big|_{x^0=y^0=\tilde{t}} = \big[\pi^\dagger(\tilde{t}, \mathbf{x}), \chi^\dagger(\tilde{t}, \mathbf{y})\big] = -i\delta^{(3)}(\mathbf{x} - \mathbf{y}), \tag{13.1.7b}$$

$$\partial_{y_0} i\Delta(x, y; m^2)\big|_{x^0=y^0=\tilde{t}} = \big[\chi(\tilde{t}, \mathbf{x}), \pi(\tilde{t}, \mathbf{y})\big] = i\delta^{(3)}(\mathbf{x} - \mathbf{y}), \tag{13.1.7c}$$

$$\partial_{x_0}\partial_{y_0} i\Delta(x, y; m^2)\big|_{x^0=y^0=\tilde{t}} = \big[\pi^\dagger(\tilde{t}, \mathbf{x}), \pi(t, \mathbf{y})\big] = 0, \tag{13.1.7d}$$

where $\pi(\tilde{t}, \mathbf{x}) = \partial_{\tilde{t}}\chi^\dagger(\tilde{t}, \mathbf{x})$ is the conjugate momentum operator. The particle and anti-particle creation and annihilation operators necessarily satisfy the algebra

$$\big[a(\mathbf{p}, \tilde{t}), a^\dagger(\mathbf{p}', \tilde{t})\big] = \big[b(\mathbf{p}, \tilde{t}), b^\dagger(\mathbf{p}', \tilde{t})\big] = (2\pi)^3 2E(\mathbf{p})\delta^{(3)}(\mathbf{p} - \mathbf{p}'), \tag{13.1.8}$$

with all other commutators vanishing.

In addition to the propagators listed in Appendix A, we also define the C-violating propagator

$$i\not{\Delta}(x,y) = \frac{1}{2}\langle\{\chi(x),\chi(y)\}\rangle, \tag{13.1.9}$$

which satisfies

$$\not{\Delta}(x,y) = \not{\Delta}(y,x) = -\eta^2\not{\Delta}^{c*}(x,y). \tag{13.1.10}$$

Clearly this is vanishing at zero-temperature and in thermodynamic equilibrium. However, such correlations cannot be ruled out for general non-homogeneous EEVs.

In analogy to (10.3.4), we write the following set of EEVs of two-point products of particle and anti-particle creation and annihilation operators:

$$\langle a^\dagger(\mathbf{p}',0)a(\mathbf{p},0)\rangle_t = 2\mathscr{E}(\mathbf{p},\mathbf{p}')f(\mathbf{p},\mathbf{p}',t)e^{i[E(\mathbf{p})-E(\mathbf{p}')]t/2}, \tag{13.1.11a}$$

$$\langle b(\mathbf{p}',0)a(\mathbf{p},0)\rangle_t = 2\mathscr{E}(\mathbf{p},\mathbf{p}')g(\mathbf{p},\mathbf{p}',t)e^{i[E(\mathbf{p})+E(\mathbf{p}')]t/2}, \tag{13.1.11b}$$

$$\langle a(\mathbf{p}',0)a(\mathbf{p},0)\rangle_t = 2\mathscr{E}(\mathbf{p},\mathbf{p}')h(\mathbf{p},\mathbf{p}',t)e^{i[E(\mathbf{p})+E(\mathbf{p}')]t/2}, \tag{13.1.11c}$$

$$\langle b^\dagger(\mathbf{p}',0)a(\mathbf{p},0\rangle_t = 2\mathscr{E}(\mathbf{p},\mathbf{p}')d(\mathbf{p},\mathbf{p}',t)e^{i[E(\mathbf{p})-E(\mathbf{p}')]t/2}, \tag{13.1.11d}$$

where f, g, h and d are consistent with the identities in Appendix A and satisfy

$$f(\mathbf{p},\mathbf{p}',t) = f(\mathbf{p}',\mathbf{p},t), \tag{13.1.12a}$$

$$g(\mathbf{p},\mathbf{p}',t) = g^c(\mathbf{p}',\mathbf{p},t), \tag{13.1.12b}$$

$$h(\mathbf{p},\mathbf{p}',t) = h(\mathbf{p}',\mathbf{p},t), \tag{13.1.12c}$$

$$d(\mathbf{p},\mathbf{p}',t) = \eta^2 d^{c*}(\mathbf{p}',\mathbf{p},t). \tag{13.1.12d}$$

The elements of the free CTP propagator, as well as the retarded, advanced, Pauli-Jordan and Hadamard propagators, may be written in the same forms as (10.3.12), (10.3.14) and (10.3.15), described in Chapter 10, with the substitution

$$\begin{aligned}\tilde{f}(p,p',t) = {}& \theta(p_0)\theta(p_0')f(\mathbf{p},\mathbf{p}',t) + \theta(-p_0)\theta(-p_0')f^c(-\mathbf{p},-\mathbf{p}',t)\\ &+ \theta(p_0)\theta(-p_0')g(\mathbf{p},-\mathbf{p}',t) + \theta(-p_0)\theta(p_0')g^c(-\mathbf{p},\mathbf{p}',t),\end{aligned} \tag{13.1.13}$$

satisfying $\tilde{f}(p,p',t) = \tilde{f}(p',p,t) = \tilde{f}^c(-p',-p,t)$, as required. The charge-violating propagator may be written

$$\not{\Delta}(p,p',t) = -i2\pi\delta(p^2-m^2)|2p_0|^{1/2}2\tilde{d}(p,p',t)e^{i(p_0-p_0')t/2}|2p_0'|^{1/2}2\pi\delta(p'^2-m^2), \tag{13.1.14}$$

where

$$\begin{aligned}\tilde{d}(p,p',t) = {}& \theta(p_0)\theta(p_0')d(\mathbf{p},\mathbf{p}',t) + \theta(-p_0)\theta(-p_0')\eta^2 d^{c*}(-\mathbf{p},-\mathbf{p}',t) \\ & + \theta(p_0)\theta(-p_0')h(\mathbf{p},-\mathbf{p}',t) + \theta(-p_0)\theta(p_0')\eta^2 h^{c*}(-\mathbf{p},\mathbf{p}',t).\end{aligned} \tag{13.1.15}$$

The inclusion of the C-violating distribution functions requires the addition to the expansion of the density matrix in the *in-in* generating functional the C-violating source l_{ab}. Hence, the in-in generating functional of connected Green's functions for the complex scalar field takes the form

$$\begin{aligned}\mathcal{W}[j_a,k_{ab},l_{ab}] = {}& -i\hbar\ln\iint[\mathrm{d}\chi^{a\dagger},\chi^a] \\ & \times\exp\left[\frac{i}{\hbar}\left(S\big[\chi^{a\dagger},\chi^a\big] + \int_{\Omega_t}\mathrm{d}^4x\left\{j_a^\dagger(x)\chi^a(x) + \chi_a^\dagger(x)j^a(x)\right\}\right.\right. \\ & + \frac{1}{2}\iint_{\Omega_t}\mathrm{d}^4x\,\mathrm{d}^4x'\left\{\chi^{a\dagger}(x)k_{ab}(x,x')\chi^b(x') + \chi^a(x)k_{ab}^c(x,x')\chi^{b\dagger}(x')\right. \\ & \left.\left.\left. + \chi^a(x)l_{ab}^\dagger(x,x')\chi^b(x') + \chi^{a\dagger}(x)l_{ab}(x,x')\chi^{b\dagger}(x')\right\} + \cdots\right)\right].\end{aligned} \tag{13.1.16}$$

The bi-local sources necessarily satisfy the identities

$$k_{ab}(x,x') = k_{ba}^\dagger(x',x), \tag{13.1.17a}$$

$$l_{ab}(x,x') = l_{ba}(x',x) = \eta^2 l_{ab}^{c\dagger}(x,x'), \tag{13.1.17b}$$

to ensure that the exponent of the generating functional is Hermitian and C-invariant. The subsequent derivation of the effective action then follows analogously to Chapter 10.

The Lagrangian in (13.1.1) is invariant under the global $U(1)$ transformation

$$\chi(x) \to \chi'(x) = e^{-i\alpha}\chi(x), \tag{13.1.18a}$$

$$\chi^\dagger(x) \to \chi'^\dagger(x) = e^{i\alpha}\chi^\dagger(x) \tag{13.1.18b}$$

and as such we obtain the conserved, Noether current

$$j_\mu(x) = i\Big[\chi^\dagger(x)\partial_\mu\chi(x) - [\partial_\mu\chi^\dagger(x)]\chi(x)\Big] \tag{13.1.19}$$

with corresponding conserved charge

$$: \mathcal{Q}(x_0) := \int \mathrm{d}^3\mathbf{x} \; : j_0(x) := \int \mathrm{d}\Pi_{\mathbf{p}} \left[a^\dagger(\mathbf{p},0)a(\mathbf{p},0) - b^\dagger(\mathbf{p},0)b(\mathbf{p},0)\right]. \tag{13.1.20}$$

The existence of this conserved charge necessitates the introduction of the chemical potential μ and, as such, the equilibrium density matrix is of the grand-canonical form

$$\rho(\beta, N) = e^{-\beta(H-\mu N)}. \tag{13.1.21}$$

The KMS relation then generalises to

$$\Delta_>(x^0 - y^0; \mathbf{x}-\mathbf{y}) = e^{-\beta\mu}\Delta_<(x^0 - y^0 + i\beta; \mathbf{x}-\mathbf{y}) \tag{13.1.22}$$

or, in the momentum representation,

$$\Delta_>(p) = e^{\beta(p_0-\mu)}\Delta_<(p). \tag{13.1.23}$$

Proceeding as in Chapter 9, we find that the final constraint on $\tilde{f}(p)$, generalising (11.0.16), is

$$\tilde{f}(p) = \theta(p_0)f_{\mathrm{B}}(p_0) + \theta(-p_0)f^c_{\mathrm{B}}(-p_0), \tag{13.1.24}$$

where $f^{(c)}_{\mathrm{B}}(p_0) = [e^{\beta[p_0-(+)\mu]} - 1]^{-1}$ is the particle (anti-particle) Bose-Einstein distribution function. In equilibrium, translational invariance is restored and the elements

of the free CTP propagator take the single-momentum forms

$$i\Delta_{\mathrm{F}}(p) = i\big[p^2 - m^2 + i\varepsilon\big]^{-1} + 2\pi\big\{\theta(p_0)f_{\mathrm{B}}(p_0) + \theta(-p_0)f^c_{\mathrm{B}}(-p_0)\big]\delta(p^2 - m^2), \tag{13.1.25a}$$

$$i\Delta_{>}(p) = 2\pi\big\{\theta(p_0)\big[1 + f_{\mathrm{B}}(p_0)\big] + \theta(-p_0)f^c_{\mathrm{B}}(-p_0)\big\}\delta(p^2 - m^2), \tag{13.1.25b}$$

$$i\Delta_{<}(p) = 2\pi\big\{\theta(p_0)f_{\mathrm{B}}(p_0) + \theta(-p_0)\big[1 + f^c_{\mathrm{B}}(-p_0)\big]\big\}\delta(p^2 - m^2). \tag{13.1.25c}$$

13.2 Connection with the Imaginary-Time Formalism

In order to define the ITF generating functional for the grand canonical partition function in (13.1.21), it is necessary to consider the Hamiltonian form of the path integral directly (see for instance [82]). We may write

$$\begin{aligned}\mathcal{Z}[j] = \iint[\mathrm{d}(\pi^\dagger,\pi)][\mathrm{d}(\chi^\dagger,\chi)]\,\exp\bigg[-\int_0^\beta \mathrm{d}\tau_x \int \mathrm{d}^3\mathbf{x}\,\Big\{\mathcal{H}(\pi^{(\dagger)},\chi^{(\dagger)}) \\ - i\Big[\pi(\bar{x})\partial_{\tau_x}\chi(\bar{x}) + \pi^\dagger(\bar{x})\partial_{\tau_x}\chi^\dagger(\bar{x})\Big] \\ - i\mu\Big[\pi^\dagger(\bar{x})\chi^\dagger(\bar{x}) - \pi(\bar{x})\chi(\bar{x})\Big] - j^\dagger(\bar{x})\chi(\bar{x}) - j(\bar{x})\chi(\bar{x})\Big\}\bigg].\end{aligned} \tag{13.2.1}$$

Expanding the fields and conjugate momenta in terms of two real degrees of freedom

$$\chi(\bar{x}) = \frac{1}{\sqrt{2}}\left[\chi_1(\bar{x}) + i\chi_2(\bar{x})\right], \tag{13.2.2a}$$

$$\pi(\bar{x}) = \frac{1}{\sqrt{2}}\left[\pi_1(\bar{x}) - i\pi_2(\bar{x})\right], \tag{13.2.2b}$$

we may perform the Gaussian integrals over π_1 and π_2, yielding

$$\begin{aligned}\mathcal{Z}[j] = \int[\mathrm{d}(\chi^\dagger,\chi)]\,\exp\bigg[-\int_0^\beta \mathrm{d}\tau_x \int \mathrm{d}^3\mathbf{x}\,\Big[(\partial_{\tau_x} + \mu)\chi^\dagger(\bar{x})(\partial_{\tau_x} - \mu)\chi(\bar{x}) \\ + \nabla\chi^\dagger(\bar{x})\cdot\nabla\chi(\bar{x}) + m^2\chi^\dagger(\bar{x})\chi(\bar{x}) - j^\dagger(\bar{x})\chi(\bar{x}) - j(\bar{x})\chi(\bar{x})\Big]\bigg].\end{aligned} \tag{13.2.3}$$

Inserting the Fourier transform,

$$\chi(\bar{x}) = \frac{1}{\beta} \sum_{\ell=-\infty}^{+\infty} \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3}\, e^{i[\omega_\ell \tau_x + \mathbf{p}\cdot\mathbf{x}]} \chi(i\omega_\ell, \mathbf{p}), \tag{13.2.4}$$

we see that the effect of the chemical potential is to shift the poles of the Matsubara propagator, which becomes

$$\bar{\Delta}^0(i\omega_\ell - \mu, \mathbf{p}) = \frac{1}{(\omega_\ell + i\mu)^2 + \mathbf{p}^2 + m^2}. \tag{13.2.5}$$

The retarded propagator is then obtained by the continuation

$$\bar{\Delta}^0(i\omega_\ell - \mu \to p_0 + i\varepsilon, \mathbf{p}) = -\Delta^0_{\mathrm{R}}(p) \tag{13.2.6}$$

and the retarded self-energy by

$$\bar{\Pi}(i\omega_\ell - \mu \to p_0 + i\varepsilon) = -\Pi_{\mathrm{R}}(p), \tag{13.2.7}$$

cf. (11.1.9) and (11.1.10).

14 The Number Density

In order to derive equations governing the evolution of the statistical distribution functions, so far appearing as unknowns in the perturbative expansion, we must first arrive at an unambiguous definition of the number density of particles in terms of the EEV of two-point correlations of field operators. We begin by considering the conserved charge for the scalar field

$$\mathcal{Q}(x_0) = i\int \mathrm{d}^3\mathbf{x}\left[\Phi^\dagger(x)\pi^\dagger(x) - \pi(x)\Phi(x)\right], \tag{14.0.1}$$

which we may interpret in terms of the difference between the number of particles and the number of anti-particles. We recall that $\pi(x) = \partial_0\Phi^\dagger(x)$ is the conjugate momentum operator. Of course, for the real scalar field, this is zero (up to a zero-point contribution) and herein lies the difficulty: we need somehow to extract from this charge the particle and anti-particle contributions.

In order to describe the number density of particles of a spatially-inhomogeneous, time-dependent system, we firstly need a generalisation of this operator with sufficient degrees-of-freedom that we may write a mixed momentum- and coordinate-space representation. We proceed by inserting unity in the form

$$1 = \int \mathrm{d}^4y \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3}\, e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}\delta(x_0 - y_0) \tag{14.0.2}$$

and subsequently symmetrising the integrand in x and y. This yields

$$\mathcal{Q}(x_0) = \frac{i}{2}\int \mathrm{d}^3\mathbf{x} \int \mathrm{d}^4 y \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3}\, e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}\delta(x_0-y_0)\Big[\Phi^\dagger(x)\pi^\dagger(y)-\pi(x)\Phi(y)+(x\leftrightarrow y)\Big], \tag{14.0.3}$$

Introducing the relative and central coordinates, R^μ and X^μ respectively, we may write the charge density

$$\begin{aligned}\mathcal{Q}(\mathbf{p},\mathbf{X},X_0) = \frac{i}{2}\int \mathrm{d}^3\mathbf{R}\, e^{-i\mathbf{p}\cdot\mathbf{R}}\,\delta(R_0) \\ \times\Big[\Phi^\dagger(X+\tfrac{R}{2})\pi^\dagger(X-\tfrac{R}{2}) - \pi(X+\tfrac{R}{2})\Phi(X-\tfrac{R}{2}) + (R\to -R)\Big].\end{aligned} \tag{14.0.4}$$

Recalling the discussion of physical, equal-time observables in Chapter 9, the EEV of the charge density at the macroscopic time t is obtained by taking the trace with the density matrix in the equal-time limit $X_0 = t/2$, such that

$$\langle\mathcal{Q}(\mathbf{p},\mathbf{X},t/2)\rangle_t = \lim_{X_0\to t/2} -i\int \mathrm{d}^3\mathbf{R}\, e^{-i\mathbf{p}\cdot\mathbf{R}}\,\delta(R_0)\,\partial_{R_0}\Big[i\Delta_>(R,X,t) - i\Delta_>(-R,X,t)\Big], \tag{14.0.5}$$

where we have used the short-hand

$$i\Delta_>(R,X,t) = \langle\Phi^\dagger(X+\tfrac{R}{2})\Phi(X-\tfrac{R}{2})\rangle_t \tag{14.0.6}$$

for the resummed CTP Wightman propagators.

Looking more closely at the two terms in (14.0.4), we see that the first comprises the difference of the forward-in-time propagation of *background plus one* positive-frequency, particle modes and *background* negative-frequency, anti-particle modes. The second comprises the difference of the forward-in-time propagation of *background* positive-frequency, anti-particle modes and *background plus one* negative-frequency, particle modes. For the real scalar field, the particle and anti-particle contributions cancel, leaving only a zero-point term, which is removed by imposing normal-ordering. The conserved charge of the real scalar field is then vanishing as we would expect.

We may then extract the number density of particles by adding the charge-conjugate of the negative-frequency contribution from the first term in (14.0.5) and the charge-conjugate of the positive-frequency contribution from the second, with an overall minus sign for our convention on the charge of particles. We may separate the positive- and negative-frequency parts by decomposing the delta function in the form

$$\delta(R_0) = \frac{1}{2\pi i}\left[\frac{1}{R_0 - i\epsilon} - \frac{1}{R_0 + i\epsilon}\right], \tag{14.0.7}$$

where the limit $\epsilon \to 0^+$ is understood. At this point, it is important to note that in separating out and combining the correct positive- and negative-frequency parts, we have removed the zero-point term, effectively imposing normal ordering on the definition of the number density. We may then define the number density of particles at the macroscopic time t as

$$\begin{aligned} n(\mathbf{p}, \mathbf{X}, t) = &- \lim_{X_0 \to t/2} \int \mathrm{d}^3\mathbf{R}\, e^{-i\mathbf{p}\cdot\mathbf{R}} \\ &\times \int \frac{\mathrm{d}R_0}{2\pi}\left[\frac{1}{R_0 - i\epsilon}\partial_{R_0} i\Delta^c_>(R, X, t) + \frac{1}{R_0 + i\epsilon}\partial_{R_0} i\Delta^c_>(-R, X, t)\right]. \end{aligned} \tag{14.0.8}$$

This may be recast in terms of the Wigner representation of the Wightman propagators as

$$n(\mathbf{p}, \mathbf{X}, t) = \lim_{X_0 \to t/2} \int \frac{\mathrm{d}p_0}{2\pi}\, p_0 \big[\theta(p_0) i\Delta^c_>(-p, X, t) - \theta(-p_0) i\Delta^c_>(p, X, t)\big], \tag{14.0.9}$$

from which we may obtain the number density of anti-particles by charge-conjugation, see Appendix A and Chapter 13. Using the identities in Appendix A, we may rewrite this in terms of the negative-frequency Wightman propagators as

$$n(\mathbf{p}, \mathbf{X}, t) = \lim_{X_0 \to t/2} \int \frac{\mathrm{d}p_0}{2\pi}\, p_0 \big[\theta(p_0) i\Delta_<(p, X, t) - \theta(-p_0) i\Delta_<(-p, X, t)\big], \tag{14.0.10}$$

We interpret this number density as the number of excitations with three-momentum $\mathbf{p}$ in a unit volume centred on $\mathbf{X}$ at macroscopic time t. Trivially, the total number

per unit volume is obtained by summing over all momentum modes, i.e.,

$$n(\mathbf{X},t) = \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3}\, n(\mathbf{p},\mathbf{X},t). \tag{14.0.11}$$

By inserting the Wigner transform, this may be expressed in terms of the double-momentum representation of the propagators as

$$n(\mathbf{X},t) = \lim_{X_0\to t/2} 2 \iint \frac{\mathrm{d}^4p}{(2\pi)^4}\frac{\mathrm{d}^4P}{(2\pi)^4}\, e^{-iP\cdot X}\, \theta(p_0)p_0 i\Delta_<(p+\tfrac{P}{2}, p-\tfrac{P}{2}, t). \tag{14.0.12}$$

If f is indeed to be interpreted as a distribution function, it follows also that

$$n(\mathbf{X},t) = \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3}\int \frac{\mathrm{d}^3\mathbf{P}}{(2\pi)^3}\, e^{i\mathbf{P}\cdot\mathbf{X}} f(\mathbf{p}+\mathbf{P}/2, \mathbf{p}-\mathbf{P}/2, t). \tag{14.0.13}$$

Substituting into (14.0.10) for the free, equilibrium Wightman propagators of the complex scalar field, we obtain

$$n^{(c)}(\mathbf{p},\mathbf{X},t) = f_{\mathrm{B}}^{(c)}\big(E(\mathbf{p})\big), \tag{14.0.14}$$

exactly as we would expect for the number density of particles (anti-particles). Inserting instead the resummed equilibrium Wightman propagators in the narrow-width limit, we obtain

$$n^{(c)}(\mathbf{p},\mathbf{X},t) = f_{\mathrm{B}}^{(c)}\big(\mathcal{E}(\mathbf{p})\big), \tag{14.0.15}$$

where $\mathcal{E}(\mathbf{p})$ is the solution to the gap equation

$$\mathcal{E}^2(\mathbf{p}) = \mathbf{p}^2 + M^2 - \mathrm{Re}\,\Pi_{\mathrm{R}}(\mathcal{E}(\mathbf{p}) + i\epsilon, \mathbf{p}), \tag{14.0.16}$$

where $n(\mathbf{p},\mathbf{X},t)$ is then the number density of quasi-particles.

15 Perturbative Time-Evolution Equations

In this chapter, we arrive at the discussion of the ultimate goal of this work: to generalise the classical Boltzmann transport equation of Chapter 3 to quantum field-theoretic systems.

The FD series alone is insufficient to describe the evolution of the distribution function $f(\mathbf{p},\mathbf{p}',t)$, since it appears as an unknown in the expansion. We proceed then in analogy to the derivation of the well-known Kadanoff-Baym equations [45,46] by using the inverse relation to constrain the statistical evolution of the two-point functions. Our approach will nevertheless have a significant difference: we will truncate the perturbative expansion in terms of the double momentum representation of the free propagators, not the gradient expansion of the Wigner representation of the resummed propagators, cf. Chapter 10 and Appendix C.

Beginning with the double-momentum representation of the SD equation (10.1.25), we convolute from the right with the resummed CTP propagator and the weight function δ_t, making use of the inverse relation (9.3.2). This yields

$$\begin{aligned}&\iint\frac{\mathrm{d}^4q_1}{(2\pi)^4}\frac{\mathrm{d}^4q_2}{(2\pi)^4}\,\Delta^{0,\,-1}_{ac}(p_1,q_1)(2\pi)^4\delta_t^{(4)}(q_1-q_2)\Delta^{c}{}_{b}(q_2,p_2,t)\\&=\eta_{ab}(2\pi)^4\delta_t(p_1-p_2)-\iint\frac{\mathrm{d}^4q_1}{(2\pi)^4}\frac{\mathrm{d}^4q_2}{(2\pi)^4}\,\Pi_{ac}(p_1,q_1,t)(2\pi)^4\delta_t(q_1-q_2)\Delta^{c}{}_{b}(q_2,p_2,t),\end{aligned}\tag{15.0.1}$$

where we have safely taken K_{ab} to zero. Recalling that the self-energy contains δ_t functions in the vertices, we may perform the q_1 integral on the right-hand side, making use of (9.3.6). Inserting the explicit form of the inverse propagator on the left, we may also perform the q_1 integral on the left-hand side. We then obtain the more manageable form

$$\int \mathrm{d}^4 q_2 \left[p_1^2 - M^2\right] \delta_t^{(4)}(p_1 - q_2) \Delta_{ab}(q_2, p_2, t) \\ = \eta_{ab}(2\pi)^4 \delta_t^{(4)}(p_1 - p_2) - \int \frac{\mathrm{d}^4 q_2}{(2\pi)^4} \, \Pi_{ac}(p_1, q_2, t) \Delta^c{}_b(q_2, p_2, t). \quad (15.0.2)$$

Outside the time interval $[-t/2, t/2]$, the resummed propagators must satisfy the Klein-Gordon equations in (9.1.21) and (9.1.22) and, as such, we may extend the time integral to infinity in all but the right-most term in the coordinate-space representation of (15.0.2), containing the self-energy. Correspondingly in (15.0.2), we may replace the δ_t functions in all but the right-most, self-energy-dependent term by exact delta functions, yielding

$$\left[p_1^2 - M^2\right] \Delta_{ab}(p_1, p_2, t) = \eta_{ab}(2\pi)^4 \delta^{(4)}(p_1 - p_2) - \int \frac{\mathrm{d}^4 q}{(2\pi)^4} \, \Pi_{ac}(p_1, q, t) \Delta^c{}_b(q, p_2, t). \quad (15.0.3)$$

With the definition of the number density (14.0.10) in mind, we equate the 21-element of each side to extract the interacting Klein-Gordon equation of the positive-frequency, resummed Wightman propagator:

$$\left[p_1^2 - M^2\right] \Delta_<(p_1, p_2, t) = -\int \frac{\mathrm{d}^4 q}{(2\pi)^4} \left[\Pi_<(p_1, q, t) \Delta_{\mathrm{F}}^*(q, p_2, t) + \Pi(p_1, q, t) \Delta_<(q, p_2, t)\right]. \quad (15.0.4)$$

Using the identities listed in Appendix A, we may show that

$$\Delta_{\mathrm{F}}(x, y) = \frac{1}{2}\left[\Delta_>(x, y) + \Delta_<(x, y) + 2\Delta_{\mathcal{P}}(x, y)\right], \quad (15.0.5)$$

with an analogous relation holding for the self-energies. Subsequently decomposing

the right-hand side of (15.0.4), we may write

$$\begin{aligned}&\big[p_1^2 - M^2\big]\Delta_<(p_1,p_2,t) + \frac{1}{2}\int\frac{\mathrm{d}^4q}{(2\pi)^4}\,\Pi_{\mathcal{P}}(p_1,q,t)\Delta_<(q,p_2,t)\\ &= -\frac{1}{2}\int\frac{\mathrm{d}^4q}{(2\pi)^4}\,\big[\Pi_>(p_1,q,t)\Delta_<(q,p_2,t) - \Pi_<(p_1,q,t)\big(\Delta_>(q,p_2,t) - 2\Delta_{\mathcal{P}}(q,p_2,t)\big)\big],\end{aligned} \tag{15.0.6}$$

where we recall that the subscript $\mathcal{P}$ denotes the principal-part functions in (7.1.29) and (10.1.22b). We now re-introduce the central and relative momenta, $p = (p_1 + p_2)/2$ and $P = p_1 - p_2$, writing

$$\big[(p_0+\tfrac{P_0}{2})^2 - E^2(\mathbf{p}+\tfrac{\mathbf{P}}{2})\big]\Delta_<(p+\tfrac{P}{2},p-\tfrac{P}{2},t) + \mathscr{F}(p+\tfrac{P}{2},p-\tfrac{P}{2},t) = \mathscr{C}(p+\tfrac{P}{2},p-\tfrac{P}{2},t), \tag{15.0.7}$$

where we have defined

$$\mathscr{F}(p+\tfrac{P}{2},p-\tfrac{P}{2},t) \equiv -\int\frac{\mathrm{d}^4q}{(2\pi)^4}\,i\Pi_{\mathcal{P}}(p+\tfrac{P}{2},q,t)i\Delta_<(q,p-\tfrac{P}{2},t) \tag{15.0.8}$$

and

$$\begin{aligned}\mathscr{C}(p+\tfrac{P}{2},p-\tfrac{P}{2},t) \equiv \frac{1}{2}\int\frac{\mathrm{d}^4q}{(2\pi)^4}\,&\big[i\Pi_>(p_1,q,t)i\Delta_<(q,p_2,t)\\ &- i\Pi_<(p_1,q,t)\big(i\Delta_>(q,p_2,t) - 2i\Delta_{\mathcal{P}}(q,p_2,t)\big)\big].\end{aligned} \tag{15.0.9}$$

Still keeping the number density (14.0.10) firmly in mind, we integrate with the measure

$$\iint\frac{\mathrm{d}^4p}{(2\pi)^4}\frac{\mathrm{d}^4P}{(2\pi)^4}\,e^{-iP\cdot X}\,\theta(p_0). \tag{15.0.10}$$

We then obtain

$$\iint\frac{\mathrm{d}^4p}{(2\pi)^4}\frac{\mathrm{d}^4P}{(2\pi)^4}\,e^{-iP\cdot X}\,\theta(p_0)\big[(p_0+\tfrac{P_0}{2})^2-E^2(\mathbf{p}+\tfrac{\mathbf{P}}{2})\big]\Delta_<(p+\tfrac{P}{2},p-\tfrac{P}{2},t)$$
$$+\iint\frac{\mathrm{d}^4p}{(2\pi)^4}\frac{\mathrm{d}^4P}{(2\pi)^4}\,e^{-iP\cdot X}\,\theta(p_0)\,\mathscr{F}(p+\tfrac{P}{2},p-\tfrac{P}{2},t)$$
$$=\iint\frac{\mathrm{d}^4p}{(2\pi)^4}\frac{\mathrm{d}^4P}{(2\pi)^4}\,e^{-iP\cdot X}\,\theta(p_0)\,\mathscr{C}(p+\tfrac{P}{2},p-\tfrac{P}{2},t). \quad (15.0.11)$$

Adding to this result the complex conjugate of the same expression with $P\to -P$, using the identities in Appendix A, we may extract the pieces bi-linear in p and P to obtain

$$2\iint\frac{\mathrm{d}^4p}{(2\pi)^4}\frac{\mathrm{d}^4P}{(2\pi)^4}\,e^{-iP\cdot X}\,\theta(p_0)\,p\cdot P\,\Delta_<(p+\tfrac{P}{2},p-\tfrac{P}{2},t)$$
$$+\iint\frac{\mathrm{d}^4p}{(2\pi)^4}\frac{\mathrm{d}^4P}{(2\pi)^4}\,e^{-iP\cdot X}\,\theta(p_0)\big[\mathscr{F}(p+\tfrac{P}{2},p-\tfrac{P}{2},t)+\mathscr{F}^*(p-\tfrac{P}{2},p+\tfrac{P}{2},t)\big]$$
$$=\iint\frac{\mathrm{d}^4p}{(2\pi)^4}\frac{\mathrm{d}^4P}{(2\pi)^4}\,e^{-iP\cdot X}\,\theta(p_0)\big[\mathscr{C}(p+\tfrac{P}{2},p-\tfrac{P}{2},t)+\mathscr{C}^*(p-\tfrac{P}{2},p+\tfrac{P}{2},t)\big]. \quad (15.0.12)$$

The first term of the left-hand side may be rewritten as

$$2\iint\frac{\mathrm{d}^4p}{(2\pi)^4}\frac{\mathrm{d}^4P}{(2\pi)^4}\theta(p_0)\big[ip_0\partial_{X_0}-\mathbf{p}\cdot\mathbf{P}\big]e^{-iP\cdot X}\,\Delta_<(p+\tfrac{P}{2},p-\tfrac{P}{2},t). \quad (15.0.13)$$

Taking the limit $X_0\to\tilde{t}_f=t/2$, replacing ∂_{X_0} with ∂_t and comparing with (14.0.10), we recognise the derivative term as precisely the time-derivative of the number density. The propagators and self-energies in the $\mathscr{F}$ and $\mathscr{C}$ terms depend on $f(\mathbf{p}+\frac{\mathbf{p}}{2},\mathbf{p}+\frac{\mathbf{p}}{2},t)$ and we have therefore obtained an evolution equation for the distribution function akin to the classical Boltzmann equation.

Truncating to leading order in perturbation theory, we obtain

$$\begin{aligned}\partial_t n(\mathbf{X},t) - 2\iint\frac{\mathrm{d}^4p}{(2\pi)^4}\frac{\mathrm{d}^4P}{(2\pi)^4}\,e^{-iP\cdot X}\,\mathbf{p}\cdot\mathbf{P}\,\theta(p_0)\Delta^{(1)}_<(p+\tfrac{P}{2},p-\tfrac{P}{2},t)\\ + \iint\frac{\mathrm{d}^4p}{(2\pi)^4}\frac{\mathrm{d}^4P}{(2\pi)^4}\,e^{-iP\cdot X}\,\theta(p_0)\big[\mathscr{F}^{(1)}(p+\tfrac{P}{2},p-\tfrac{P}{2},t)+\mathscr{F}^{(1)*}(p-\tfrac{P}{2},p+\tfrac{P}{2},t)\big]\\ = \iint\frac{\mathrm{d}^4p}{(2\pi)^4}\frac{\mathrm{d}^4P}{(2\pi)^4}\,e^{-iP\cdot X}\theta(p_0)\big[\mathscr{C}^{(1)}(p+\tfrac{P}{2},p-\tfrac{P}{2},t)+\mathscr{C}^{(1)*}(p-\tfrac{P}{2},p+\tfrac{P}{2},t)\big],\end{aligned} \tag{15.0.14}$$

where $X_0 = t/2$. Recalling (14.0.13), we may rewrite this in terms of the distribution function f as

$$\begin{aligned}\partial_t f(\mathbf{p}+\tfrac{\mathbf{P}}{2},\mathbf{p}-\tfrac{\mathbf{P}}{2},t) - 2\iint\frac{\mathrm{d}p_0}{2\pi}\frac{\mathrm{d}P_0}{2\pi}\,e^{-iP_0t/2}\,\mathbf{p}\cdot\mathbf{P}\,\theta(p_0)\Delta^{(1)}_<(p+\tfrac{P}{2},p-\tfrac{P}{2},t)\\ + \iint\frac{\mathrm{d}p_0}{2\pi}\frac{\mathrm{d}P_0}{2\pi}\,e^{-iP_0t/2}\,\theta(p_0)\big[\mathscr{F}^{(1)}(p+\tfrac{P}{2},p-\tfrac{P}{2},t)+\mathscr{F}^{(1)*}(p-\tfrac{P}{2},p+\tfrac{P}{2},t)\big]\\ = \iint\frac{\mathrm{d}p_0}{2\pi}\frac{\mathrm{d}P_0}{2\pi}\,e^{-iP_0t/2}\,\theta(p_0)\big[\mathscr{C}^{(1)}(p+\tfrac{P}{2},p-\tfrac{P}{2},t)+\mathscr{C}^{(1)*}(p-\tfrac{P}{2},p+\tfrac{P}{2},t)\big],\end{aligned} \tag{15.0.15}$$

where, for instance,

$$\begin{aligned}\mathscr{C}^{(1)}(p+\tfrac{P}{2},p-\tfrac{P}{2},t) \equiv \frac{1}{2}\int\frac{\mathrm{d}^4q}{(2\pi)^4}\,\big[i\Pi^{(1)}_>(p+\tfrac{P}{2},q,t)i\Delta^0_<(q,p-\tfrac{P}{2},t)\\ - i\Pi^{(1)}_<(p+\tfrac{P}{2},q,t)\big(i\Delta^0_>(q,p-\tfrac{P}{2},t) - 2i\Delta^0_{\mathcal{P}}(q,p-\tfrac{P}{2},t)\big)\big].\end{aligned} \tag{15.0.16}$$

The first two terms of the left-hand side of (15.0.14), originating from (15.0.13) generalise the *drift* term $\partial_t + \mathbf{v}\cdot\nabla$ of the Boltzmann equation to this non-homogeneous double momentum representation, cf. (3.6.11). We see that it is possible to write the spatial part of this drift term in terms of the distribution function f only when we take the limit of on-shell, massless particles, in which case $p_0 = |\mathbf{p}|$. The $\mathscr{F}$ terms then are the *force* terms generated by a potential due to the dispersive part of the self-energy. The $\mathscr{C}$ terms are the *collision* terms where the principal-part contribution encodes off-shell processes. Comparing with the full, non-truncated form of Kadanoff-Baym kinetic equation in (C.4b), we see that the resummed prop-

agators have been replaced by the one-loop inserted propagators and the series of nested Poisson brackets has been replaced by the single convolution integral over the central momentum P.

Imposing energy conservation, we may replace the time-dependent weight functions of the vertices with exact delta functions. Subsequently imposing spatial homogeneity, we recall that all propagators and self-energies are proportional to four-dimensional delta functions of the momenta. In the same limit, the distribution function satisfies the correspondence

$$f(\mathbf{p}+\tfrac{\mathbf{P}}{2},\mathbf{p}-\tfrac{\mathbf{P}}{2},t) = (2\pi)^3\delta^{(3)}(\mathbf{P})f(|\mathbf{p}|,t). \tag{15.0.17}$$

Working then in the single-momentum representation and integrating over the three momentum $\mathbf{P}$, we find the following evolution equation for the number density $f(|\mathbf{p}|,t)$:

$$\partial_t f(|\mathbf{p}|,t) = \int \frac{\mathrm{d}p_0}{2\pi}\,\theta(p_0)\big[i\Pi^{(1)}_{>}(p,t)i\Delta^0_{<}(p,t) - i\Pi^{(1)}_{<}(p,t)i\Delta^0_{>}(p,t)\big], \tag{15.0.18}$$

where the force term and off-shell effects have vanished. In the following section, we will show that this is precisely the Boltzmann equation for the evolution of the distribution function to leading order in perturbation theory. This equation is to be compared with the truncated Kadanoff-Baym kinetic equation in (C.5b)

16 Non-Homogeneous Loop Integrals

In this chapter, we side step the development of our approach, in order to outline the techniques necessary to perform loop integrals in the presence of the energy-non-conserving vertices and non-homogeneous free propagators introduced in Chapters 9 and 10. We do not discuss the generalisation of the A-function (see [100]), however an explicit calculation of tadpole graphs is described with reference to the toy model and the inclusion of thermal masses in Chapter 17.

16.1 The Non-Homogeneous B_0 Function

Let us define by

$$\begin{aligned} B_0^{ab}(q_1,q_2,m_1,m_2,t) \equiv (2\pi\mu)^{4-d} e^{i(q_1^0-q_2^0)t/2} \int\cdots\int \frac{\mathrm{d}^d k_1}{i\pi^2}\frac{\mathrm{d}^4 k_1'}{(2\pi)^4}\frac{\mathrm{d}^4 k_2}{(2\pi)^4}\frac{\mathrm{d}^4 k_2'}{(2\pi)^4} \\ \times (2\pi)^4\delta_t^{(4)}(q_1-k_1+k_2)(2\pi)^4\delta_t^{(4)}(q_2-k_1'+k_2') \\ \times \eta^{acd}\Delta^0_{ce}(k_1,k_1',t;m_1)\Delta^0_{fd}(k_2',k_2,t;m_2)\eta^{efb}, \end{aligned} \tag{16.1.1}$$

where

$$B_0^{ab} = \begin{bmatrix} B_0 & B_0^< \\ B_0^> & -B_0^* \end{bmatrix}, \tag{16.1.2}$$

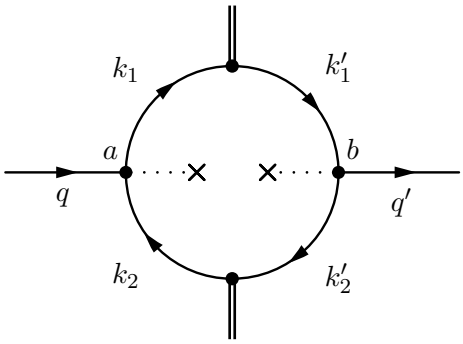


Figure 16.1: The non-homogeneous B_0^{ab} function.

the generalisation of the more familiar zero-temperature B_0 function (see, for instance, [100]):

$$B_0^{T=0}(q, m_1, m_2) = (2\pi\mu)^{4-d} \int \frac{\mathrm{d}^d k}{i\pi^2} \frac{1}{k^2 - m_1^2 + i\epsilon} \frac{1}{(k-q)^2 - m_1^2 + i\epsilon}. \tag{16.1.3}$$

Under the assumption that the statistical distribution functions are appropriately cut-off in the ultra-violet and in anticipation that any such divergence will result from the homogeneous zero-temperature contribution, we have restricted the dimensional regularisation of the integral only to the k_1 dependence.

In order to deal with the product of t-dependent sinusoidal terms in the vertex functions, we make the following replacement

$$\delta_t(x)\delta_t(y) = \int_{\sigma-i\infty}^{\sigma+i\infty} \frac{\mathrm{d}s}{2\pi i}\, e^{st}\, \frac{2}{\pi^2} \frac{4s}{(x-y)^2 + 4s^2} \frac{1}{(x+y)^2 + 4s^2}, \tag{16.1.4}$$

where the right-hand side is the inverse Laplace transform and $s \in \mathbb{C}$. The Bromwich contour is chosen so that $\sigma \in \mathbb{R}$ is larger than the real part of the right-most pole in the integrand to ensure convergence. We then introduce the representation $B_0^{ab}(q_1, q_2, m_1, m_2, s)$ through

$$B^{ab}(q_1, q_2, m_1, m_2, t) = \int_{\sigma-i\infty}^{\sigma+i\infty} \frac{\mathrm{d}s}{2\pi i}\, e^{st}\, B_0^{ab}(q_1, q_2, m_1, m_2, s). \tag{16.1.5}$$

We note that $B_0^{ab}(q_1, q_2, m_1, m_2, s)$ is not the Laplace transform of $B_0^{ab}(q_1, q_2, m_1, m_2, t)$ as we do not transform the t dependence of the distribution functions.

Accordingly, we then obtain

$$\begin{aligned}
B_0^{ab}(q_1, q_2, m_1, m_2, s) &= 8(2\pi\mu)^{4-d} e^{i(q_1^0 - q_2^0)t/2} \int \cdots \int \frac{\mathrm{d}^d k_1}{i\pi^2} \frac{\mathrm{d}^4 k_1'}{(2\pi)^4} \frac{\mathrm{d}^4 k_2}{(2\pi)^4} \frac{\mathrm{d}^4 k_2'}{(2\pi)^4} \\
&\times (2\pi)^3 \delta^{(3)}(\mathbf{q}_1 - \mathbf{k}_1 + \mathbf{k}_2)(2\pi)^3 \delta^{(3)}(\mathbf{q}_2 - \mathbf{k}_1' + \mathbf{k}_2') \\
&\times 4s \Big[\big[q_1^0 - q_2^0 - k_1^0 + k_1^{0\prime} + k_2^0 - k_2^{0\prime} \big]^2 + 4s^2 \Big]^{-1} \\
&\times \Big[\big[q_1^0 + q_2^0 - k_1^0 - k_1^{0\prime} + k_2^0 + k_2^{0\prime} \big]^2 + 4s^2 \Big]^{-1} \\
&\times \eta^{acd} \Delta_{ce}^0(k_1, k_1', t; m_1) \Delta_{fd}^0(k_2', k_2, t; m_2) \eta^{efb},
\end{aligned} \tag{16.1.6}$$

in which the analytic structure of the product of formerly t-dependent vertex functions is now manifest.

Recalling the relations in Appendix A, we may fix all four components of this generalised B_0 function by the explicit evaluation of only two: one from the diagonal and one from the anti-diagonal; specifically one of the time- or anti-time-ordered functions and one of the positive- or negative-frequency absolutely-ordered functions. Proceeding in the most nominal and aesthetic fashion, we opt to evaluate the time-ordered and positive-frequency absolutely-ordered functions in the first instance.

16.1.1 Time-Ordered Functions

The 11-element coincides with the time-ordered function, which we immediately separate into four contributions, that is

$$B_0 = I^{(\mathrm{i})} + I^{(\mathrm{ii})} + I^{(\mathrm{iiia})} + I^{(\mathrm{iiib})}, \tag{16.1.7}$$

corresponding to the zero-temperature, purely thermal and cross terms, respectively:

(i) **The zero-temperature part** may be extracted from the product of terms

non-vanishing in the limit of vanishing statistical distribution functions and is

$$
\begin{aligned}
I^{(\mathrm{i})}(q_1,q_2,m_1,m_2,s) &= 8(2\pi\mu)^{4-d}e^{i(q_1^0-q_2^0)t/2}\int\cdots\int\frac{\mathrm{d}^d k_1}{i\pi^2}\frac{\mathrm{d}^4 k_1'}{(2\pi)^4}\frac{\mathrm{d}^4 k_2}{(2\pi)^4}\frac{\mathrm{d}^4 k_2'}{(2\pi)^4}\\
&\times(2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times 4s\Big[\big[q_1^0-q_2^0-k_1^0+k_1^{0\prime}+k_2^0-k_2^{0\prime}\big]^2+4s^2\Big]^{-1}\\
&\times\Big[\big[q_1^0+q_2^0-k_1^0-k_1^{0\prime}+k_2^0+k_2^{0\prime}\big]^2+4s^2\Big]^{-1}\\
&\times\frac{1}{k_1^2-m_1^2+i\epsilon}(2\pi)^4\delta^{(4)}(k_1-k_1')\frac{1}{k_2'^2-m_2^2+i\epsilon}(2\pi)^4\delta^{(4)}(k_2'-k_2).
\end{aligned}
\tag{16.1.8}
$$

The $k_1^{0\prime}$ and k_2^0 integrations are performed by means of the delta functions in the final line, giving

$$
\begin{aligned}
I^{(\mathrm{i})}(q_1,q_2,m_1,m_2,s) &= (2\pi\mu)^{4-d}e^{i(q_1^0-q_2^0)t/2}\int\cdots\int\frac{\mathrm{d}^{d-1} k_1}{i\pi^2}\frac{\mathrm{d}^3\mathbf{k}_1'}{(2\pi)^3}\frac{\mathrm{d}^3\mathbf{k}_2}{(2\pi)^3}\frac{\mathrm{d}^3\mathbf{k}_2'}{(2\pi)^3}\,\mathrm{d}k_1^0\,\mathrm{d}k_2^{0\prime}\\
&\times(2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times\frac{4s}{\pi}\Big[\big[q_1^0-q_2^0\big]^2+4s^2\Big]^{-1}\Big[\big[\tfrac{q_1^0+q_2^0}{2}-k_1^0+k_2^{0\prime}\big]^2+s^2\Big]^2\Big]^{-1}\\
&\times\frac{1}{(k_1^0)^2-E_1^2(\mathbf{k}_1)+i\epsilon}\frac{1}{(k_2^{0\prime})^2-E_2'^2(\mathbf{k}_2')+i\epsilon}\\
&\times(2\pi)^3\delta^{(3)}(\mathbf{k}_1-\mathbf{k}_1')(2\pi)^3\delta^{(3)}(\mathbf{k}_2'-\mathbf{k}_2).
\end{aligned}
\tag{16.1.9}
$$

The reason for the seemingly-gratuitous retention of the trivial phase-space integrals and three-dimensional delta functions will become evident in the forthcoming evaluation of the remaining contributions to the time-ordered function.

By virtue of the residue theorem, we may perform the k_1^0 and $k_2^{0\prime}$ integrations by closing contours in the lower-halves of the k_1^0 and $k_2^{0\prime}$ complex-planes. After collecting together the resulting terms and re-expressing the result with more illus-

trative partial fractions, we find

$$
\begin{aligned}
I^{(\mathrm{i})}(q_1,q_2,m_1,m_2,s) &= -2(2\pi)^3\mu^{4-d}\sum_{\alpha_1=\pm1}\int\cdots\int\frac{\mathrm{d}^{d-1}k_1}{(2\pi)^{d-1}}\frac{\mathrm{d}^3\mathbf{k}_1'}{(2\pi)^3}\frac{\mathrm{d}^3\mathbf{k}_2}{(2\pi)^3}\frac{\mathrm{d}^3\mathbf{k}_2'}{(2\pi)^3}\\
&\times(2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times\frac{1}{\pi}\Big[\big[q_1^0-q_2^0\big]^2+4s^2\Big]^{-1}\frac{\alpha_1}{E_1(\mathbf{k}_1)E_2'(\mathbf{k}_2')}\Big[\tfrac{q_1^0+q_2^0}{2}-\alpha_1\big[E_1(\mathbf{k}_1)+E_2'(\mathbf{k}_2')-is\big]\Big]^{-1}\\
&\times(2\pi)^3\delta^{(3)}(\mathbf{k}_1-\mathbf{k}_1')(2\pi)^3\delta^{(3)}(\mathbf{k}_2'-\mathbf{k}_2),
\end{aligned}
\tag{16.1.10}
$$

or, in terms of the Lorentz-invariant phase-spaces,

$$
\begin{aligned}
I^{(\mathrm{i})}(q_1,q_2,m_1,m_2,s) &= -8(2\pi)^3\mu^{4-d}\sum_{\alpha_1=\pm1}e^{i(q_1^0-q_2^0)t/2}\int\cdots\int\mathrm{d}\Pi_{\mathbf{k}_1}^{d-1}\,\mathrm{d}\Pi_{\mathbf{k}_1'}\,\mathrm{d}\Pi_{\mathbf{k}_2}\,\mathrm{d}\Pi_{\mathbf{k}_2'}\\
&\times(2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times\frac{1}{\pi}\Big[\big[q_1^0-q_2^0\big]^2+4s^2\Big]^{-1}\Big[\tfrac{q_1^0+q_2^0}{2}-\alpha_1\big[E_1(\mathbf{k}_1)+E_2'(\mathbf{k}_2')-is\big]\Big]^{-1}\\
&\times\alpha_1(2\pi)^3 2E_1'(\mathbf{k}_1')\delta^{(3)}(\mathbf{k}_1-\mathbf{k}_1')(2\pi)^3 2E_2(\mathbf{k}_2)\delta^{(3)}(\mathbf{k}_2'-\mathbf{k}_2),
\end{aligned}
\tag{16.1.11}
$$

where the superscript $d-1$ identifies that the $\mathbf{k}_1$ integration is to be made over a $(d-1)$-dimensional phase-space.

Using the fact that the Laplace transform satisfies

$$
\mathcal{L}_t[\mathrm{Re}\,F](s)=\frac{1}{2}\Big[\mathcal{F}(s)+\big[\mathcal{F}(s^*)\big]^*\Big],
\tag{16.1.12a}
$$

$$
\mathcal{L}_t[\mathrm{Im}\,F](s)=\frac{1}{2i}\Big[\mathcal{F}(s)-\big[\mathcal{F}(s^*)\big]^*\Big],
\tag{16.1.12b}
$$

we may separate this result into the dispersive and absorptive parts of the original t-dependent function, that is to say the parts symmetric and anti-symmetric in s

respectively. In this form,

$$
\begin{aligned}
I^{(\mathrm{i})}(q_1,q_2,m_1,m_2,s) &= 8(2\pi)^3\mu^{4-d}\sum_{\alpha_1=\pm1} e^{i(q_1^0-q_2^0)t/2}\int\cdots\int \mathrm{d}\Pi_{k_1}^{d-1}\,\mathrm{d}\Pi_{\mathbf{k}_1'}\,\mathrm{d}\Pi_{\mathbf{k}_2}\,\mathrm{d}\Pi_{\mathbf{k}_2'}\\
&\times (2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times \frac{1}{\pi}\Big[\big[q_1^0-q_2^0\big]^2+4s^2\Big]^{-1}\Big[\big[\tfrac{q_1^0+q_2^0}{2}-\alpha_1\big(E_1(\mathbf{k}_1)+E_2'(\mathbf{k}_2')\big)\big]^2+s^2\Big]^{-1}\\
&\times\Big\{-\alpha_1\Big[\tfrac{q_1^0+q_2^0}{2}-\alpha_1\big(E_1(\mathbf{k}_1)+E_2'(\mathbf{k}_2')\big)\Big]+is\Big\}\\
&\times (2\pi)^3 2E_1'(\mathbf{k}_1')\delta^{(3)}(\mathbf{k}_1-\mathbf{k}_1')(2\pi)^3 2E_2(\mathbf{k}_2)\delta^{(3)}(\mathbf{k}_2'-\mathbf{k}_2),
\end{aligned}
\tag{16.1.13}
$$

where the delineation is identified within the braces of the fourth line.

Isolating the dispersive part of this result and performing the superfluous phase-space integrals, we find

$$
\begin{aligned}
\mathrm{Disp}\,B_0(q_1,q_2,m_1,m_2,s) &= -(2\pi)^4\frac{1}{\pi}\frac{1}{\big[q_1^0-q_2^0\big]^2+4s^2}\delta^{(3)}(\mathbf{q}_1-\mathbf{q}_2)\\
&\times(2\pi\mu)^{4-d}e^{i(q_1^0-q_2^0)t/2}\sum_{\alpha=\pm1}\int\mathrm{d}^{d-1}k_1\,\frac{E_1(\mathbf{k}_1)+E_2(\mathbf{k}_1-\mathbf{q}_1)}{E_1(\mathbf{k}_1)E_2(\mathbf{k}_1-\mathbf{q}_1)}\\
&\times\frac{1}{\pi}\frac{1}{\big[q_0-i\alpha s\big]^2-\big[E_1(\mathbf{k}_1)+E_2(\mathbf{q}_1-\mathbf{k}_1)\big]^2},
\end{aligned}
\tag{16.1.14}
$$

where Disp denotes that this is the dispersive part. We compare this result to the form of the zero-temperature B_0 function (16.1.3) after the k_0 integration has been performed:

$$
\begin{aligned}
B_0^{T=0}(q,m_1,m_2) &= -(2\pi\mu)^{4-d}\int\mathrm{d}^{d-1}k_1\,\frac{E_1(\mathbf{k}_1)+E_2(\mathbf{k}_1-\mathbf{q}_1)}{E_1(\mathbf{k}_1)E_2(\mathbf{k}_1-\mathbf{q}_1)}\\
&\times\frac{1}{\pi}\frac{1}{q_0^2-\big[E_1(\mathbf{k}_1)+E_2(\mathbf{q}_1-\mathbf{k}_1)\big]^2}.
\end{aligned}
\tag{16.1.15}
$$

Hence, we may write

$$\begin{aligned}&\mathrm{Disp}\, I^{(\mathrm{i})}(q_1,q_2,m_1,m_2,s)\\&=(2\pi)^4\frac{1}{\pi}\frac{1}{\left[q_1^0-q_2^0\right]^2+4s^2}\delta^{(3)}(\mathbf{q}_1-\mathbf{q}_2)e^{i(q_1^0-q_2^0)t/2}\sum_{\alpha=\pm1}B_0^{T=0}(q_1^0+i\alpha s,\mathbf{q},m_1,m_2),\end{aligned}\tag{16.1.16}$$

where, for $d=4$,

$$\begin{aligned}B_0^{T=0}(q_1^0+i\alpha s,\mathbf{q},m_1,m_2)&=\Big[\frac{1}{\epsilon}-\gamma_{\mathrm{E}}+\ln\frac{4\pi\mu^2}{m_1m_2}\Big]+\frac{1}{(q^0-i\alpha s)^2-\mathbf{q}^2}\Big[(m_2^2-m_1^2)\ln\frac{m_1^2}{m_2^2}\\&+\lambda^{1/2}((q^0-i\alpha s)^2-\mathbf{q}^2,m_1^2,m_2^2)\cosh^{-1}\Big(\frac{m_1^2+m_2^2-(q^0-i\alpha s)^2+\mathbf{q}^2}{2m_1m_2}\Big)\Big],\end{aligned}\tag{16.1.17}$$

containing the familiar zero-temperature UV divergence [100]. γ_{E} is the Euler gamma.

(ii) **The product of ensemble contributions** is more straightforward:

$$\begin{aligned}&I^{(\mathrm{ii})}(q_1,q_2,m_1,m_2,s)=-8(2\pi\mu)^{4-d}e^{i(q_1^0-q_2^0)t/2}\int\cdots\int\frac{\mathrm{d}^dk_1}{i\pi^2}\frac{\mathrm{d}^4k_1'}{(2\pi)^4}\frac{\mathrm{d}^4k_2}{(2\pi)^4}\frac{\mathrm{d}^4k_2'}{(2\pi)^4}\\&\times(2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\&\times4s\Big[\big[q_1^0-q_2^0-k_1^0+k_1^{0\prime}+k_2^0-k_2^{0\prime}\big]^2+4s^2\Big]^{-1}\\&\times\Big[\big[q_1^0+q_2^0-k_1^0-k_1^{0\prime}+k_2^0+k_2^{0\prime}\big]^2+4s^2\Big]^{-1}\\&\times2\pi\delta(k_1^2-m_1^2)|2k_1^0|^{1/2}\tilde{f}_1(k_1,k_1',t)e^{i(k_1^0-k_1^{0\prime})t/2)}|2k_1^{0\prime}|^{1/2}2\pi\delta(k_1'^2-m_1^2)\\&\times2\pi\delta(k_2'^2-m_2^2)|2k_2^{0\prime}|^{1/2}\tilde{f}_2(k_2',k_2,t)e^{i(k_2^{0\prime}-k_2{}^0)t/2)}|2k_2^0|^{1/2}2\pi\delta(k_2^2-m_2^2).\end{aligned}\tag{16.1.18}$$

Performing the four zeroth-component integrations, we find

$$
\begin{aligned}
I^{(\mathrm{ii})}(q_1,q_2,m_1,m_2,s) &= 8(2\pi)^3\mu^{4-d}e^{i(q_1^0-q_2^0)t/2}\sum_{\{\alpha\}=\pm1}\int\cdots\int \mathrm{d}\Pi_{k_1}^{d-1}\,\mathrm{d}\Pi_{\mathbf{k}_1'}\,\mathrm{d}\Pi_{\mathbf{k}_2}\,\mathrm{d}\Pi_{\mathbf{k}_2'}\\
&\times(2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times\Big[\big[q_1^0-q_2^0-\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')+\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')\big]^2+4s^2\Big]^{-1}\\
&\times\Big[\big[\tfrac{q_1^0+q_2^0}{2}-\tfrac{\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')}{2}+\tfrac{\alpha_2E_2(\mathbf{k}_2)+\alpha_2'E_2'(\mathbf{k}_2')}{2}\big]^2+s^2\Big]^{-1}\\
&\times\Big\{is\Big\}2\sqrt{2E_1(\mathbf{k}_1)2E_1'(\mathbf{k}_1')}\,\tilde f_1(k_1(\mathbf{k}_1),k_1'(\mathbf{k}_1'),t)e^{i[\alpha_1E_1(\mathbf{k}_1)-\alpha_1'E_1'(\mathbf{k}_1')]t/2)}\\
&\times\sqrt{2E_2(\mathbf{k}_2)2E_2'(\mathbf{k}_2')}\,\tilde f_2(k_2'(\mathbf{k}_2'),k_2(\mathbf{k}_2),t)e^{i[\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')]t},
\end{aligned}
\tag{16.1.19}
$$

where $\{\alpha\}\equiv\{\alpha_1,\alpha_1',\alpha_2,\alpha_2'\}$ and

$$
k_i(\mathbf{k}_i)\equiv(\alpha_iE_i(\mathbf{k}_i),\mathbf{k}_i) \tag{16.1.20}
$$

identifies on-shell four-momenta. The braces of the fifth line are included for comparison with the separation of dispersive and absorptive parts in (16.1.13).

(iii) **The cross-terms** yield both dispersive and absorptive contributions. The first yields

$$
\begin{aligned}
I^{(\mathrm{iiia})}(q_1,q_2,m_1,m_2,s) &= -8i(2\pi\mu)^{4-d}e^{i(q_1^0-q_2^0)t/2}\int\cdots\int\frac{\mathrm{d}^dk_1}{i\pi^2}\frac{\mathrm{d}^4k_1'}{(2\pi)^4}\frac{\mathrm{d}^4k_2}{(2\pi)^4}\frac{\mathrm{d}^4k_2'}{(2\pi)^4}\\
&\times(2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times 4s\Big[\big[q_1^0-q_2^0-k_1^0+k_1^{0\prime}+k_2^0-k_2^{0\prime}\big]^2+4s^2\Big]^{-1}\\
&\times\Big[\big[q_1^0+q_2^0-k_1^0-k_1^{0\prime}+k_2^0+k_2^{0\prime}\big]^2+4s^2\Big]^{-1}\\
&\times\frac{1}{k_1^2-m_1^2+i\epsilon}(2\pi)^4\delta^{(4)}(k_1-k_1')\\
&\times 2\pi\delta(k_2'^{\,2}-m_2^2)|2k_2^{0\prime}|^{1/2}\tilde f_2(k_2',k_2,t)e^{i(k_2^{0\prime}-k_2^0)t/2}|2k_2{}^0|^{1/2}2\pi\delta(k_2^2-m_2^2).
\end{aligned}
\tag{16.1.21}
$$

After evaluating the trivial $k_1{}'^0$, k_2^0, $k_2^{0\prime}$ and finally the k_1^0 integrals, with some

transposition of the result, we find

$$
\begin{aligned}
&I^{(\mathrm{iiia})}(q_1,q_2,m_1,m_2,s) = -8(2\pi)^3\mu^{4-d}e^{i(q_1^0-q_2^0)t/2}\\
&\times \sum_{\alpha_1,\alpha_2,\alpha_2'=\pm1}\int\cdots\int \mathrm{d}\Pi_{\mathbf{k}_1}^{d-1}\,\mathrm{d}\Pi_{\mathbf{k}_1'}\,\mathrm{d}\Pi_{\mathbf{k}_2}\,\mathrm{d}\Pi_{\mathbf{k}_2'}\\
&\times (2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times \frac{1}{\pi}\Big[\big[q_1^0-q_2^0+\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')\big]^2+4s^2\Big]^{-1}\\
&\times \Big[\tfrac{q_1^0+q_2^0}{2}+\tfrac{\alpha_2E_2(\mathbf{k}_2)+\alpha_2'E_2'(\mathbf{k}_2')}{2}-\alpha_1\big[E_1(\mathbf{k}_1)-is\big]\Big]^{-1}\\
&\times \alpha_1(2\pi)^3 2E_1'(\mathbf{k}_1')\delta^{(3)}(\mathbf{k}_1-\mathbf{k}_1')\\
&\times \sqrt{2E_2(\mathbf{k}_2)2E_2'(\mathbf{k}_2')}\,\tilde{f}_2(k_2'(\mathbf{k}_2'),k_2(\mathbf{k}_2),t)e^{i[\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')]t/2}.
\end{aligned}
\tag{16.1.22}
$$

Separating again into dispersive and absorptive parts as in (16.1.13), this may be written

$$
\begin{aligned}
&I^{(\mathrm{iiia})}(q_1,q_2,m_1,m_2,s) = 8(2\pi)^3\mu^{4-d}e^{i(q_1^0-q_2^0)t/2}\\
&\times \sum_{\alpha_1,\alpha_2,\alpha_2'=\pm1}\int\cdots\int \mathrm{d}\Pi_{\mathbf{k}_1}^{d-1}\,\mathrm{d}\Pi_{\mathbf{k}_1'}\,\mathrm{d}\Pi_{\mathbf{k}_2}\,\mathrm{d}\Pi_{\mathbf{k}_2'}\\
&\times (2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times \frac{1}{\pi}\Big[\big[q_1^0-q_2^0+\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')\big]^2+4s^2\Big]^{-1}\\
&\times \Big[\big[\tfrac{q_1^0+q_2^0}{2}-\alpha_1E_1(\mathbf{k}_1)+\tfrac{\alpha_2E_2(\mathbf{k}_2)+\alpha_2'E_2'(\mathbf{k}_2')}{2}\big]^2+s^2\Big]^{-1}\\
&\times \Big\{-\alpha_1\Big[\tfrac{q_1^0+q_2^0}{2}-\alpha_1E_1(\mathbf{k}_1)+\tfrac{\alpha_2E_2(\mathbf{k}_2)+\alpha_2'E_2'(\mathbf{k}_2')}{2}\Big]+is\Big\}\\
&\times (2\pi)^3 2E_1'(\mathbf{k}_1')\delta^{(3)}(\mathbf{k}_1-\mathbf{k}_1')\\
&\times \sqrt{2E_2(\mathbf{k}_2)2E_2'(\mathbf{k}_2')}\,\tilde{f}_2(k_2'(\mathbf{k}_2'),k_2(\mathbf{k}_2),t)e^{i[\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')]t/2}.
\end{aligned}
\tag{16.1.23}
$$

Similarly, from the second of the cross terms, we obtain

$$
\begin{aligned}
&I^{(\mathrm{iiib})}(q_1,q_2,m_1,m_2,s) = 8(2\pi)^3\mu^{4-d}e^{i(q_1^0-q_2^0)t/2}\\
&\times \sum_{\alpha_1,\alpha_1',\alpha_2'=\pm1}\int\cdots\int \mathrm{d}\Pi_{\mathbf{k}_1}^{d-1}\,\mathrm{d}\Pi_{\mathbf{k}_1'}\,\mathrm{d}\Pi_{\mathbf{k}_2}\,\mathrm{d}\Pi_{\mathbf{k}_2'}\\
&\times (2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times \frac{1}{\pi}\Big[\big[q_1^0-q_2^0-\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')\big]^2+4s^2\Big]^{-1}\\
&\times \Big[\big[\tfrac{q_1^0+q_2^0}{2}-\tfrac{\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')}{2}+\alpha_2E_2(\mathbf{k}_2)\big]^2+s^2\Big]^{-1}\\
&\times \Big\{\alpha_2\Big[\tfrac{q_1^0+q_2^0}{2}-\tfrac{\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')}{2}+\alpha_2E_2(\mathbf{k}_2)\Big]+is\Big\}\\
&\times \sqrt{2E_1(\mathbf{k}_1)2E_1'(\mathbf{k}_1')}\,\tilde{f}_1(k_1(\mathbf{k}_1),k_1'(\mathbf{k}_1'),t)e^{i[\alpha_1E_1(\mathbf{k}_1)-\alpha_1'E_1'(\mathbf{k}_1')]t/2}\\
&\times (2\pi)^3 2E_2(\mathbf{k}_2)\delta^{(3)}(\mathbf{k}_2'-\mathbf{k}_2),
\end{aligned}
\tag{16.1.24}
$$

as we would expect from the symmetry of the original integral under the interchange: $k_1 \leftrightarrow -k_2$, $k_1' \leftrightarrow -k_2'$ and $m_1 \leftrightarrow m_2$.

Concatenating these four contributions, after some convenient introductions, we find the time-ordered function

$$
\begin{aligned}
&B_0(q_1,q_2,m_1,m_2,s) = 8(2\pi)^3\mu^{4-d}e^{i(q_1^0-q_2^0)t/2}\sum_{\{\alpha\}=\pm1}\int\cdots\int \mathrm{d}\Pi_{\mathbf{k}_1}^{d-1}\,\mathrm{d}\Pi_{\mathbf{k}_1'}\,\mathrm{d}\Pi_{\mathbf{k}_2}\,\mathrm{d}\Pi_{\mathbf{k}_2'}\\
&\times (2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times \frac{1}{\pi}\Big[\big[q_1^0-q_2^0-\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')+\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')\big]^2+4s^2\Big]^{-1}\\
&\times \Big[\big[\tfrac{q_1^0+q_2^0}{2}-\tfrac{\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')}{2}+\tfrac{\alpha_2E_2(\mathbf{k}_2)+\alpha_2'E_2'(\mathbf{k}_2')}{2}\big]^2+s^2\Big]^{-1}\\
&\times \sqrt{2E_1(\mathbf{k}_1)2E_1'(\mathbf{k}_1')2E_2(\mathbf{k}_2)2E_2'(\mathbf{k}_2')}\,e^{i[\alpha_1E_1(\mathbf{k}_1)-\alpha_1'E_1'(\mathbf{k}_1')]t/2}e^{i[\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')]t/2}\\
&\times \Big\{-\Big[\tfrac{q_1^0+q_2^0}{2}-\tfrac{\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')}{2}+\tfrac{\alpha_2E_2(\mathbf{k}_2)+\alpha_2'E_2'(\mathbf{k}_2')}{2}\Big]F^{\mathrm{R}}_{\{\alpha\}}(\{k\},t)+isF^{1}_{\{\alpha\}}(\{k\},t)\Big\},
\end{aligned}
\tag{16.1.25}
$$

where $\{k\} \equiv \{k_1(\mathbf{k}_1), k_1'(\mathbf{k}_1'), k_2(\mathbf{k}_2), k_2'(\mathbf{k}_2')\}$. We have kept the spectral information explicit, whereas all statistical information has been condensed into the distributions

$F^{\mathrm{R}}_{\{\alpha\}}(\{k\},t)$ and $F^{1}_{\{\alpha\}}(\{k\},t)$:

$$\begin{aligned}
F^{\mathrm{R}}_{\{\alpha\}}(\{k\},t) &= (2\pi)^3\delta^{(3)}(\mathbf{k}_1-\mathbf{k}'_1)(2\pi)^3\delta^{(3)}(\mathbf{k}_2-\mathbf{k}'_2)\\
&\qquad\times\big[\theta(\alpha_1,\alpha'_1)\theta(-\alpha_2,-\alpha'_2)-\theta(-\alpha_1,-\alpha'_1)\theta(\alpha_2,\alpha'_2)\big]\\
&\quad+(2\pi)^3\delta^{(3)}(\mathbf{k}_1-\mathbf{k}'_1)\tilde{f}_2(k'_2(\mathbf{k}'_2),k_2(\mathbf{k}_2),t)\big[\theta(\alpha_1,\alpha'_1)-\theta(-\alpha_1,-\alpha'_1)\big]\\
&\quad+\tilde{f}_1(k_1(\mathbf{k}_1),k'_1(\mathbf{k}'_1),t)(2\pi)^3\delta^{(3)}(\mathbf{k}_2-\mathbf{k}'_2)\big[\theta(-\alpha_2,-\alpha'_2)-\theta(\alpha_2,\alpha'_2)\big],
\end{aligned}\tag{16.1.26a}$$

$$\begin{aligned}
F^{1}_{\{\alpha\}}(\{k\},t) &= (2\pi)^3\delta^{(3)}(\mathbf{k}_1-\mathbf{k}'_1)(2\pi)^3\delta^{(3)}(\mathbf{k}_2-\mathbf{k}'_2)\\
&\qquad\times\big[\theta(\alpha_1,\alpha'_1)\theta(-\alpha_2,-\alpha'_2)+\theta(-\alpha_1,-\alpha'_1)\theta(\alpha_2,\alpha'_2)\big]\\
&\quad+(2\pi)^3\delta^{(3)}(\mathbf{k}_1-\mathbf{k}'_1)\tilde{f}_2(k'_2(\mathbf{k}'_2),k_2(\mathbf{k}_2),t)\big[\theta(\alpha_1,\alpha'_1)+\theta(-\alpha_1,-\alpha'_1)\big]\\
&\quad+\tilde{f}_1(k_1(\mathbf{k}_1),k'_1(\mathbf{k}'_1),t)(2\pi)^3\delta^{(3)}(\mathbf{k}_2-\mathbf{k}'_2)\big[\theta(-\alpha_2,-\alpha'_2)+\theta(\alpha_2,\alpha'_2)\big]\\
&\quad+2\tilde{f}_1(k_1(\mathbf{k}_1),k'_1(\mathbf{k}'_1),t)\tilde{f}_2(k'_2(\mathbf{k}'_2),k_2(\mathbf{k}_2),t).
\end{aligned}\tag{16.1.26b}$$

We have introduced the short-hand

$$\theta(x,y)=\theta(x)\theta(y)\tag{16.1.27}$$

for the product of step functions. The reason for our choice of notation of these F's will soon become apparent. We note that the statistical contributions to the dispersive and absorptive parts of this function differ.

For completeness, the anti-time-ordered function, obtained by taking $s \to -s$ and multiplying by an overall minus sign, is

$$
\begin{aligned}
-B_0^*(q_1,q_2,m_1,m_2,s) &= 8(2\pi)^3\mu^{4-d}e^{i(q_1^0-q_2^0)t/2}\sum_{\{\alpha\}=\pm1}\int\cdots\int \mathrm{d}\Pi_{\mathbf{k}_1}^{d-1}\,\mathrm{d}\Pi_{\mathbf{k}_1'}\,\mathrm{d}\Pi_{\mathbf{k}_2}\,\mathrm{d}\Pi_{\mathbf{k}_2'}\\
&\times (2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times \frac{1}{\pi}\Big[\big[q_1^0-q_2^0-\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')+\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')\big]^2+4s^2\Big]^{-1}\\
&\times \Big[\big[\tfrac{q_1^0+q_2^0}{2}-\tfrac{\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')}{2}+\tfrac{\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')}{2}\big]^2+s^2\Big]^{-1}\\
&\times \sqrt{2E_1(\mathbf{k}_1)2E_1'(\mathbf{k}_1')2E_2(\mathbf{k}_2)2E_2'(\mathbf{k}_2')}\,e^{i[\alpha_1E_1(\mathbf{k}_1)-\alpha_1'E_1'(\mathbf{k}_1')]t/2}e^{i[\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')]t/2}\\
&\times \Big\{\Big[\tfrac{q_1^0+q_2^0}{2}-\tfrac{\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')}{2}+\tfrac{\alpha_2E_2(\mathbf{k}_2)+\alpha_2'E_2'(\mathbf{k}_2')}{2}\Big]F^{\mathrm{R}}_{\{\alpha\}}(\{k\},t)+isF^1_{\{\alpha\}}(\{k\},t)\Big\}.
\end{aligned}
\tag{16.1.28}
$$

It follows then from (10.1.22a) that the 'Hadamard' self-energy is

$$
\begin{aligned}
B_0^1(q_1,q_2,m_1,m_2,s) &= 16(2\pi)^3\mu^{4-d}e^{i(q_1^0-q_2^0)t/2}\sum_{\{\alpha\}=\pm1}\int\cdots\int \mathrm{d}\Pi_{\mathbf{k}_1}^{d-1}\,\mathrm{d}\Pi_{\mathbf{k}_1'}\,\mathrm{d}\Pi_{\mathbf{k}_2}\,\mathrm{d}\Pi_{\mathbf{k}_2'}\\
&\times (2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times \sqrt{2E_1(\mathbf{k}_1)2E_1'(\mathbf{k}_1')2E_2(\mathbf{k}_2)2E_2'(\mathbf{k}_2')}\,e^{i[\alpha_1E_1(\mathbf{k}_1)-\alpha_1'E_1'(\mathbf{k}_1')]t/2}e^{i[\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')]t/2}\\
&\times \frac{1}{\pi}\Big[\big[q_1^0-q_2^0-\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')+\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')\big]^2+4s^2\Big]^{-1}\\
&\times \Big[\big[\tfrac{q_1^0+q_2^0}{2}-\tfrac{\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')}{2}+\tfrac{\alpha_2E_2(\mathbf{k}_2)+\alpha_2'E_2'(\mathbf{k}_2')}{2}\big]^2+s^2\Big]^{-1}isF^1_{\{\alpha\}}(\{k\},t),
\end{aligned}
\tag{16.1.29}
$$

in which the conspiracy of our choice of notation for the F's becomes clear.

16.1.2 Absolutely-Ordered Functions

We turn our attention now to the 21-element; the positive-frequency, absolutely-ordered function:

$$
\begin{aligned}
&B_0^{>}(q_1,q_2,m_1,m_2,s) = -8(2\pi\mu)^{4-d}e^{i(q_1^0-q_2^0)t/2}\int\cdots\int\frac{\mathrm{d}^d k_1}{i\pi^2}\frac{\mathrm{d}^4 k_1'}{(2\pi)^4}\frac{\mathrm{d}^4 k_2}{(2\pi)^4}\frac{\mathrm{d}^4 k_2'}{(2\pi)^4}\\
&\times(2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times 4s\Big[\big[q_1^0-q_2^0-k_1^0+k_1^{0\prime}+k_2^0-k_2^{0\prime}\big]^2+4s^2\Big]^{-1}\\
&\times\Big[\big[q_1^0+q_2^0-k_1^0-k_1^{0\prime}+k_2^0+k_2^{0\prime}\big]^2+4s^2\Big]^{-1}\\
&\times 2\pi\delta(k_1^2-m_1^2)|2k_1^0|^{1/2}\Big[\theta(k_1^0,k_1^{0\prime})(2\pi)^3\delta^{(3)}(\mathbf{k}_1-\mathbf{k}_1')\\
&\qquad\qquad+\tilde{f}_1(k_1,k_1',t)\Big]e^{i(k_1^0-k_1^{0\prime})t/2}|2k_1^{0\prime}|^{1/2}2\pi\delta(k_1'^2-m_1^2)\\
&\times 2\pi\delta(k_2'^2-m_2^2)|2k_2^{0\prime}|^{1/2}\Big[\theta(k_2^{0\prime},k_2^0)(2\pi)^3\delta^{(3)}(\mathbf{k}_2'-\mathbf{k}_2)\\
&\qquad\qquad+\tilde{f}_2(k_2',k_2,t)\Big]e^{i(k_2^{0\prime}-k_2^0)t/2}|2k_2^0|^{1/2}2\pi\delta(k_2^2-m_2^2).
\end{aligned}
\tag{16.1.30}
$$

After completing the zeroth-component momentum integrals, this may be written

$$
\begin{aligned}
&B_0^{>}(q_1,q_2,m_1,m_2,s) = 16(2\pi)^3\mu^{4-d}e^{i(q_1^0-q_2^0)t/2}\\
&\times\sum_{\{\alpha\}=\pm1}\int\cdots\int\mathrm{d}\Pi_{\mathbf{k}_1}^{d-1}\,\mathrm{d}\Pi_{\mathbf{k}_1'}\,\mathrm{d}\Pi_{\mathbf{k}_2}\,\mathrm{d}\Pi_{\mathbf{k}_2'}\\
&\times(2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times\sqrt{2E_1(\mathbf{k}_1)2E_1'(\mathbf{k}_1')2E_2(\mathbf{k}_2)2E_2'(\mathbf{k}_2')}e^{i[\alpha_1E_1(\mathbf{k}_1)-\alpha_1'E_1'(\mathbf{k}_1')]t/2}e^{i[\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')]t/2}\\
&\times\frac{1}{\pi}\Big[\big[q_1^0-q_2^0-\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')+\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')\big]^2+4s^2\Big]^{-1}\\
&\times\Big[\big[\tfrac{q_1^0+q_2^0}{2}-\tfrac{\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')}{2}+\tfrac{\alpha_2E_2(\mathbf{k}_2)+\alpha_2'E_2'(\mathbf{k}_2')}{2}\big]^2+s^2\Big]^{-1}isF_{\{\alpha\}}^{>}(\{k\},t),
\end{aligned}
\tag{16.1.31}
$$

where

$$
\begin{aligned}
F_{\{\alpha\}}^{>}(\{k\},t) = &\Big[\theta(\alpha_1,\alpha_1')(2\pi)^3\delta^{(3)}(\mathbf{k}_1-\mathbf{k}_1')+\tilde{f}_1(k_1(\mathbf{k}_1),k_1'(\mathbf{k}_1'),t)\Big]\\
&\times\Big[\theta(-\alpha_2,-\alpha_2')(2\pi)^3\delta^{(3)}(\mathbf{k}_2'-\mathbf{k}_2)+\tilde{f}_2(k_2'(\mathbf{k}_2'),k_2(\mathbf{k}_2),t)\Big].
\end{aligned}
\tag{16.1.32}
$$

It follows from the discussions of Appendix A that the negative-frequency absolutely-ordered function is simply

$$
\begin{aligned}
&B_0^{<}(q_1,q_2,m_1,m_2,s) = 16(2\pi)^3\mu^{4-d}e^{i(q_1^0-q_2^0)t/2}\\
&\times\sum_{\{\alpha\}=\pm1}\int\cdots\int \mathrm{d}\Pi_{\mathbf{k}_1}^{d-1}\,\mathrm{d}\Pi_{\mathbf{k}_1'}\,\mathrm{d}\Pi_{\mathbf{k}_2}\,\mathrm{d}\Pi_{\mathbf{k}_2'}\\
&\times(2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times\sqrt{2E_1(\mathbf{k}_1)2E_1'(\mathbf{k}_1')2E_2(\mathbf{k}_2)2E_2'(\mathbf{k}_2')}e^{i[\alpha_1E_1(\mathbf{k}_1)-\alpha_1'E_1'(\mathbf{k}_1')]t/2}e^{i[\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')]t/2}\\
&\times\frac{1}{\pi}\Big[\big[q_1^0-q_2^0-\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')+\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')\big]^2+4s^2\Big]^{-1}\\
&\times\Big[\big[\tfrac{q_1^0+q_2^0}{2}-\tfrac{\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')}{2}+\tfrac{\alpha_2E_2(\mathbf{k}_2)+\alpha_2'E_2'(\mathbf{k}_2')}{2}\big]^2+s^2\Big]^{-1}isF_{\{\alpha\}}^{<}(\{k\},t),
\end{aligned}
\tag{16.1.33}
$$

where

$$
\begin{aligned}
F_{\{\alpha\}}^{<}(\{k\},t) = &\Big[\theta(-\alpha_1,-\alpha_1')(2\pi)^3\delta^{(3)}(\mathbf{k}_1-\mathbf{k}_1')+\tilde{f}_1(k_1(\mathbf{k}_1),k_1'(\mathbf{k}_1'),t)\Big]\\
&\times\Big[\theta(\alpha_2,\alpha_2')(2\pi)^3\delta^{(3)}(\mathbf{k}_2'-\mathbf{k}_2)+\tilde{f}_2(k_2'(\mathbf{k}_2'),k_2(\mathbf{k}_2),t)\Big].
\end{aligned}
\tag{16.1.34}
$$

16.1.3 Causal Functions

Having established the functions that we intended, we are now in a position to obtain their causal counterparts. Given the relations in (A.6c), the retarded and advanced B-functions are

$$
\begin{aligned}
&B_0^{\mathrm{R(A)}}(q_1,q_2,m_1,m_2,s) = -8(2\pi)^3\mu^{4-d}e^{i(q_1^0-q_2^0)t/2}\\
&\times\sum_{\{\alpha\}=\pm1}\int\cdots\int \mathrm{d}\Pi_{\mathbf{k}_1}^{d-1}\,\mathrm{d}\Pi_{\mathbf{k}_1'}\,\mathrm{d}\Pi_{\mathbf{k}_2}\,\mathrm{d}\Pi_{\mathbf{k}_2'}\\
&\times(2\pi)^3\delta^{(3)}(\mathbf{q}_1-\mathbf{k}_1+\mathbf{k}_2)(2\pi)^3\delta^{(3)}(\mathbf{q}_2-\mathbf{k}_1'+\mathbf{k}_2')\\
&\times\sqrt{2E_1(\mathbf{k}_1)2E_1'(\mathbf{k}_1')2E_2(\mathbf{k}_2)2E_2'(\mathbf{k}_2')}e^{i[\alpha_1E_1(\mathbf{k}_1)-\alpha_1'E_1'(\mathbf{k}_1')]t/2}e^{i[\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')]t/2}\\
&\times\frac{1}{\pi}\Big[\big[q_1^0-q_2^0-\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')+\alpha_2E_2(\mathbf{k}_2)-\alpha_2'E_2'(\mathbf{k}_2')\big]^2+4s^2\Big]^{-1}\\
&\times\Big[\tfrac{q_1^0+q_2^0}{2}-\tfrac{\alpha_1E_1(\mathbf{k}_1)+\alpha_1'E_1'(\mathbf{k}_1')}{2}+\tfrac{\alpha_2E_2(\mathbf{k}_2)+\alpha_2'E_2'(\mathbf{k}_2')}{2}+(-)is\Big]^{-1}F_{\{\alpha\}}^{\mathrm{R(A)}}(\{k\},t),
\end{aligned}
\tag{16.1.35}
$$

where $F_{\{\alpha\}}^{\mathrm{R}}(\{k\},t) = -F_{\{\alpha\}}^{\mathrm{A}}(\{k\},t)$.

16.2 The Thermodynamic Equilibrium Limit

In the limit of thermodynamic equilibrium, we expect to be able to recover the results from the discussions of Chapter 11, using the correspondence identified in (11.0.8). It follows that the various distribution functions satisfy the factorisation:

$$\begin{aligned} F_{\{\alpha\}}(\{k\},t) \to{}& (2\pi)^3\delta^{(3)}(\mathbf{k}_1-\mathbf{k}_1')\Big[\theta(\alpha_1,\alpha_1')-\theta(-\alpha_1,-\alpha_1')\Big] \\ &\times(2\pi)^3\delta^{(3)}(\mathbf{k}_2-\mathbf{k}_2')\Big[\theta(-\alpha_2,-\alpha_2')-\theta(\alpha_2,\alpha_2')\Big] \\ &\times F_{\rm eq}(\alpha_1,-\alpha_2,\mathbf{k}_1,\mathbf{k}_2), \end{aligned} \tag{16.2.1}$$

and

$$\begin{aligned} F^1_{\rm eq}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{k}_2) &= \Big[1+f_{\rm B}\big(\alpha_1E_1(\mathbf{k}_1)\big)\Big]\Big[1+f^c_{\rm B}\big(\alpha_2E_2(\mathbf{k}_2)\big)\Big] \\ &\quad + f_{\rm B}\big(\alpha_1E_1(\mathbf{k}_1)\big)f^c_{\rm B}\big(\alpha_2E_2(\mathbf{k}_2)\big) && \text{(16.2.2a)} \\ F^{>}_{\rm eq}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{k}_2) &= \Big[1+f_{\rm B}\big(\alpha_1E_1(\mathbf{k}_1)\big)\Big]\Big[1+f^c_{\rm B}\big(\alpha_2E_2(\mathbf{k}_2)\big)\Big], && \text{(16.2.2b)} \\ F^{<}_{\rm eq}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{k}_2) &= f_{\rm B}\big(\alpha_1E_1(\mathbf{k}_1)\big)f^c_{\rm B}\big(\alpha_2E_2(\mathbf{k}_2)\big), && \text{(16.2.2c)} \\ F^{\rm R}_{\rm eq}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{k}_2) &= 1+f_{\rm B}\big(\alpha_1E_1(\mathbf{k}_1)\big)+f^c_{\rm B}\big(\alpha_2E_2(\mathbf{k}_2)\big), && \text{(16.2.2d)} \end{aligned}$$

After performing the now superfluous phase-space integrations and summations and redefining $\alpha_2 \to -\alpha_2$ for aesthetics, we obtain the following set of 'equilibrium' functions:

$$\begin{aligned} &B_0(-B_0^*)(q_1,q_2,m_1,m_2,s) = (2\pi)^4\frac{1}{\pi}\frac{1}{\big[q_1^0-q_2^0\big]^2+4s^2}e^{i(q_1^0-q_2^0)t/2}\delta^{(3)}(\mathbf{q}_1-\mathbf{q}_2) \\ &\times(2\pi\mu)^{4-d}\sum_{\alpha_1,\alpha_2=\pm1}\int \mathrm{d}^{d-1}\mathbf{k}_1\,\frac{1}{\pi}\frac{\alpha_1\alpha_2}{E_1(\mathbf{k}_1)E_2(\mathbf{q}_1-\mathbf{k}_1)} \\ &\times\Big[\big[\tfrac{q_1^0+q_2^0}{2}-\alpha_1E_1(\mathbf{k}_1)-\alpha_2E_2(\mathbf{q}_1-\mathbf{k}_1)\big]^2+s^2\Big]^{-1} \\ &\times\Big\{-(+)\Big[\tfrac{q_1^0+q_2^0}{2}-\alpha_1E_1(\mathbf{k}_1)-\alpha_2E_2(\mathbf{q}_1-\mathbf{k}_1)\Big]F^{\rm R}_{\rm eq}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{q}_1-\mathbf{k}_1) \\ &+isF^1_{\rm eq}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{q}_1-\mathbf{k}_1)\Big\}, \end{aligned} \tag{16.2.3}$$

$$B_0^{>,<,1}(q_1,q_2,m_1,m_2,s) = 2(2\pi)^4\frac{1}{\pi}\frac{1}{\left[q_1^0-q_2^0\right]^2+4s^2}e^{i(q_1^0-q_2^0)t/2}\delta^{(3)}(\mathbf{q}_1-\mathbf{q}_2)$$
$$\times(2\pi\mu)^{4-d}\sum_{\alpha_1,\alpha_2=\pm1}\int \mathrm{d}^{d-1}\mathbf{k}_1\,\frac{1}{\pi}\frac{\alpha_1\alpha_2}{E_1(\mathbf{k}_1)E_2(\mathbf{q}_1-\mathbf{k}_1)}$$
$$\times\left[\left[\tfrac{q_1^0+q_2^0}{2}-\alpha_1E_1(\mathbf{k}_1)-\alpha_2E_2(\mathbf{q}_1-\mathbf{k}_1)\right]^2+s^2\right]^{-1}$$
$$\times isF_{\mathrm{eq}}^{>,<,1}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{q}_1-\mathbf{k}_1), \tag{16.2.4}$$
$$B_0^{\mathrm{R(A)}}(q_1,q_2,m_1,m_2,s) = -(2\pi)^4\frac{1}{\pi}\frac{1}{\left[q_1^0-q_2^0\right]^2+4s^2}e^{i(q_1^0-q_2^0)t/2}\delta^{(3)}(\mathbf{q}_1-\mathbf{q}_2)$$
$$\times(2\pi\mu)^{4-d}\sum_{\alpha_1,\alpha_2=\pm1}\int \mathrm{d}^{d-1}\mathbf{k}_1\,\frac{1}{\pi}\frac{\alpha_1\alpha_2}{E_1(\mathbf{k}_1)E_2(\mathbf{q}_1-\mathbf{k}_1)}$$
$$\times\left[\tfrac{q_1^0+q_2^0}{2}-\alpha_1E_1(\mathbf{k}_1)-\alpha_2E_2(\mathbf{q}_1-\mathbf{k}_1)+(-)is\right]^{-1}$$
$$\times F_{\mathrm{eq}}^{\mathrm{R}}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{q}_1-\mathbf{k}_1). \tag{16.2.5}$$

The word 'equilibrium' has deliberately been singled-out with inverted commas, because this is in fact *not* an equilibrium result. For late times, we may use the final value theorem

$$\lim_{t\to\infty}F(t)=\lim_{s\to0}s\mathcal{L}_t\big[F\big](s) \tag{16.2.6}$$

to obtain the true, time-invariant equilibrium functions:

$$B_0(-B_0^*)(q_1,q_2,m_1,m_2) = (2\pi)^4\delta^{(4)}(q_1-q_2)(2\pi\mu)^{4-d}$$
$$\times\sum_{\alpha_1,\alpha_2=\pm1}\int \mathrm{d}^{d-1}\mathbf{k}_1\,\frac{\alpha_1\alpha_2}{E_1(\mathbf{k}_1)E_2(\mathbf{q}_1-\mathbf{k}_1)}\Bigg[-(+)\frac{1}{2\pi}\frac{F_{\mathrm{eq}}^{\mathrm{R}}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{q}_1-\mathbf{k}_1)}{q_1^0-\alpha_1E_1(\mathbf{k}_1)-\alpha_2E_2(\mathbf{q}_1-\mathbf{k}_1)}$$
$$+\frac{i}{2}\,\delta\big(q_1^0-\alpha_1E_1(\mathbf{k}_1)-\alpha_2E_2(\mathbf{q}_1-\mathbf{k}_1)\big)F_{\mathrm{eq}}^{1}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{q}_1-\mathbf{k}_1)\Bigg], \tag{16.2.7}$$
$$B_0^{>,<,1}(q_1,q_2,m_1,m_2) = i(2\pi)^4\delta^{(4)}(q_1-q_2)(2\pi\mu)^{4-d}$$
$$\times\sum_{\alpha_1,\alpha_2=\pm1}\int \mathrm{d}^{d-1}\mathbf{k}_1\,\frac{\alpha_1\alpha_2}{E_1(\mathbf{k}_1)E_2(\mathbf{q}_1-\mathbf{k}_1)}$$
$$\times\delta\big(q_1^0-\alpha_1E_1(\mathbf{k}_1)-\alpha_2E_2(\mathbf{q}_1-\mathbf{k}_1)\big)F_{\mathrm{eq}}^{>,<,1}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{q}_1-\mathbf{k}_1), \tag{16.2.8}$$

$$B_0^{\mathrm{R(A)}}(q_1,q_2,m_1,m_2) = -(2\pi)^4\delta^{(4)}(q_1-q_2)(2\pi\mu)^{4-d}$$
$$\times \sum_{\alpha_1,\alpha_2=\pm1}\int \mathrm{d}^{d-1}\mathbf{k}_1\,\frac{\alpha_1\alpha_2}{E_1(\mathbf{k}_1)E_2(\mathbf{q}_1-\mathbf{k}_1)}$$
$$\times \frac{1}{2\pi}\frac{1}{q_1^0-\alpha_1E_1(\mathbf{k}_1)-\alpha_2E_2(\mathbf{k}_2)+(-)i\epsilon}F^{\mathrm{R}}_{\mathrm{eq}}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{q}_1-\mathbf{k}_1), \tag{16.2.9}$$

all of which are consistent with known results calculated in the imaginary-time formalism or the more familiar equilibrium CTP formalism.

Returning to (16.2.3) and making the inverse Laplace transformations, we find

$$B_0(-B_0^*)s(q_1,q_2,m_1,m_2,t) = (2\pi)^4\delta^{(3)}(\mathbf{q}_1-\mathbf{q}_2)(2\pi\mu)^{4-d}e^{i(q_1^0-q_2^0)t/2}$$
$$\times \sum_{\alpha_1,\alpha_2=\pm1}\int \mathrm{d}^{d-1}\mathbf{k}_1\,\frac{\alpha_1\alpha_2}{E_1E_2}$$
$$\times\Bigg\{-(+)\frac{1}{2\pi}\frac{\frac{q_1^0+q_2^0}{2}-\alpha_1E_1-\alpha_2E_2}{\big[q_1^0-\alpha_1E_1-\alpha_2E_2\big]\big[q_2^0-\alpha_1E_1-\alpha_2E_2\big]}$$
$$\times\Big[\delta_t(q_1^0-q_2^0)-\delta_t\big(q_1^0+q_2^0-2\alpha_1E_1-2\alpha_2E_2\big)\Big]F^{\mathrm{R}}_{\mathrm{eq}}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{q}_1-\mathbf{k}_1)$$
$$+\frac{i}{2}\delta_t\big(q_1^0-\alpha_1E_1-\alpha_2E_2\big)\delta_t\big(q_2^0-\alpha_1E_1-\alpha_2E_2\big)F^{1}_{\mathrm{eq}}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{q}_1-\mathbf{k}_1)\Bigg\}, \tag{16.2.10}$$

$$B_0^{>,<,1}(q_1,q_2,m_1,m_2,t) = i(2\pi)^4\delta^{(3)}(\mathbf{q}_1-\mathbf{q}_2)(2\pi\mu)^{4-d}e^{i(q_1^0-q_2^0)t/2}$$
$$\times \sum_{\alpha_1,\alpha_2=\pm1}\int \mathrm{d}^{d-1}\mathbf{k}_1\,\frac{\alpha_1\alpha_2}{E_1E_2}$$
$$\times\,\delta_t\big(q_1^0-\alpha_1E_1-\alpha_2E_2\big)\delta_t\big(q_2^0-\alpha_1E_1-\alpha_2E_2\big)F^{>,<,1}_{\mathrm{eq}}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{q}_1-\mathbf{k}_1), \tag{16.2.11}$$

$$
\begin{aligned}
B_0^{\mathrm{R(A)}}(q_1,q_2,m_1,m_2,t) &= (2\pi)^4\delta^{(3)}(\mathbf{q}_1-\mathbf{q}_2)(2\pi\mu)^{4-d}e^{i(q_1^0-q_2^0)t/2} \\
&\times \sum_{\alpha_1,\alpha_2=\pm 1}\int \mathrm{d}^{d-1}\mathbf{k}_1\,\frac{\alpha_1\alpha_2}{E_1E_2} \\
&\times \Bigg\{ -\frac{1}{2\pi}\frac{\frac{q_1^0+q_2^0}{2}-\alpha_1E_1-\alpha_2E_2}{\big[q_1^0-\alpha_1E_1-\alpha_2E_2\big]\big[q_2^0-\alpha_1E_1-\alpha_2E_2\big]} \\
&\qquad \times\Big[\delta_t(q_1^0-q_2^0)-\delta_t\big(q_1^0+q_2^0-2\alpha_1E_1-2\alpha_2E_2\big)\Big] \\
&+(-)\frac{i}{2}\delta_t\big(q_1^0-\alpha_1E_1-\alpha_2E_2\big)\delta_t\big(q_2^0-\alpha_1E_1-\alpha_2E_2\big)\Bigg\}F_{\mathrm{eq}}^{\mathrm{R}}(\alpha_1,\alpha_2,\mathbf{k}_1,\mathbf{q}_1-\mathbf{k}_1).
\end{aligned}
\tag{16.2.12}
$$

We have omitted the arguments of $E_1 \equiv E_1(\mathbf{k}_1)$ and $E_2 \equiv E_2(\mathbf{q}_1-\mathbf{k}_1)$ for convenience.

17 Thermalisation of a Massive Scalar

With the formalism now in place, we shall consider a simple toy model involving one massive real scalar field (Φ) and one less-massive pair of complex scalar fields ($\chi^\dagger$, χ), described by the Lagrangian density

$$\begin{aligned}\mathcal{L}(x) = &\tfrac{1}{2}\partial_\mu\Phi(x)\partial^\mu\Phi(x) - \tfrac{1}{2}M^2\Phi^2(x) + \partial_\mu\chi^\dagger(x)\partial^\mu\chi(x) - m^2\chi^\dagger(x)\chi(x) \\ &- g\Phi(x)\chi^\dagger(x)\chi(x) - \tfrac{1}{4}\lambda\big[\chi^\dagger(x)\chi(x)\big]^2, \end{aligned} \tag{17.0.1}$$

where $M \gg m$.

17.1 Feynman Rules

Following the arguments of Chapters 9 and 10, we obtain the following *modified* Feynman rules for this toy model:

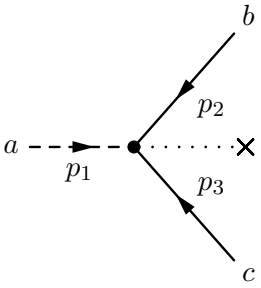
- sum over all topologically-distinct diagrams at a given order in perturbation theory;
- to each Φ line assign a factor of

$$= i\Delta_\Phi^{0,ab}(p, p', t); \tag{17.1.1}$$

- to each χ line assign a factor of

$$= i\Delta_{\chi}^{0,ab}(p,p',t); \tag{17.1.2}$$

- to each three-point Φ vertex assign a factor of

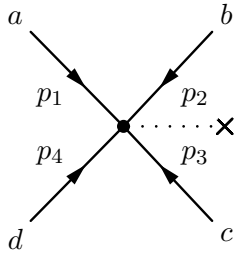


$$= -ig\eta_{abc}(2\pi)^4\delta_t\big(\textstyle\sum_{i=1}^3 p_{0,i}\big)\delta^{(3)}\big(\textstyle\sum_{i=1}^3 \mathbf{p}_i\big),$$

where we recall the definition

$$\delta_t(p_0 - p_0') = \frac{t}{2\pi}\,\mathrm{sinc}\Big[\Big(\frac{p_0 - p_0'}{2}\Big)t\Big]; \tag{17.1.3}$$

- to each four-point χ vertex assign a factor of



$$= -i\lambda\eta_{abcd}(2\pi)^4\delta_t\big(\textstyle\sum_{i=1}^4 p_{0,i}\big)\delta^{(3)}\big(\textstyle\sum_{i=1}^4 \mathbf{p}_i\big);$$

- for each vertex attached to an external leg (amputated or otherwise) with four momentum p, associate a phase factor

$$e^{ip_0 t/2},$$

where p is the momentum flowing into the vertex, see Chapter 10;

- contract all internal CTP indices;

- for each contracted pair of CTP indices, integrate over the corresponding four-momentum with the measure,
$$\int \frac{\mathrm{d}^4 p}{(2\pi)^4};$$
- multiply by the symmetry factor.

We emphasise the modification that has occurred in the vertices, where the more familiar energy-conserving delta function has been replaced by the weight function in (9.3.3). This loss of microscopic energy conservation results from Heisenberg's uncertainty principle due to our finite, macroscopic observation time t. As a result, the vertices are now time-dependent, vanishing in the limit $t \to 0$ as we should expect. We also note that this modification has resulted in a doubling of the number of integrations with respect to the zero-temperature case.

At one-loop, we have three diagrams: the local χ self-energy, shown in Figure 17.1:

$$\begin{aligned} i\Pi^{\chi(1)}_{\mathrm{loc},ab}(q,q',t) = \frac{-i\lambda}{2!}(2\pi\mu)^{2\epsilon} e^{i(q_0-q_0')t/2} \iint \frac{\mathrm{d}^d k}{(2\pi)^d}\frac{\mathrm{d}^4 k'}{(2\pi)^4} \\ \times (2\pi)^4 \delta_t^{(4)}(q-q'-k+k')\eta_{abcd} i\Delta_\chi^{0,cd}(k,k',t); \end{aligned} \tag{17.1.4}$$

and the non-local diagrams, shown in Figure 17.2:

$$\begin{aligned} i\Pi^{\Phi(1)}_{ab}(q,q',t) = \frac{(-ig)^2}{2!}(2\pi\mu)^{2\epsilon} e^{i(q_0-q_0')t/2} \int\cdots\int \frac{\mathrm{d}^d k_1}{(2\pi)^d}\frac{\mathrm{d}^4 k_1'}{(2\pi)^4}\frac{\mathrm{d}^4 k_2}{(2\pi)^4}\frac{\mathrm{d}^4 k_2'}{(2\pi)^4} \\ \times (2\pi)^4 \delta_t^{(4)}(q-k_1-k_2)(2\pi)^4\delta_t^{(4)}(q'-k_1'-k_2') \\ \times \eta_{acd} i\Delta_\chi^{0,ce}(k_1,k_1',t) i\Delta_\chi^{0,fd}(k_2',k_2,t)\eta_{efb}. \end{aligned} \tag{17.1.5}$$

and

$$\begin{aligned} i\Pi^{\chi(1)}_{ab}(q,q',t) = \frac{(-ig)^2}{2!}(2\pi\mu)^{2\epsilon} e^{i(q_0-q_0')t/2} \int\cdots\int \frac{\mathrm{d}^d k_1}{(2\pi)^d}\frac{\mathrm{d}^4 k_1'}{(2\pi)^4}\frac{\mathrm{d}^4 k_2}{(2\pi)^4}\frac{\mathrm{d}^4 k_2'}{(2\pi)^4} \\ \times (2\pi)^4 \delta_t^{(4)}(q-k_1-k_2)(2\pi)^4\delta_t^{(4)}(q'-k_1'-k_2') \\ \times \eta_{acd} i\Delta_\chi^{0,fd}(k_1,k_1',t) i\Delta_\Phi^{0,fd}(k_2',k_2,t)\eta_{efb}. \end{aligned} \tag{17.1.6}$$

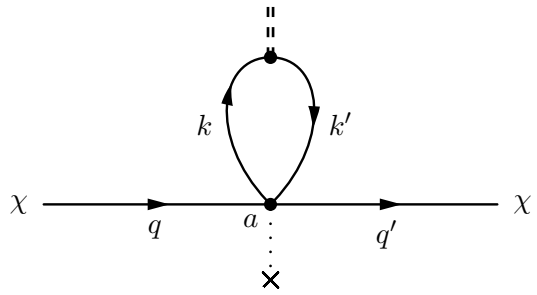
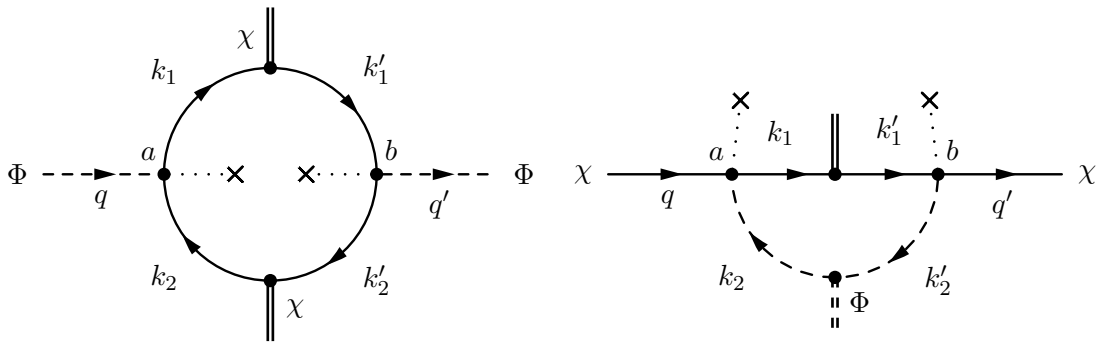


Figure 17.1: One-loop, local χ self-energy: $i\Pi^{\chi(1)}_{\mathrm{loc},ab}(q,q',t) \propto \eta_{ab}$.



(a) $i\Pi^{\Phi(1)}_{ab}(q,q',t)$ (b) $i\Pi^{\chi(1)}_{ab}(q,q',t)$

Figure 17.2: One-loop, non-local Φ and χ self-energies.

These loop integrals may be performed using the techniques and results outlined in Chapter 16.

17.2 Time-Dependent Width

We consider the following situation: we imagine preparing two isolated but coincident subsystems $\mathscr{S}_\Phi$ and $\mathscr{S}_\chi$, both separately in thermodynamic equilibrium and at the same temperature T, with all interactions turned off. $\mathscr{S}_\Phi$ comprises only the real scalar field and $\mathscr{S}_\chi$, only the complex scalar. At macroscopic time $t = 0$, we

turn on the interactions and allow the system $\mathscr{S} = \mathscr{S}_\Phi \cup \mathscr{S}_\chi$ to re-thermalise. For definiteness, we shall take the thermodynamic temperature $T = 10\,\mathrm{GeV}$, the mass of the massive scalar $M = 1\,\mathrm{GeV}$ and the mass of complex scalar $m = 0.01\,\mathrm{GeV}$. When it is relevant to do so, we shall take $g = 0.1\,\mathrm{GeV}$.

The free propagators of both fields at time $t = 0$ are the equilibrium propagators in (11.0.9) and (13.1.25), containing the Bose-Einstein distributions at temperature T. We shall take the chemical potential of the complex scalar to be vanishingly small in comparison to its mass, i.e. $\mu \ll m$, and ignore the local self-interactions, such that $f_\chi(|\mathbf{p}|, 0) = f^c_\chi(|\mathbf{p}|, 0) = f_{\mathrm{B}}\big(E_\chi(\mathbf{p})\big)$. In order to get a handle on the behaviour of the time-dependent vertices, let us first assume that the heat bath of χ's is sufficiently large that it is unperturbed by the addition of the real scalar. In this case, we may assume that the number density of χ's remains unchanged, so that the free equilibrium χ propagators in (13.1.25) persist for all times.

By the optical theorem, the width of the massive scalar Φ is defined in terms of the absorptive part of the retarded self-energy via

$$\Gamma^\Phi(q_1, q_2, t) = \frac{1}{M}\mathrm{Im}\,\Pi^\Phi_{\mathrm{R}}(q_1, q_2, t), \tag{17.2.1}$$

in which we recall that

$$\mathrm{Im}\,\Pi^\Phi_{\mathrm{R}}(q_1, q_2, t) = \frac{1}{2i}\Big(\Pi^\Phi_{>}(q_1, q_2, t) - \Pi^\Phi_{<}(q_1, q_2, t)\Big). \tag{17.2.2}$$

At one-loop, these self-energies are given by (17.1.5).

Introducing the relative and central momenta $Q = q_1 - q_2$ and $q = (q_1 + q_2)/2$ and using the results in Appendix 16.2, the Laplace transform with respect to t of

the one-loop, massive scalar width is

$$\Gamma^{\Phi(1)}(q+Q/2,q-Q/2,s) = (2\pi)^4\frac{1}{\pi}\frac{s}{Q_0^2+4s^2}e^{iQ_0t/2}\delta^{(3)}(\mathbf{Q})$$
$$\times\frac{g^2}{32\pi^2M}\sum_{\alpha_1,\alpha_2=\pm1}\int \mathrm{d}^3\mathbf{k}\frac{1}{\pi}\frac{\alpha_1\alpha_2}{E_\chi(\mathbf{k})E_\chi(\mathbf{q}-\mathbf{k})}\frac{1+f_\mathrm{B}\big(\alpha_1E(\mathbf{k})\big)+f_\mathrm{B}\big(\alpha_2E_\chi(\mathbf{q}-\mathbf{k})\big)}{\big(q_0^2-\alpha_1E_\chi(\mathbf{k})-\alpha_2E_\chi(\mathbf{q}-\mathbf{k})\big)^2+s^2}. \tag{17.2.3}$$

Taking the inverse Wigner transform with respect to Q in the equal-time limit and performing the inverse Laplace transform with respect to s, we obtain

$$\Gamma^{\Phi(1)}(q,t) = \frac{g^2}{64\pi^2M}\sum_{\alpha_1,\alpha_2=\pm1}\int \mathrm{d}^3\mathbf{k}\,\frac{\alpha_1\alpha_2}{E_\chi(\mathbf{k})E_\chi(\mathbf{q}-\mathbf{k})}$$
$$\times\frac{t}{\pi}\,\mathrm{sinc}\big[\big(q_0-\alpha_1E_\chi(\mathbf{k})-\alpha_2E_\chi(\mathbf{q}-\mathbf{k})\big)t\big]\big[1+f_\mathrm{B}\big(\alpha_1E(\mathbf{k})\big)+f_\mathrm{B}\big(\alpha_2E_\chi(\mathbf{q}-\mathbf{k})\big)\big]. \tag{17.2.4}$$

In the limit, $t\to\infty$, the sinc function yields the more familiar delta function

$$\lim_{t\to\infty}\frac{t}{\pi}\,\mathrm{sinc}\big[\big(q_0-\alpha_1E_1(\mathbf{k})-\alpha_2E_2(\mathbf{q}-\mathbf{k})\big)t\big] = \delta\big(q_0-\alpha_1E_1(\mathbf{k})-\alpha_2E_2(\mathbf{q}-\mathbf{k})\big) \tag{17.2.5}$$

and we may quickly convince ourselves that we do indeed obtain the correct equilibrium result. We have generalised

$$E_1 = \sqrt{|\mathbf{k}|^2+m_1^2}, \tag{17.2.6a}$$
$$E_2 = \sqrt{|\mathbf{k}|^2-2|\mathbf{k}||\mathbf{q}|\cos\theta+|\mathbf{q}|^2+m_2^2} \tag{17.2.6b}$$

to different masses for later convenience. For clarity, however, we emphasise that we ultimately take $m_1=m_2=m$ in all numerical analyses.

Figure 17.3 contains a series of contour plots of the differential, one-loop on-shell Φ width evaluated over the dominant region of the $|\mathbf{k}|$, θ phase space. For late times, the integrand is highly oscillatory and, as we should expect, the dominant peak of the sinc function approaches the region of phase space permitted in the limit

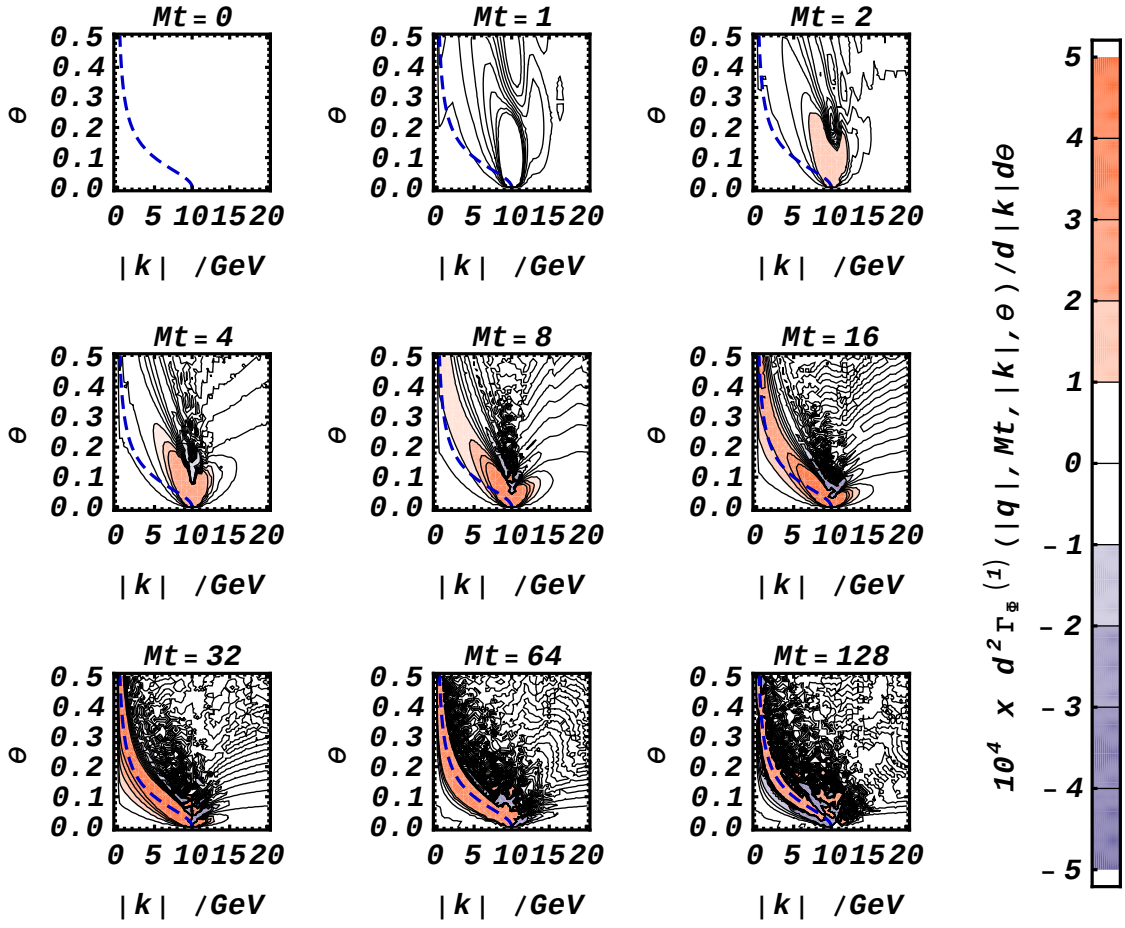


Figure 17.3: Contour plots of the differential, one-loop Φ width, evaluated for a series of dimensionless times Mt over the dominant region of the $|\mathbf{k}|, \theta$ phase space for $q^2 = M^2$ on-shell and $|\mathbf{q}| = 10\,\mathrm{GeV}$. The region of phase-space permitted in the $t \to \infty$ limit is shown by the blue, dashed line, corresponding to the delta function in (17.2.5).

$t \to \infty$, cf. (17.2.5), defined by

$$|\mathbf{k}| = \frac{M^2|\mathbf{q}|\cos\theta + \sqrt{\left[|\mathbf{q}|^2 + M^2\right]\left[M^4 - 4m^2\left(M^2 + |\mathbf{q}|^2\sin^2\theta\right)\right]}}{2\left(M^2 + |\mathbf{q}|^2\sin^2\theta\right)}. \tag{17.2.7}$$

For early times, the permitted region of phase space is greatly expanded. For later times, the increasing frequency of oscillation and the narrowing peak, lying along a curve in the phase space, leaves Monte Carlo methods unsuitable for performing these phase-space integrals in their initial form—the integral is systematically underestimated. In order to proceed further, we need a means of dealing with the kinematics in the absence of the more familiar delta-function constraint.

17.3 Generalised Two-Body Decay Kinematics

At zero temperature and density, we normally determine the two-body decay kinematics by Lorentz-boosting to the rest frame of the decaying particle. However, at finite temperature, the dependence on the thermodynamic temperature of the heat bath breaks the Lorentz covariance of the integral and as such, we cannot eliminate dependence upon the the three-momentum of the decaying particle by an appropriate Lorentz boost — the dependence will reappear in the 'boosted' temperature:

$$T' = \gamma\, T, \tag{17.3.1}$$

where, for the massive scalar,

$$\gamma = \left(1 + \frac{|\mathbf{q}|^2}{M^2}\right)^{1/2}. \tag{17.3.2}$$

As a result, we are forced to analyse the kinematics of the two-body decay in the rest frame of the heat bath (or *laboratory frame*), which we shall define to be the frame in which $\langle\mathbf{k}\rangle$ (the EEV of the three-momentum operator) is minimised. For an isotropic heat bath, this is the frame in which $\langle\mathbf{k}\rangle = \mathbf{0}$, that is the *comoving* frame.

We proceed by making the time-dependent Jacobian transformation

$$u \equiv \big(q_0 - \alpha_1 E_1 - \alpha_2 E_2\big)t, \tag{17.3.3}$$

which may be interpreted in terms of energy *borrowed from* or *lent to* the heat bath and which we shall hereafter refer to as the *evanescent action* of the process for the reason that its non-zero values extend the kinematically-allowed region of phase space beyond that permitted by energy-momentum conservation. We define the *evanescent energy*

$$q_u(t) \equiv q_0 - \frac{u}{t}, \tag{17.3.4}$$

which satisfies

$$\lim_{u/t\to 0} q_u(t) = q_0. \tag{17.3.5}$$

With this substitution, we obtain the more familiar-looking kinematic constraint

$$q_u(t) - \alpha_1 E_1 - \alpha_2 E_2 = 0. \tag{17.3.6}$$

Since u can take large positive values, $q_u(t)$ is not necessarily restricted to positive values for early times even for $q_0 = \sqrt{|\mathbf{q}|^2 + M^2}$ on-shell.

Solving for the internal momentum of the loop, we find

$$|\mathbf{k}|(t) = \frac{1}{2\big(q_u^2(t) - |\mathbf{q}|^2\cos^2\theta\big)}\Big[|\mathbf{q}|\cos\theta\big(q_u^2(t) - |\mathbf{q}|^2 + m_1^2 - m_2^2\big) \pm q_u(t)\sqrt{\lambda\big(q_u^2(t) - |\mathbf{q}|^2, m_1^2, m_2^2\big) - 4m_1^2|\mathbf{q}|^2\sin^2\theta}\Big], \tag{17.3.7}$$

where

$$\lambda(x,y,z) = (x-y-z)^2 - 4yz. \tag{17.3.8}$$

After some manipulation, we then obtain the energies

$$E_1(t) = \frac{\alpha_1}{2\big(q_u^2(t) - |\mathbf{q}|^2\cos^2\theta\big)}\Big[q_u(t)\big(q_u^2(t) - |\mathbf{q}|^2 + m_1^2 - m_2^2\big) \pm |\mathbf{q}|\cos\theta\sqrt{\lambda\big(q_u^2(t) - |\mathbf{q}|^2, m_1^2, m_2^2\big) - 4m_1^2|\mathbf{q}|^2\sin^2\theta}\Big], \quad (17.3.9a)$$

$$E_2(t) = \frac{\alpha_2}{2\big(q_u^2(t) - |\mathbf{q}|^2\cos^2\theta\big)}\Big[q_u(t)\big(q_u^2(t) - |\mathbf{q}|^2\cos 2\theta - m_1^2 + m_2^2\big) \mp |\mathbf{q}|\cos\theta\sqrt{\lambda\big(q_u^2(t) - |\mathbf{q}|^2, m_1^2, m_2^2\big) - 4m_1^2|\mathbf{q}|^2\sin^2\theta}\Big], \quad (17.3.9b)$$

where the overall factors of α_1 and α_2 are necessary to satisfy the initial constraint (17.3.6). It is clear that these results collapse to the familiar kinematics of equilibrium field theory in the limit $u/t \to 0$.

For $t > 0$, the width of the massive scalar, keeping for now m_1 and m_2 distinct, is then

$$\Gamma_\Phi^{(1)}(q, Z_0 = 0, t) = \frac{g^2}{64\pi^2 M}\sum_{\alpha_1,\alpha_2,b=\pm 1}\int_0^\pi \mathrm{d}\theta\int_{u_-(t)}^{u_+(t)}\mathrm{d}u\ \mathrm{sinc}(u)\,\frac{\sin\theta}{\big(q_u^2(t) - |\mathbf{q}|^2\cos^2\theta\big)^2} \times \frac{1}{\sqrt{\lambda\big(q_u^2(t) - |\mathbf{q}|^2, m_1^2, m_2^2\big) - 4m_1^2|\mathbf{q}|^2\sin^2\theta}}\Big[|\mathbf{q}|\cos\theta\big(q_u^2(t) - |\mathbf{q}|^2 + m_1^2 - m_2^2\big) + bq_u(t)\sqrt{\lambda\big(q_u^2(t) - |\mathbf{q}|^2, m_1^2, m_2^2\big) - 4m_1^2|\mathbf{q}|^2\sin^2\theta}\Big]^2 \times \alpha_1\alpha_2\big[1 + f_\mathrm{B}\big(\alpha_1 E_1(t)\big) + f_\mathrm{B}\big(\alpha_2 E_2(t)\big)\big]. \quad (17.3.10)$$

The reality of the internal momentum requires that the discriminant

$$\lambda\big(q_u^2(t) - |\mathbf{q}|^2, m_1^2, m_2^2\big) - 4m_1^2|\mathbf{q}|^2\sin^2\theta \geq 0. \quad (17.3.11)$$

Furthermore, we require $|\mathbf{k}|(t) \geq 0$, $E_1(t) \geq m_1$ and $E_2(t) \geq m_2$. For $t = 0$, the range of integration over u collapses to zero and given the analytic behaviour of the integrand at these bounds, the integral vanishing, as we should expect. For $t > 0$,

	$\alpha_1 = \alpha_2 = +1$	$\alpha_1 = -\alpha_2$	$\alpha_1 = \alpha_2 = -1$
$u_+(t)$	$\omega_0(q, \alpha_1, \alpha_2)t$	$\omega_0(q, \alpha_1, \alpha_2)t$	$+\infty$
$u_-(t)$	$-\infty$	0	$\omega_0(q, \alpha_1, \alpha_2)t$

Table 17.1: Limits of integration of the evanescent action u for each of the four processes contributing to the non-equilibrium thermal width for $t > 0$, where the angular frequency $\omega_0(q, \alpha_1, \alpha_2)$ is as defined in (17.3.12).

the limits of integration are given in Table 17.1, where we have defined

$$\omega_0(q, \alpha_1, \alpha_2) = q_0 - \big(\alpha_1 m_1 + \alpha_2 m_2\big)\left(1 + \frac{|\mathbf{q}|^2}{\big(m_1 + m_2\big)^2}\right)^{1/2}, \tag{17.3.12}$$

which is the angular frequency of the sine-integral-like oscillations of the integral. It follows for on-shell decay modes that

$$\omega_0(|\mathbf{q}|, \alpha_1, \alpha_2) \equiv \omega_0(q, \alpha_1, \alpha_2)\big|_{q^2=M^2} = \sqrt{|\mathbf{q}|^2 + M^2} - \sqrt{|\mathbf{q}|^2 + \big(m_1 + m_2\big)^2}, \tag{17.3.13}$$

such that the evolution of the phase space for on-threshold decays with $M^2 = (m_1 + m_2)^2$ is *critically damped*. We note that in the large momentum limit, $|\mathbf{q}| >> M$,

$$\omega_0(|\mathbf{q}|, \alpha_1, \alpha_2) = \frac{M^2 - \big(m_1 + m_2\big)^2}{2|\mathbf{q}|}, \tag{17.3.14}$$

such that the evolution of the phase space for high-momentum modes is similarly critically damped.

The summation over α_1 and α_2 yields four distinct contributions to the decay width: for $\alpha_1 = \alpha_2 = +1$, we obtain the contribution from the familiar $1 \to 2$-body decay process (see Figure 17.5a); for $\alpha_1 = -\alpha_2$, we obtain the $2 \to 1$-body *Landau damping* contributions (see Figure 17.5b and [82]); and for $\alpha_1 = \alpha_2 = -1$, we obtain the $3 \to 0$-body process shown in Figure 17.5c, in which the decay 'products' appear in the *initial state* along with the decaying particle — we shall refer to this process as *annihilation*. It is important to note that this contribution is not the production

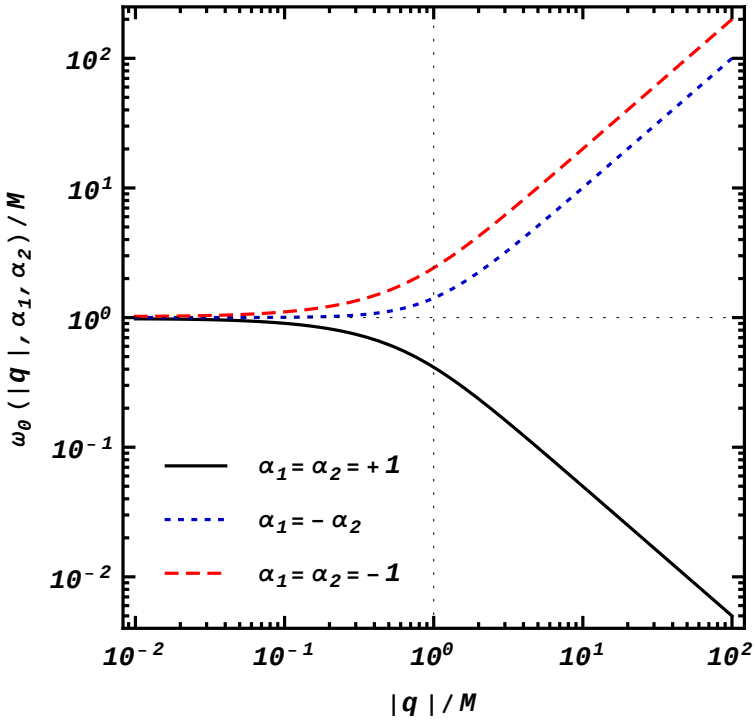
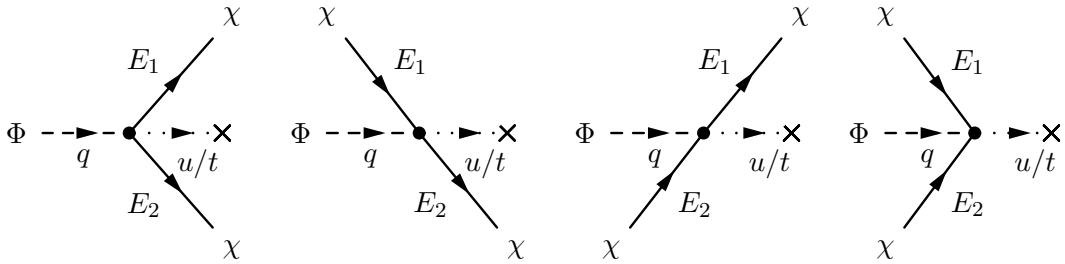


Figure 17.4: Plot of $\omega_0(|\mathbf{q}|, \alpha_1, \alpha_2)/M$ *against* $|\mathbf{q}|/M$ *for* $q^2 = M^2$ *on-shell and* $m_1 = m_2 = m = 0.01\,\mathrm{GeV}$. *We see that the phase-space for Landau damping (blue dashed) and* $3 \to 0$ *annihilation (red dotted) processes is highly oscillatory. On the other hand, the same modulation in the* $1 \to 2$ *decay process (solid black) is critically damped for large momenta, as we expect from (17.3.14).*



(a) $1 \to 2$ decay. (b) $2 \to 1$ Landau damping. (c) $3 \to 0$ annihilation.

Figure 17.5: (a): the familiar $1 \to 2$*-body decay contribution to the time-dependent thermal decay width; (b)–(d): the evanescent contributions to the time-dependent thermal decay width.*

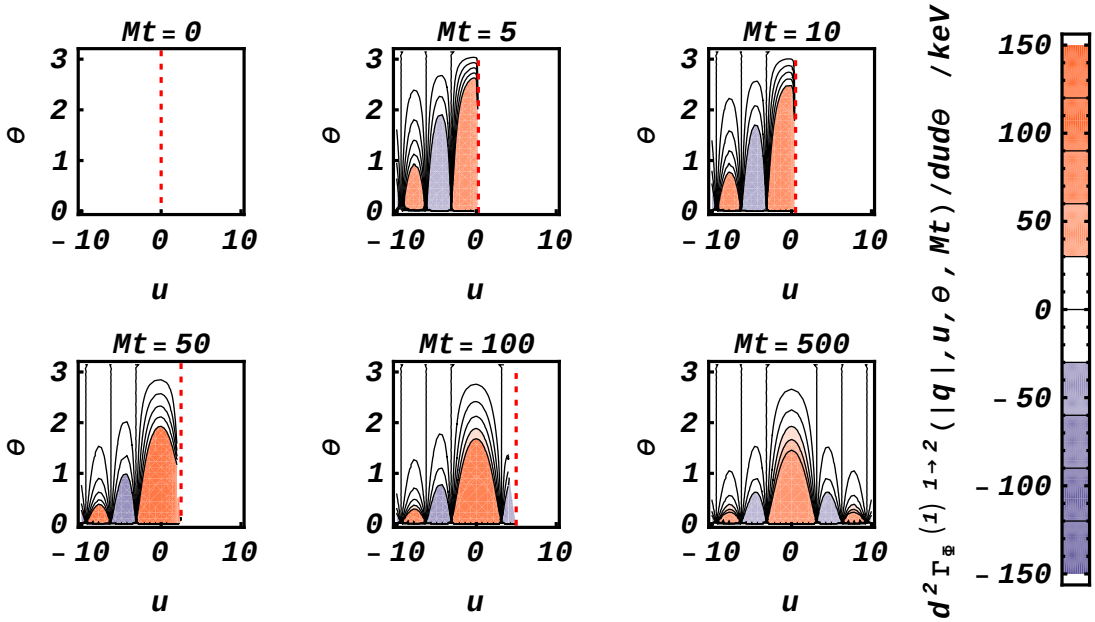


Figure 17.6: Contour plots of the $\alpha_1 = \alpha_2 = +1$, $1 \to 2$-body decay contribution to the differential, one-loop Φ width, evaluated for a series of dimensionless times Mt over the dominant region of u, θ phase space for $q^2 = M^2$ on-shell and $|\mathbf{q}| = 10\,\mathrm{GeV}$. The solid excluded regions to the right of the red-dotted line lie exterior to the limits of integration in u. We see that the domain of integration grows to encompass the full domain of the sinc function in the large-time limit.

rate, which would be given by the transformation $q \to -q$ of the decay width with $\alpha_1 = \alpha_2 = -1$. We note that for late times, the Landau damping and annihilation processes are kinematically disallowed, as we would expect, and are permitted only in the *evanescent regime* at early times.

Figures 17.6, 17.7 and 17.8 contain contour plots of the $1 \to 2$-body decay ($\alpha_1 = \alpha_2 = +1$), $3 \to 0$-body annihilation ($\alpha_1 = \alpha_2 = -1$) and Landau damping ($\alpha_1 - \alpha_2$) contributions to the integrand in the dominant region of the u, θ phase space. We see that with the coordinate transformation in terms of the evanescent action u, the oscillation of the integrand is far better behaved. We see also how the equilibrium limit is obtained in the large-time limit. For the $1 \to 2$ decay process, the limits of integration grow to encompass the full range of the sinc function. At the same time, the u dependence of the phase-space pre-factors vanishes. For the $3 \to 0$

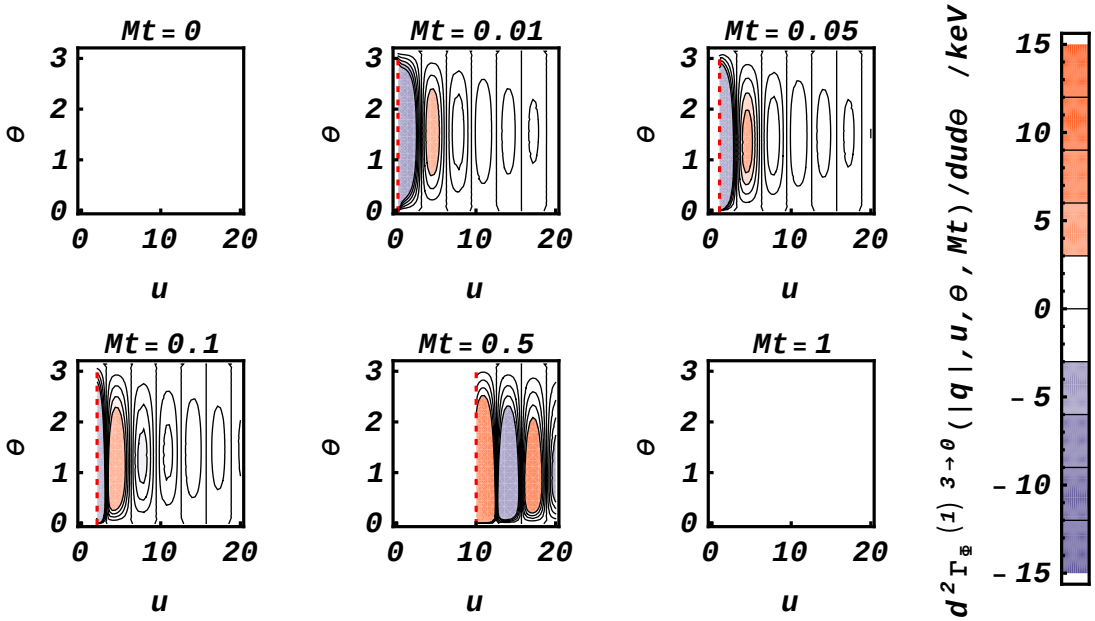


Figure 17.7: Contour plots of the $\alpha_1 = \alpha_2 = -1$, $3 \to 0$-body annihilation contribution to the differential, one-loop Φ width, evaluated for a series of dimensionless times Mt over the dominant region of u, θ phase space for $q^2 = M^2$ on-shell and $|\mathbf{q}| = 10\,\mathrm{GeV}$. The solid excluded regions to the left of the red-dotted line lie exterior to the limits of integration in u. We see that in the large-time limit, the domain of integration shrinks to zero and the contribution vanishes.

annihilation process, the domain of integration vanishes at infinity in the large-time limit. Given that the integrand is finite in this limit, the contribution therefore vanishes as we would hope. For the Landau damping contributions, the behaviour is more subtle: for large times, the domain of integration covers approximately all positive u. However, we see a reduction in the kinematically-allowed phase-space, such that these contributions also vanish in the large-time limit, leaving only the familiar $1 \to 2$ decay contribution.

In order to reduce the statistical error in the Monte Carlo integration (see Appendix D), we use Gaussian importance sampling to ensure that the majority of sampling points fall over the dominant region of the sinc function in u. We define the weight function

$$\frac{\mathrm{d}u}{\mathrm{d}r} \equiv \exp\left[-\frac{(u-u_0)^2}{2\sigma_u^2} \right] \tag{17.3.15}$$

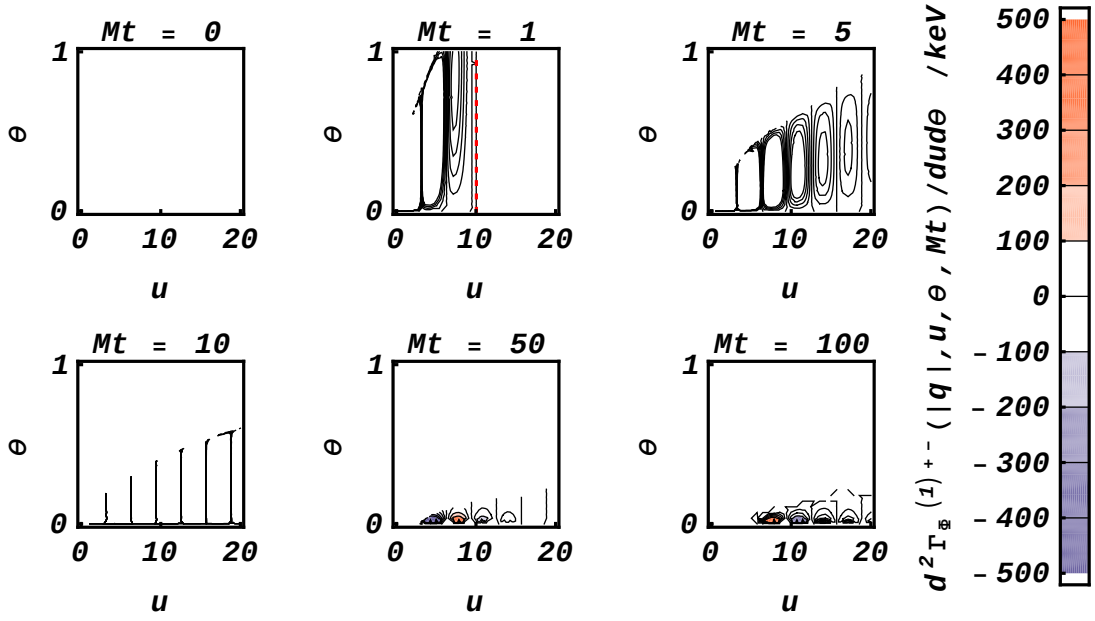
where

$$r(u) \equiv \frac{\mathrm{erf}\left(\frac{1}{\sqrt{2}}\frac{u-u_0}{\sigma_u}\right) - \mathrm{erf}\left(\frac{1}{\sqrt{2}}\frac{u_- - u_0}{\sigma_u}\right)}{\mathrm{erf}\left(\frac{1}{\sqrt{2}}\frac{u_+ - u_0}{\sigma_u}\right) - \mathrm{erf}\left(\frac{1}{\sqrt{2}}\frac{u_- - u_0}{\sigma_u}\right)} \in [0,1]. \tag{17.3.16}$$

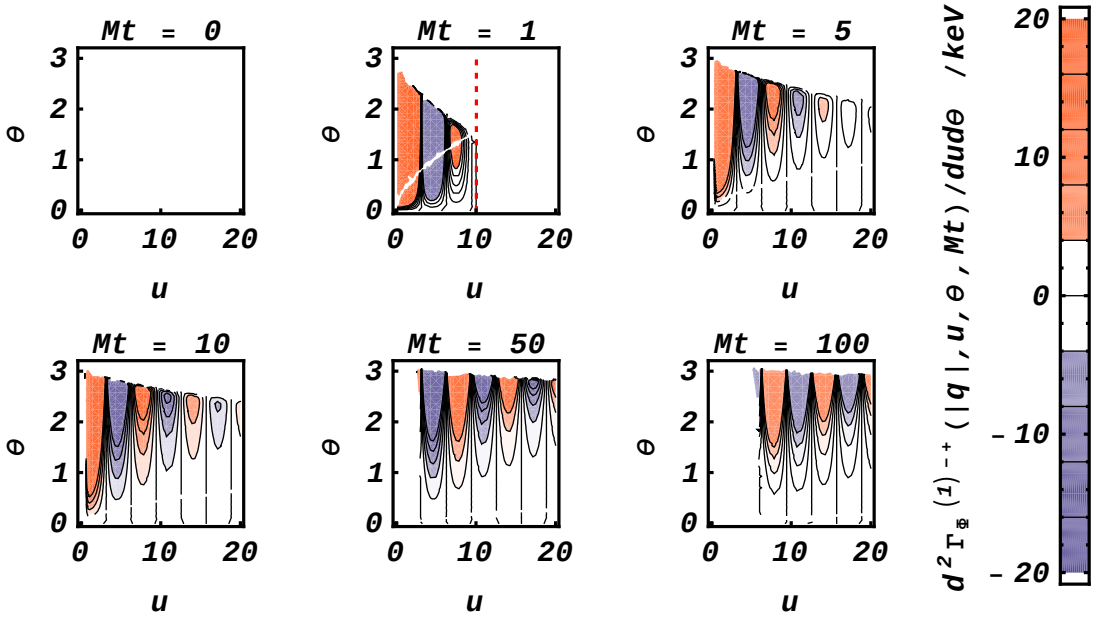
After performing the change of variables, we obtain the added convenience that the limits of integration lose their time dependence and become the same across the decay, production and Landau-damping contributions, with the dependence upon u_+ and u_- appearing in the integrand itself. We may then reduce the required number of integrations by moving the summation over the contributions inside the integral.

We centre the Gaussian on the central maximum of the sinc function, that is $u_0 = 0$. The width of the dominant region is taken to be the distance between maxima at which the amplitude of the sinc function has fallen to 0.1% of its amplitude at the central maximum (i.e. unity), such that we require $0 < \mathrm{sinc}\, u_n \leq 0.001$. Stationary points of the sinc function satisfy the transcendental equation

$$u_n = \tan u_n, \tag{17.3.17}$$



(a) $\alpha_1 = -\alpha_2 = +1$



(b) $\alpha_1 = -\alpha_2 = -1$

Figure 17.8: Contour plots of the $\alpha_1 = -\alpha_2$, Landau damping contributions to the differential, one-loop Φ width, evaluated for a series of dimensionless times Mt over the dominant region of u, θ phase space for $q^2 = M^2$ on-shell and $|\mathbf{q}| = 10\,\mathrm{GeV}$.

with solution (see [101])

$$u_n = \pm n\pi \exp\left\{\frac{1}{\pi}\int_0^1 \mathrm{d}\xi\, \frac{1}{\xi}\arg\left[\left(1+\frac{1}{2}\xi\ln\frac{1-\xi}{1+\xi}\pm\frac{1}{2}\pi i\xi\right)^2 + n^2\pi^2\xi^2\right]\right\}, n \geq 1. \tag{17.3.18}$$

The required width is then given by $n = 318$ with $u_{318} = 1000$, that is the 159^{th} maximum. The Gaussian weight function is taken to have a variance of $(u_{318}/2)^2$, such that 95% of sampling points fall within this dominant region.

In Figure 17.9, we plot the on-shell, one-loop Φ width, normalised to its equilibrium value, as a function of the dimensionless time-scale Mt for a series of momenta, where we have defined

$$\bar{\Gamma}^{(1)}_{\Phi}(|\mathbf{q}|,t) = \frac{\Gamma^{(1)}_{\Phi}(|\mathbf{q}|,t)}{\Gamma^{(1)}_{\Phi}(|\mathbf{q}|,t\to\infty)}. \tag{17.3.19}$$

We see that the width is vanishing for $Mt = 0$, as we would expect. This is followed shortly by a sharp rise (particularly apparent in the infra-red modes), resulting from the prompt evanescent regime. This steep rise is followed by the superposition of short time-scale transient oscillations, described by the angular frequency ω_0, and longer time-scale *non-Markovian* oscillations. The latter of these modulations show time-dependent frequencies, the origin of which will be discussed in the following Section 17.4. These non-Markovian modulations are emphasised in Figure 17.10, in which we perform a moving time average over the higher-frequency oscillations for the $|\mathbf{q}| = 1\,\text{GeV}$ mode. For later times, the oscillations are damped towards the equilibrium limits. Figure 17.9 contains the summation of all four contributions [102]. These contributions are shown separately in Figure 17.11, where we see that the Landau damping terms yield a contribution to the lower momentum modes of order 10–20% at early times. The annihilation process contributes similarly at the level of about 5%.

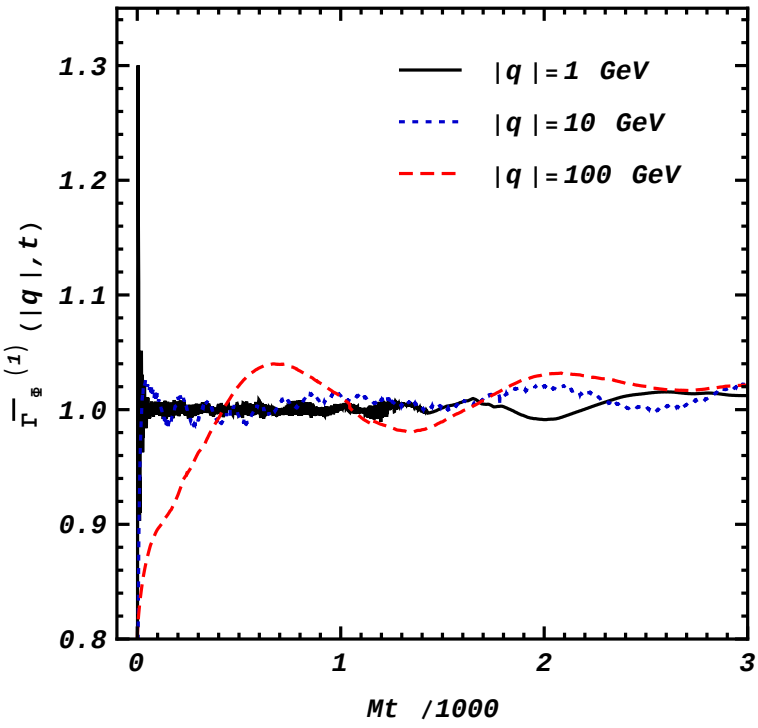


Figure 17.9: Plot of the ratio of the one-loop Φ width to its equilibrium ($t \to \infty$) value against Mt for on-shell decays with $|\mathbf{q}| = 1\,\mathrm{GeV}$ (solid black), $10\,\mathrm{GeV}$ (blue dotted) and $100\,\mathrm{GeV}$ (red dashed).

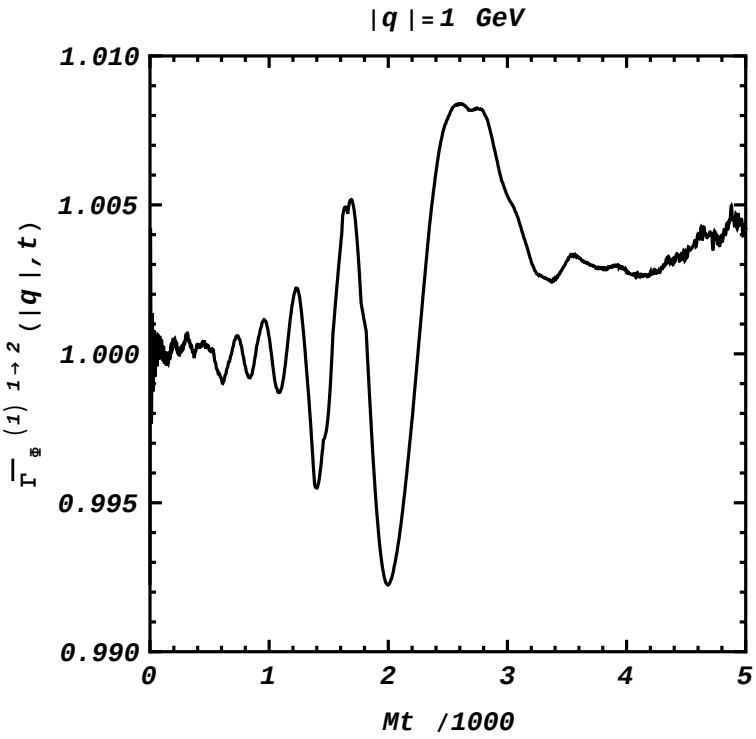


Figure 17.10: The non-Markovian modulations of the decay contribution to the one-loop Φ width by performing a moving average over intervals of $150Mt$ in order to remove the more rapid oscillations of angular frequency ω_0. With the rescaling, the numerical errors (at the level of 0.4%) from the Monte Carlo integration are apparent for late times, where the integrand is becoming highly peaked.

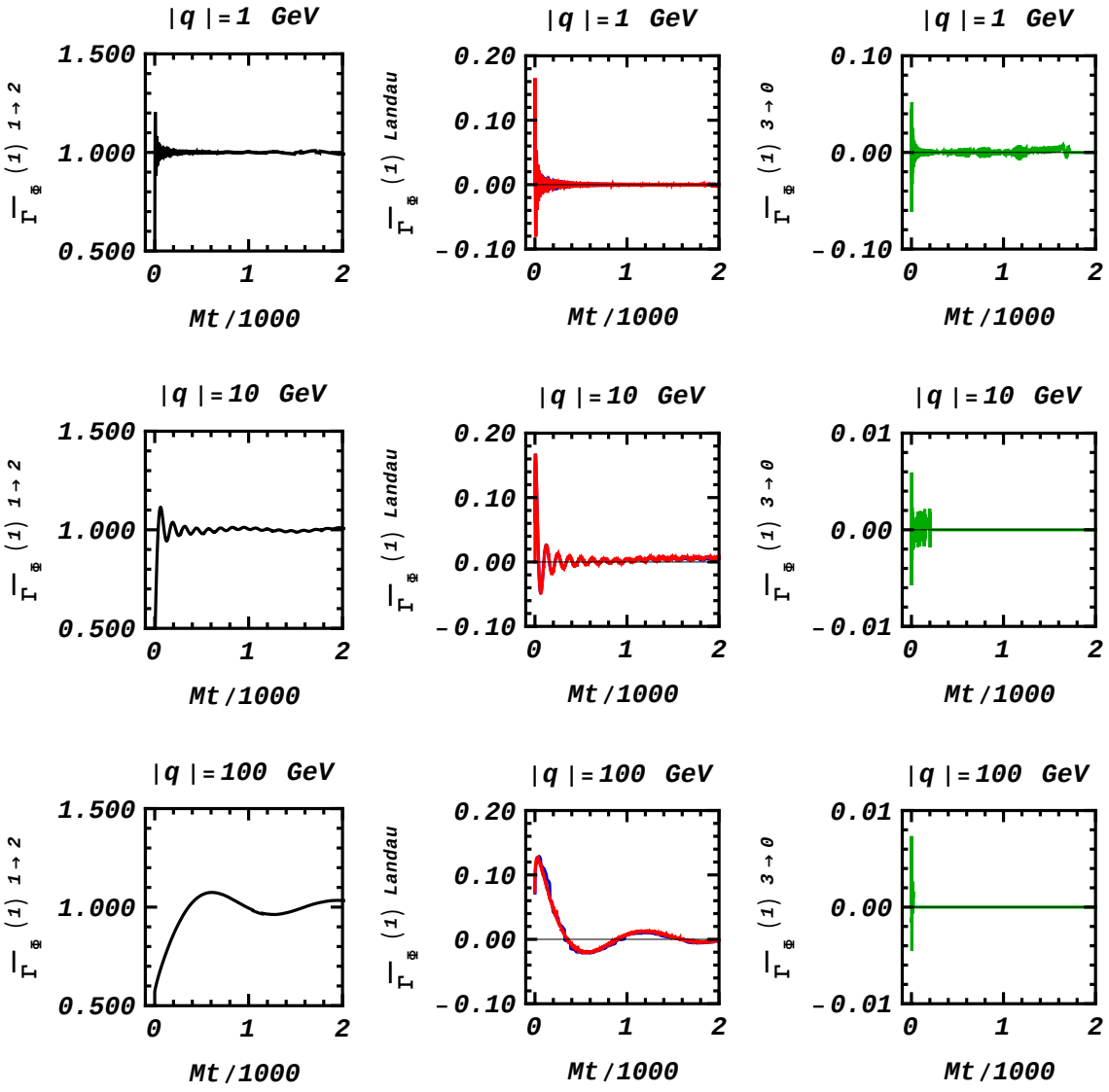


Figure 17.11: Plot of the four contributions to the the normalised one-loop Φ width against Mt for on-shell decays with $|\mathbf{q}| = 1\,\mathrm{GeV}$, $10\,\mathrm{GeV}$ and $100\,\mathrm{GeV}$. We emphasise that the two Landau damping contributions are, indeed, up to numerical errors, identical.

17.4 Non-Markovian Behaviour

In Figure 17.9, we observed that the time-dependent thermal width comprised a superposition of damped, oscillatory contributions. Furthermore, the more long-lived of these oscillations had time-dependent frequencies, see Figure 17.10. In the following section, we attempt to shed some light on the origin of these time-dependent modulations.

Returning to (17.2.4), in the high-temperature limit, for which

$$f_{\mathrm{B}}(E) \approx \frac{T}{E}, \tag{17.4.1}$$

we may perform the angular integration by making the substitution

$$\cos\theta = \frac{|\mathbf{k}|^2 + |\mathbf{q}|^2 + m_2^2}{2|\mathbf{k}||\mathbf{q}|}(1-x)^2. \tag{17.4.2}$$

We then obtain

$$\begin{aligned}\Gamma^{\Phi(1)}_{T\gg M}(q,t) = \frac{g^2}{32\pi^2 M}\sum_{\{\alpha\}=\pm 1}\alpha_1\alpha_\theta\int_0^\infty \mathrm{d}|\mathbf{k}|\,\frac{|\mathbf{k}|}{|\mathbf{q}|}\frac{1}{E_1}\\ \times\Bigg[\left(1+\frac{T}{\alpha_1 E_1}+\frac{T}{q_0-\alpha_1 E_1}\right)\mathrm{Si}\big[(q_0-\alpha_1E_1-\alpha_2E_2)t\big]\\ -\frac{T}{q_0-\alpha_1E_1}\Bigg(\sin\big[(q_0-\alpha_1E_1)t\big]\mathrm{Ci}\big(\alpha_2E_2t\big)\\ -\cos\big[(q_0-\alpha_1E_1)t\big]\mathrm{Si}\big(\alpha_2E_2t\big)\Bigg)\Bigg],\end{aligned} \tag{17.4.3}$$

where Si and Ci are respectively the sine integral and cosine integral functions, $\{\alpha\} = \{\alpha_1, \alpha_2, \alpha_\theta\}$ and

$$E_1 = \sqrt{|\mathbf{k}|^2 + m_1^2}, \tag{17.4.4}$$

$$E_2 = \sqrt{|\mathbf{k}|^2 - 2\alpha_\theta|\mathbf{k}||\mathbf{q}| + |\mathbf{q}|^2 + m_2^2}. \tag{17.4.5}$$

Again introducing the evanescent action u through the substitution in (17.3.3), we obtain

$$\begin{aligned}\Gamma^{\Phi(1)}_{T\gg M}(q,t) = \frac{g^2}{32\pi^2 Mt}\sum_{\{\alpha\},b=\pm1}\alpha_1\alpha_2\int_{u_-(t)}^{u_+(t)}\mathrm{d}u \\ \times\left\{\frac{q_u(t)}{\lambda^{1/2}\big(q_u^2(t)-|\mathbf{q}|^2,m_1^2,m_2^2\big)}\left[\frac{m_1^2+m_2^2}{q_u^2(t)-|\mathbf{q}|^2}-\left(\frac{m_1^2-m_2^2}{q_u^2(t)-|\mathbf{q}|^2}\right)^2\right]\right. \\ \left.+\frac{b\alpha_\theta}{2|\mathbf{q}|}\left(1-\frac{m_1^2-m_2^2}{q_u^2(t)-|\mathbf{q}|^2}\right)\right\} \\ \times\left[\left(1+\frac{T}{\omega_1(q,u,t)}+\frac{T}{q_u(t)-\omega_2(q,u,t)}\right)\mathrm{Si}(u)\right. \\ -\frac{T}{\omega_1(q,u,t)}\left(\sin\big(\omega_1(q,u,t)t\big)\,\mathrm{Ci}\big(\omega_2(q,u,t)t\big)\right. \\ \left.\left.-\cos\big(\omega_1(q,u,t)t\big)\,\mathrm{Si}\big(\omega_2(q,u,t)t\big)\right)\right],\end{aligned} \tag{17.4.6}$$

where we have defined

$$\omega_1(q,u,t) = q_0 - \frac{q_u(t)\big(q_u^2(t)-|\mathbf{q}|^2+m_1^2-m_2^2\big)+b\alpha_\theta|\mathbf{q}|\lambda^{1/2}\big(q_u^2(t)-|\mathbf{q}|^2,m_1^2,m_2^2\big)}{2\big(q_u^2(t)-|\mathbf{q}|^2\big)}, \tag{17.4.7a}$$

$$\omega_2(q,u,t) = \frac{q_u(t)\big(q_u^2(t)-|\mathbf{q}|^2-m_1^2+m_2^2\big)-b\alpha_\theta|\mathbf{q}|\lambda^{1/2}\big(q_u^2(t)-|\mathbf{q}|^2,m_1^2,m_2^2\big)}{2\big(q_u^2(t)-|\mathbf{q}|^2\big)}. \tag{17.4.7b}$$

It is clear then that these non-Markovian modulations contribute only for $T\neq 0$ and are, therefore, a purely statistical effect. We interpret these time-dependent oscillations as a clear signal of memory effects and the departure from thermodynamic equilibrium.

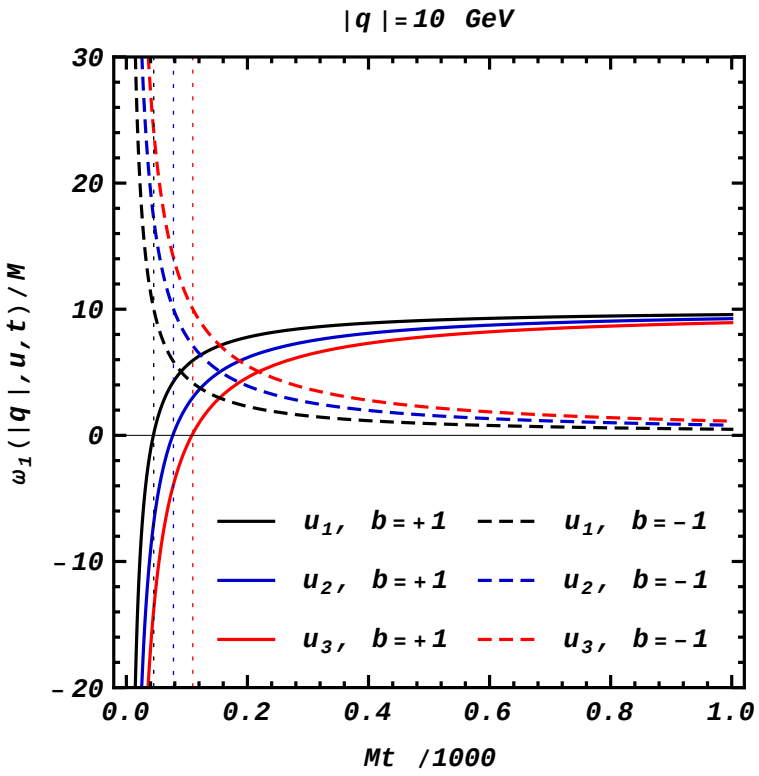


Figure 17.12: Plot of the $\alpha_\theta = +1$ contribution to $\omega_1(q,u,t)$ with $q^2 = M^2$ on-shell and $|\mathbf{q}| = 10\,\mathrm{GeV}$ for the first three extrema of $\mathrm{sinc}(u)$*: $u_1 = 4.49$ (black), $u_2 = 7.73$ (blue) and $u_3 = 10.90$ (red), as given by (17.3.18). The solid lines correspond to the $b = 1$ solution of (17.4.7a) and the dashed line to $b = -1$. The $b = 1$ contribution persists for late times, at which point the frequency of the modulations have decayed to zero. The $b = -1$ contribution is disallowed for late times, such that the amplitude of this constant-frequency modulation is damped to zero. The dotted lines mark the upper limit of the kinematically disallowed region. For $\alpha_\theta = -1$, the $b = +1$ and $b = -1$ contributions are switched, such that the frequency of the $b = -1$ contribution reduces to zero for late times. We have not plotted ω_2 as it is indistinguishable from ω_1 as plotted here.*

17.5 Time-Evolution Equations

Before developing the evolution equations for our toy model, let us return to (15.0.18) and for now maintain energy conservation. The collision terms on the right-hand side for the real scalar read as

$$\Pi^{\Phi}_{>}(p,t)\Delta^{\Phi}_{<}(p,t) - \Pi^{\Phi}_{<}(p,t)\Delta^{\Phi}_{>}(p,t). \tag{17.5.1}$$

At the initial time, the two systems are separately in thermodynamic equilibrium at the same temperature. It follows then, for $\mu \ll m$, that the Φ and χ propagators satisfy the KMS relation and the self-energies satisfy the detailed balance condition, such that

$$\Delta_{>}(p,0) = e^{\beta p_0}\Delta_{<}(p,0) \tag{17.5.2}$$

and

$$\Pi_{>}(p,0) = e^{\beta p_0}\Pi_{<}(p,0). \tag{17.5.3}$$

It is clear then that these collision terms are exactly zero. Furthermore, with nothing to then perturb the system away from this equilibrium, the number density will *not* evolve away from the initial condition. This seems somewhat counter-intuitive. Once the interactions have been switched on, energy will be stored within those interactions and as such, the system should evolve to some interacting thermodynamic equilibrium. We may see this explicitly in the one-loop-inserted propagators in Chapter 12. It is clear then that the Boltzmann equation in this form is incapable of describing this phenomenon correctly. This is true also of the truncated kinetic equation of the Kadanoff-Baym approach in (C.5b). We are forced to conclude therefore that the energy-non-conserving, *evanescent regime* outlined previously is entirely necessary to account for the evolution of this system.

We proceed then to insert into (15.0.15) the one-loop integrals with the homogeneous number densities $f_{\Phi}(|\mathbf{p}|,t)$ and $f^{(c)}_{\chi}(|\mathbf{p}|,t)$. We then obtain the evolution

equation

$$\begin{aligned}\partial_t f_\Phi(|\mathbf{p}|,t) = -\frac{g^2}{2}\sum_{\{\alpha\}}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{1}{2E_\Phi(\mathbf{p})}\frac{1}{2E_\chi(\mathbf{k})}\frac{1}{2E_\chi(\mathbf{p}-\mathbf{k})}\\ \times\frac{t}{2\pi}\,\mathrm{sinc}\big[\big(\alpha E_\Phi(\mathbf{p})-\alpha_1E_\chi(\mathbf{k})-\alpha_2E_\chi(\mathbf{p}-\mathbf{k})\big)t/2\big]\\ \times\big\{\pi+2\mathrm{Si}\big[\big(\alpha E_\Phi(\mathbf{p})+\alpha_1E_\chi(\mathbf{k})+\alpha_2E_\chi(\mathbf{p}-\mathbf{k})\big)t/2\big]\big\}\\ \times\big\{\big[\theta(-\alpha)+f_\Phi(|\mathbf{p}|,t)\big]\big[\theta(\alpha_1)\big(1+f_\chi(|\mathbf{k}|,t)\big)+\theta(-\alpha_1)f^c_\chi(|\mathbf{k}|,t)\big]\\ \times\big[\theta(\alpha_2)\big(1+f^c_\chi(|\mathbf{p}-\mathbf{k}|,t)\big)+\theta(-\alpha_2)f_\chi(|\mathbf{p}-\mathbf{k}|,t)\big]\\ -\big[\theta(\alpha)+f_\Phi(|\mathbf{p}|,t)\big]\big[\theta(\alpha_1)f_\chi(|\mathbf{k}|,t)+\theta(-\alpha_1)\big(1+f^c_\chi(|\mathbf{k}|,t)\big)\big]\\ \times\big[\theta(\alpha_2)f^c_\chi(|\mathbf{p}-\mathbf{k}|,t)+\theta(-\alpha_2)\big(1+f_\chi(|\mathbf{p}-\mathbf{k}|,t)\big)\big]\big\}.\end{aligned} \tag{17.5.4}$$

where Si is the sine integral function. The dispersive force term and off-shell collision term are vanishing in the spatially homogeneous case due to the symmetry of the self-energy under $P\to -P$.

In the large-time limit,

$$\begin{aligned}\frac{t}{2\pi}\,\mathrm{sinc}\big[\big(\alpha E_\Phi(\mathbf{p})-\alpha_1E_\chi(\mathbf{k})-\alpha_2E_\chi(\mathbf{p}-\mathbf{k})\big)t/2\big]\\ \times\big\{\pi+2\mathrm{Si}\big[\big(\alpha E_\Phi(\mathbf{p})+\alpha_1E_\chi(\mathbf{k})+\alpha_2E_\chi(\mathbf{p}-\mathbf{k})\big)t/2\big]\big\}\\ \to 2\pi\theta(\alpha)\delta\big(E_\Phi(\mathbf{p})-\alpha_1E_\chi(\mathbf{k})-\alpha_2E_\chi(\mathbf{p}-\mathbf{k})\big).\end{aligned} \tag{17.5.5}$$

The kinematic constraints then force $\alpha_1=\alpha_2=+1$ and we obtain the familiar Boltzmann equation:

$$\begin{aligned}&\partial_t f_\Phi(|\mathbf{p}|,t)\\ &\quad=-\frac{g^2}{2}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{1}{2E_\Phi(\mathbf{p})}\frac{1}{2E_\chi(\mathbf{k})}\frac{1}{2E_\chi(\mathbf{p}-\mathbf{k})}2\pi\delta\big(E_\Phi(\mathbf{p})-E_\chi(\mathbf{k})-E_\chi(\mathbf{p}-\mathbf{k})\big)\\ &\qquad\times\Big[f_\Phi(|\mathbf{p}|,t)\big(1+f_\chi(|\mathbf{k}|,t)\big)\big(1+f^c_\chi(|\mathbf{p}-\mathbf{k}|,t)\big)\\ &\qquad\quad-\big(1+f_\Phi(|\mathbf{p}|,t)\big)f_\chi(|\mathbf{k}|,t)f^c_\chi(|\mathbf{p}-\mathbf{k}|,t)\Big].\end{aligned} \tag{17.5.6}$$

At $t = 0$, the right-hand side may be written in terms of the Bose-Einstein distributions:

$$-\frac{g^2}{2}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{1}{2E_\Phi(\mathbf{p})}\frac{1}{2E_\chi(\mathbf{k})}\frac{1}{2E_\chi(\mathbf{p}-\mathbf{k})}2\pi\delta\big(E_\Phi(\mathbf{p})-E_\chi(\mathbf{k})-E_\chi(\mathbf{p}-\mathbf{k})\big)$$
$$\times\Big[f_{\mathrm{B}}\big(E_\Phi(\mathbf{p})\big)\Big(1+f_{\mathrm{B}}\big(E_\chi(\mathbf{k})\big)+f^c_{\mathrm{B}}\big(E_\chi(\mathbf{p}-\mathbf{k})\big)\Big)-f_{\mathrm{B}}\big(E_\chi(\mathbf{k})\big)f^c_{\mathrm{B}}\big(E(\mathbf{p}-\mathbf{k})\big)\Big]. \tag{17.5.7}$$

By virtue of the energy-conserving delta function, the product of distributions

$$f_{\mathrm{B}}\big(E_\Phi(\mathbf{p})\big)\Big(1+f_{\mathrm{B}}\big(E_\chi(\mathbf{k})\big)+f^c_{\mathrm{B}}\big(E_\chi(\mathbf{p}-\mathbf{k})\big)\Big)=f_{\mathrm{B}}\big(E_\chi(\mathbf{k})\big)f^c_{\mathrm{B}}\big(E(\mathbf{p}-\mathbf{k})\big) \tag{17.5.8}$$

and the right-hand side is exactly zero. We see explicitly that the Boltzmann equation is incapable of describing the evolution of the system $\mathscr{S}$, see also (C.5b).

Analogously, for the complex scalar, we obtain

$$\begin{aligned}\partial_t f_\chi(|\mathbf{p}|,t)=-\frac{g^2}{2}\sum_{\{\alpha\}}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{1}{2E_\Phi(\mathbf{p})}\frac{1}{2E_\chi(\mathbf{k})}\frac{1}{2E_\chi(\mathbf{p}-\mathbf{k})}\\
\times\frac{t}{2\pi}\,\mathrm{sinc}\big[\big(\alpha E_\chi(\mathbf{p})-\alpha_1E_\Phi(\mathbf{k})-\alpha_2E_\chi(\mathbf{p}-\mathbf{k})\big)t/2\big]\\
\times\big\{\pi+2\mathrm{Si}\big[\big(\alpha E_\chi(\mathbf{p})+\alpha_1E_\Phi(\mathbf{k})+\alpha_2E_\chi(\mathbf{p}-\mathbf{k})\big)t/2\big]\big\}\\
\times\big\{\big[\theta(\alpha)f_\chi(|\mathbf{p}|,t)+\theta(-\alpha)\big(1+f^c_\chi(|\mathbf{p}|,t)\big)\big]\big[\theta(\alpha_1)+f_\Phi(|\mathbf{k}|,t)\big]\\
\times\big[\theta(\alpha_2)\big(1+f_\chi(|\mathbf{p}-\mathbf{k}|,t)\big)+\theta(-\alpha_2)f^c_\chi(|\mathbf{p}-\mathbf{k}|,t)\big]\\
-\big[\theta(\alpha)\big(1+f_\chi(|\mathbf{p}|,t)\big)+\theta(-\alpha)f^c_\chi(|\mathbf{p}|,t)\big]\big[\theta(-\alpha_1)+f_\Phi(|\mathbf{p}|,t)\big]\\
\times\big[\theta(\alpha_2)f_\chi(|\mathbf{p}-\mathbf{k}|,t)+\theta(-\alpha_2)\big(1+f^c_\chi(|\mathbf{p}-\mathbf{k}|,t)\big)\big]\big\}.\end{aligned} \tag{17.5.9}$$

In the large-time limit, the kinematics restrict $\alpha=+1$, $\alpha_1=+1$ and $\alpha_2=-1$ and

we obtain

$$\partial_t f_\chi(|\mathbf{p}|,t) = -\frac{g^2}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{1}{2E_\Phi(\mathbf{p})}\frac{1}{2E_\chi(\mathbf{k})}\frac{1}{2E_\chi(\mathbf{p}-\mathbf{k})} \times 2\pi\delta\big(E_\Phi(\mathbf{k}) - E_\chi(\mathbf{p}) - E_\chi(\mathbf{p}-\mathbf{k})\big) \times\Big[\big(1+f_\Phi(|\mathbf{k}|,t)\big)f_\chi(|\mathbf{p}|,t)f^c_\chi(|\mathbf{p}-\mathbf{k}|,t) - f_\Phi(|\mathbf{k}|,t)\big(1+f_\chi(|\mathbf{p}|,t)\big)\big(1+f^c_\chi(|\mathbf{p}-\mathbf{k}|,t)\big)\Big]. \tag{17.5.10}$$

This is exactly the negative of $\partial_t f_\Phi$ as we would expect.

The rapidly evolving transient behaviour of the system means that the numerical solution of this system of equations is non-trivial. However, we shall show by contradiction that these equations do indeed constitute a non-trivial evolution of the system to some new interacting thermodynamic equilibrium. Let us assume then that the distribution functions on the right-hand side of (17.5.4) remain in their initial, equilibrium forms for all times. If this right-hand side evaluates to zero for all times, it is clear that this system of equations do not add to the pictures provided by the classical Boltzmann or Kadanoff-Baym approaches. If however this right-hand side does not evaluate to zero for all times, then we can be certain that the system is indeed perturbed from the non-interacting equilibrium, presumably evolving for late times to some new interacting thermodynamic equilibrium. These evaluations are shown in Figure 17.13. It is clear that the the systematic inclusion of finite-time effects and the subsequent energy-non-conserving, evanescent regime do indeed push the system away from equilibrium, forcing it to attain a new equilibrium state at late times. We emphasise that such behaviour cannot be described by existing quantum Boltzmann or Kadanoff-Baym approaches.

These time-evolution equations differ from those derived previously [39, 103] by our systematic treatment of finite-time effects and the generalised kinematics of the evanescent regime. We also do not rely on obscure and partial quasi-particle resummations.

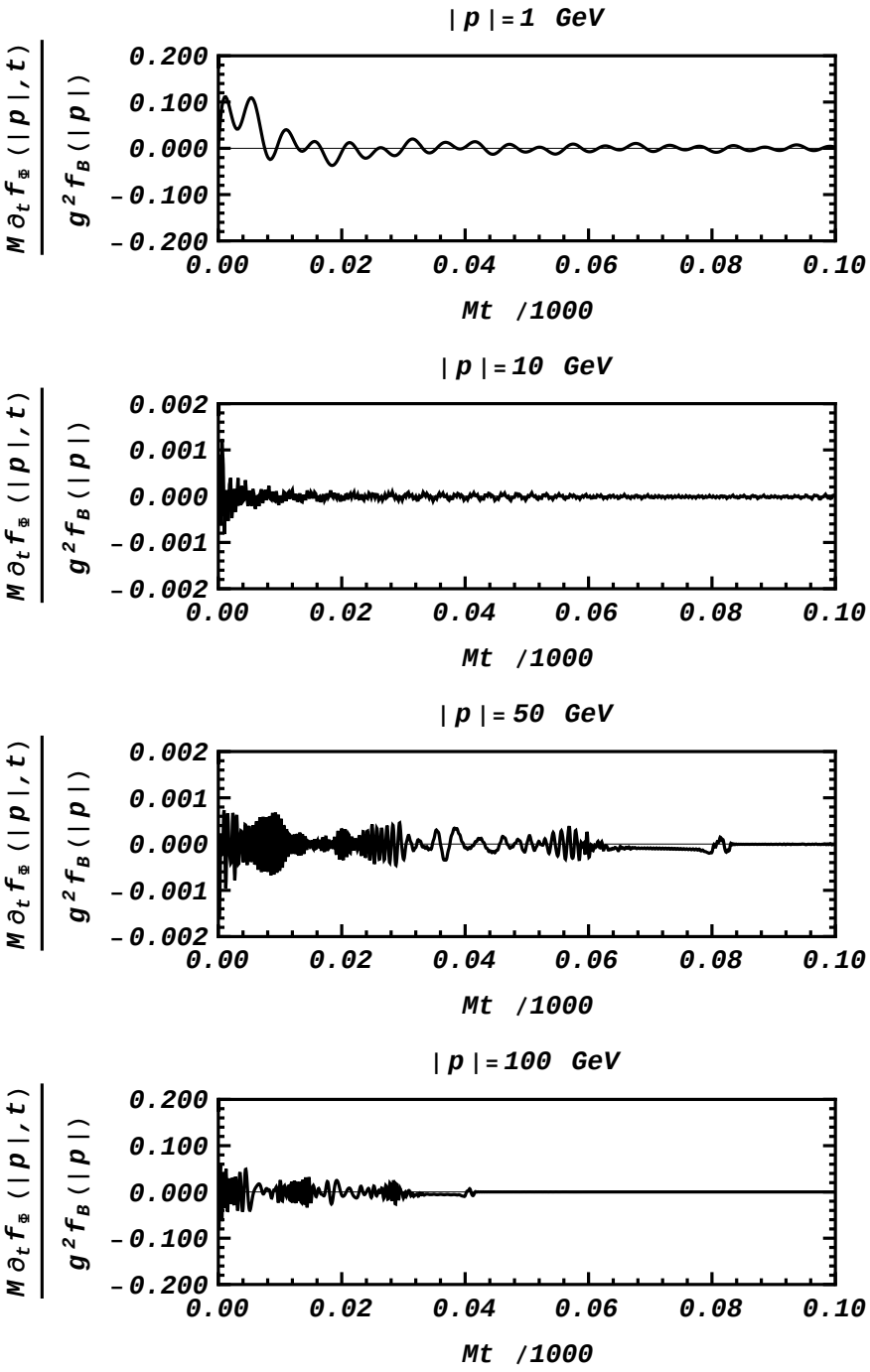


Figure 17.13: Behaviour of $\partial_t f_\Phi(|\mathbf{p}|, t)$, assuming that the distribution functions of the right-hand side of the time-evolution equation maintain their equilibrium form for all times.

17.6 Inclusion of Thermal Masses

In the following section, we describe how local, thermal-mass corrections may be incorporated consistently into this approach.

The local contribution to the one-loop χ self-energy (see Figure 17.1) is

$$\begin{aligned}\Pi_{\chi}^{\mathrm{loc}(1)}(p,p',t) = &-\frac{\lambda}{2}(2\pi)^4\delta_t^{(4)}(p-p')(2\pi\mu)^{2\varepsilon}e^{i(p_0-p_0')t/2}\\ &\times\iint\frac{\mathrm{d}^d k}{(2\pi)^d}\frac{\mathrm{d}^4 k'}{(2\pi)^4}\Big[\frac{i}{k^2-m^2+i\epsilon}(2\pi)^4\delta^{(4)}(k-k')\\ &+2\pi\delta(k^2-m^2)|2k_0|^{1/2}\tilde{f}_{\chi}(k,k',t)e^{i(k_0-k_0')t/2}|2k_0'|^2 2\pi\delta(k'^2-m^2)\Big].\end{aligned} \tag{17.6.1}$$

The first term yields the familiar zero-temperature ultra-violet divergence, which we may remove by adding to the Lagrangian the usual mass renormalisation. The second term is UV finite and yields

$$\Pi_{\chi}^{\mathrm{loc}(1)}(p,p',t) = -(2\pi)^4\delta_t^{(4)}(p-p')e^{i(p_0-p_0')t/2}m_{\mathrm{th}}^2(t), \tag{17.6.2}$$

where the time-dependent thermal mass is given by

$$\begin{aligned}m_{\mathrm{th}}^2(t) = \frac{\lambda}{2}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{1}{\sqrt{2E_{\chi}(\mathbf{k})}}\int\frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}\frac{1}{\sqrt{2E_{\chi}(\mathbf{k}')}}\\ \Big[f_{\chi}(\mathbf{k},\mathbf{k}',t)e^{i[E(\mathbf{k})-E(\mathbf{k}')]t/2}+f_{\chi}^c(-\mathbf{k},-\mathbf{k}',t)e^{-i[E(\mathbf{k})-E(\mathbf{k}')]t/2}\Big].\end{aligned} \tag{17.6.3}$$

The inverse quasi-particle χ propagator then has the form

$$\Delta_{\chi,ab}^{-1}(p,p') = (2\pi)^4\delta_t^{(4)}(p-p')e^{i(p_0-p_0')t/2}\big\{\big[p'^2-m_{\mathrm{th}}^2(t)\big]\eta_{ab}+i\epsilon\mathbb{I}_{ab}\big\}. \tag{17.6.4}$$

If the χ self-interaction is switched on sufficiently long before $t=0$, then for $t\geq 0$, we may replace the δ_t function in the inverse quasi-particle propagator by an exact

energy-conserving delta function. We then obtain the quasi-particle χ propagators

$$\begin{aligned}
&\Delta_{\chi}^{0,ab}(p,p',t) \\
&\quad = \begin{bmatrix} [p^2 - m_{\rm th}^2(t) + i\epsilon]^{-1} & -i2\pi\theta(-p_0)\delta(p^2 - m_{\rm th}^2(t)) \\ -i2\pi\theta(p_0)\delta(p^2 - m_{\rm th}^2(t)) & -\big[p^2 - m_{\rm th}^2(t) - i\epsilon\big]^{-1} \end{bmatrix} (2\pi)^4\delta^{(4)}(p-p') \\
&\quad - i\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} 2\pi|2p_0|^{1/2}\delta(p^2 - m_{\rm th}^2(t))\tilde{f}_{\chi}(p,p',t)e^{i(p_0-p_0')t/2}2\pi|2p_0'|^{1/2}\delta(p'^2 - m_{\rm th}^2(t)),
\end{aligned} \tag{17.6.5}$$

where we have assumed $m_{\rm th}(t) \gg m$.

If $\mathscr{S}_{\chi}$ is at $t = 0$ in a state of thermodynamic equilibrium, the thermal mass reduces to the familiar result

$$m_{\rm th}^2(t=0) = \frac{\lambda T^2}{24}, \tag{17.6.6}$$

where we have assumed that $m = 0$ and $\mu \ll T$. However, in order to describe completely the dynamics of the system $\mathscr{S} = \mathscr{S}_{\Phi} \cup \mathscr{S}_{\chi}$, we must couple the evolution of the local, thermal-mass corrections to the evolution equations for the number density through

$$\partial_t m_{\rm th}(t) = \frac{\lambda}{2m_{\rm th}(t)} \int \frac{{\rm d}^3\mathbf{k}}{(2\pi)^3} \frac{1}{2E_{\chi}(\mathbf{k})} \frac{1}{2}\Big[\partial_t f_{\chi}(|\mathbf{k}|,t) + \partial_t f_{\chi}^c(|\mathbf{k}|,t)\Big], \tag{17.6.7}$$

where, of course, $\partial_t f_{\chi}(|\mathbf{k}|,t)$ and $\partial_t f_{\chi}^c(|\mathbf{k}|,t)$ depend implicitly upon $m_{\rm th}(t)$. It is clear that the solution of this equation will allow the inclusion of non-perturbative effects, in fact, one would anticipate that the leading contribution to $\partial_t m_{\rm th}(t)$ is of order $\lambda^{1/2}g$.

17.7 Early-Time Regime

In this final section, we look more closely at the early-time behaviour immediately after the instant the interactions are switched on. This behaviour must dominated by the ultra-violet behaviour of the phase-space integral on the right-hand side of

(17.5.4), by uncertainty arguments.

We take $|\mathbf{p}| = 0$ and $m = 0$ and introduce the ultra-violet momentum cut-off Λ. Assuming that the χ distribution functions are tempered, vanishing in the ultra-violet, we may show that the ultra-violet contribution is

$$\partial_t f_\Phi(|\mathbf{p}| = 0, t) \sim -\frac{g^2}{32\pi^3 M}\big[1 + 2f_\Phi(|\mathbf{p}| = 0, t)\big] \lim_{\Lambda\to\infty} \mathrm{Si}^2\Lambda t. \tag{17.7.1}$$

It is clear that this vanishes in the limit $t << 1/\Lambda \to 0$ as we expect. However, expanding around $\Lambda t = 0$, i.e., for times infinitesimally close to zero, we obtain

$$\partial_t f_\Phi(|\mathbf{p}| = 0, t) \sim -\frac{g^2}{32\pi^3 M}\big[1 + 2f_\Phi(|\mathbf{p}| = 0, t)\big] \lim_{\Lambda\to\infty} (\Lambda t)^2. \tag{17.7.2}$$

We see however that for small but finite times, ultra-violet contributions yield rapidly varying contributions. What is immediately apparent in this discussion and from Figures 17.9 and 17.13 is the importance of the transient behaviour of the system to the subsequent dynamics, the memories of which persist on long time scales. The highly-oscillatory and rapidly-evolving early-time behaviour suggests that the truncation of any gradient expansion of the evolution equations is unsuitable, at least for these early times.

Furthermore, it is apparent that the numerical solution of these systems of equations constitutes in itself a technical challenge. The presence of the non-singular, but nevertheless highly-peaked phase-space integral leaves the problem unsuitable for naïve discretisation, since any lattice would need to be relatively dense in order to sample the integrand effectively; indeed, for the evaluations of Figures 17.9 and 17.13, 10×10^6 sampling points were required to minimise sufficiently the statistical error of the two-dimensional Monte Carlo integrations (performed using the `quasi Monte Carlo` algorithm in `Wolfram Mathematica` [104]), even with the Gaussian variance reduction. As such, implicit methods, i.e., Backward Euler or n-step Backward Differentiation Formula methods or explicit Runge-Kutta iterative methods, are unsuitable. On the other hand, the rapidly-oscillating transient behaviour sug-

gests a high degree of stiffness to the system and, as such, any explicit method, i.e., Forward Euler, explicit Runge-Kutta or other linear multi-step method would, for early times at least, require a small and therefore computationally-intensive step size.

18 Conclusions

We have outlined a perturbative approach to non-equilibrium thermal quantum field theory. Proceeding from the imposition of general boundary conditions on ensemble expectation values (EEVs) of interaction-picture creation and annihilation operators, we have been able to arrive at time-evolution equations for statistical distribution functions without the need for gradient expansion or quasi-particle Ansätzen of the free propagators. The form of the free propagators and the behaviour of these boundary conditions are constrained by the familiar requirements of causality, unitarity, CPT invariance and Hermiticity. Allowing elements of the density matrix off-diagonal in three-momenta, we account for initial spatial inhomogeneities in the thermal background. Further allowing elements off-diagonal in particle number, we may encode particle-non-conserving correlations in the initial conditions.

The systematic inclusion of finite-time effects ensures that the perturbation theory is free of the pinching singularities thought to spoil such approaches to non-equilibrium quantum field theory. This is achieved without prescription, but rather by accounting consistently for the finite boundary time resulting from the switching on of the interactions. In the early universe, such a switching on may result from the explosive particle production in models of preheating following some inflationary regime; in the decay of false vacua; or in phase transitions.

In systematically treating the generalised decay kinematics in the energy-non-conserving, evanescent regime at early times, we see an expansion of the available $2 \to 1$ decay phase-space and contributions from processes that are normally kinematically forbidden. For the three-body processes in the model considered, these

evanescent processes are the Landau damping and $3 \to 0$ annihilation processes. Indeed, we see for the model considered that these processes contribute promptly to the particle width as much as of order 10–20%. This early-time regime is a manifestation of the Heisenberg uncertainty principle, included consistently in this approach by careful treatment of finite-time effects. The switching on of the interactions leads to a sudden deposition of energy in the system, which we see as a rapid rise in both the particle width and the collision terms of the time-evolution equations. Notably, these early-time effects persist in the oscillations visible in the late-time behaviour. Furthermore, these late-time memory effects show evidence of non-Markovian evolution with the appearance of modulations of time-dependent frequency.

The rapid transient behaviour of the system suggests that the method of gradient expansion is unsuitable for early times. We emphasise that at no point is any assumption made as to the relative rate of thermalisation of either the statistical or spectral behaviour of the system. Indeed, for the equilibrium initial conditions considered, it is clear that the spectral evolution through the evanescent regime is critical to the evolution of the system. The system of time-evolution equations is highly stiff and their solution, in itself, presents a computational challenge. The solution of these equations is therefore a predominate area for further investigation.

Having established closed forms for the most general form of the non-homogeneous propagators, this approach may be appropriate for the consistent incorporation of particle mixing [105, 106]. The non-homogeneous loop integrals presented in Chapter 16 may be readily generalised to higher-point functions and the application of Veltman-Passarino-like [107] reduction methods to the tensor equivalents of these integrals are of interest.

The finite-time effects and the evanescent regime described by this formalism are of particular relevance to processes occurring on time-scales shorter than the thermalization time, the so-called prethermalization [108] and isotropization [109] time-scales. In particular, these effects are relevent when the evolution of the sys-

tem is driven over some finite characteristic time-scale. One such example occurs during the first-order electroweak phase transition, in which this finite time-scale is determined by the bubble wall velocity of the nucleation. For a bubble wall of width $L \gg 1/T$, where T is the thermodynamic temperature, and velocity v_w, the characteristic time-scale is of order $Mt_c \sim Mv_w/L$. For mass-scales of order the Higgs mass $M \sim m_H \sim 100\,\mathrm{GeV}$ and bubble wall widths of order $L \sim 8\,\mathrm{GeV}^{-1}$, the authors of [110] find values of $v_w \sim 0.55$ for Standard Model scenarios, giving $Mt_c \sim 7$. This time-scale is consistent with those over which we have found the finite-time effects to be prominent, see Figure 17.9. One can anticipate that the energy-non-conserving evanescent regime may contribute a rich phenomenology of exotic processes.

Appendices

A Propagator Properties and Identities

In the following appendix, we summarise the transformation properties and identities between the various propagators defined in Section 7.1, which we list below for the complex-scalar field χ:

$$i\Delta(x,y) \equiv \langle[\chi(x),\chi^\dagger(y)]\rangle\,, \tag{A.1a}$$

$$i\Delta_1(x,y) \equiv \langle\{\chi(x),\chi^\dagger(y)\}\rangle\,, \tag{A.1b}$$

$$i\Delta_{\mathrm{R}}(x,y) \equiv \theta(x_0-y_0)i\Delta(x,y), \tag{A.1c}$$

$$i\Delta_{\mathrm{A}}(x,y) \equiv -\theta(y_0-x_0)i\Delta(x,y), \tag{A.1d}$$

$$i\Delta_{\mathcal{P}}(x,y) \equiv \tfrac{1}{2}\varepsilon(x_0-y_0)\,\langle[\chi(x),\chi^\dagger(y)]\rangle\,, \tag{A.1e}$$

$$i\Delta_{>}(x,y) \equiv \langle\chi(x)\chi^\dagger(y)\rangle\,, \tag{A.1f}$$

$$i\Delta_{<}(x,y) \equiv \langle\chi^\dagger(y)\chi(x)\rangle\,, \tag{A.1g}$$

$$i\Delta_{\mathrm{F}}(x,y) \equiv \langle\mathrm{T}[\chi(x)\chi^\dagger(y)]\rangle\,, \tag{A.1h}$$

$$i\Delta_{\mathrm{D}}(x,y) \equiv \langle\bar{\mathrm{T}}[\chi(x)\chi^\dagger(y)]\rangle\,. \tag{A.1i}$$

The definitions of the charge-conjugate propagators follow from the unitary transformation

$$C\chi(x) \equiv U_c^\dagger\chi(x)U_c = \chi^c(x) = \eta\chi^\dagger(x), \tag{A.2a}$$

$$C\chi^\dagger(x) \equiv U_c^\dagger\chi^\dagger(x)U_c = \chi^{c\dagger}(x) = \eta^*\chi(x), \tag{A.2b}$$

where the complex phase η satisfies $|\eta|^2 = 1$.

It follows from the definitions that the propagators satisfy the transformations

listed below under charge- and Hermitian-conjugation:

$$\Delta(x,y) = -\Delta^*(y,x) = -\Delta^c(y,x), \tag{A.3a}$$

$$\Delta_1(x,y) = -\Delta_1^*(y,x) = \Delta_1^c(y,x), \tag{A.3b}$$

$$\Delta_{\mathcal{P}}(x,y) = \Delta_{\mathcal{P}}^*(y,x) = \Delta_{\mathcal{P}}^c(y,x), \tag{A.3c}$$

$$\Delta_{\mathrm{R}}(x,y) = \Delta_{\mathrm{R}}^{c*}(x,y) = \Delta_{\mathrm{A}}^*(y,x) = \Delta_{\mathrm{A}}^c(y,x), \tag{A.3d}$$

$$\Delta_{>}(x,y) = -\Delta_{>}^*(y,x) = \Delta_{<}^c(y,x) = -\Delta_{<}^{c*}(x,y), \tag{A.3e}$$

$$\Delta_{\mathrm{F}}(x,y) = \Delta_{\mathrm{F}}^c(y,x) = -\Delta_{\mathrm{D}}^*(y,x) = -\Delta_{\mathrm{D}}^{c*}(x,y), \tag{A.3f}$$

where the action of charge-conjugation is trivial in the case of the real-scalar field. In the double-momentum representation, these identities take the form:

$$\Delta(p,p') = -\Delta^*(p',p) = -\Delta^c(-p',-p), \tag{A.4a}$$

$$\Delta_1(p,p') = -\Delta_1^*(p',p) = \Delta_1^c(-p',-p), \tag{A.4b}$$

$$\Delta_{\mathcal{P}}(p,p') = \Delta_{\mathcal{P}}^*(p',p) = \Delta_{\mathcal{P}}^c(-p',-p), \tag{A.4c}$$

$$\Delta_{\mathrm{R}}(p,p') = \Delta_{\mathrm{R}}^{c*}(-p,-p') = \Delta_{\mathrm{A}}^*(p',p) = \Delta_{\mathrm{A}}^c(-p',-p), \tag{A.4d}$$

$$\Delta_{>}(p,p') = -\Delta_{>}^*(p',p) = \Delta_{<}^c(-p',-p) = -\Delta_{<}^{c*}(-p,-p'), \tag{A.4e}$$

$$\Delta_{\mathrm{F}}(p,p') = \Delta_{\mathrm{F}}^c(-p',-p) = -\Delta_{\mathrm{D}}^*(p',p) = -\Delta_{\mathrm{D}}^{c*}(-p,-p'). \tag{A.4f}$$

Finally, in the Wigner representation, the propagators satisfy the following:

$$\Delta(q,X) = -\Delta^*(q,X) = -\Delta^c(-q,X), \tag{A.5a}$$

$$\Delta_1(q,X) = -\Delta_1^*(q,X) = \Delta_1^c(-q,X), \tag{A.5b}$$

$$\Delta_{\mathrm{R}}(q,X) = \Delta_{\mathrm{R}}^{c*}(-q,X) = \Delta_{\mathrm{A}}^*(q,X) = \Delta_{\mathrm{A}}^c(-q,X), \tag{A.5c}$$

$$\Delta_{>}(q,X) = -\Delta_{>}^*(q,X) = \Delta_{<}^c(-q,X) = -\Delta_{<}^{c*}(-q,X), \tag{A.5d}$$

$$\Delta_{\mathrm{F}}(q,X) = \Delta_{\mathrm{F}}^c(-q,X) = -\Delta_{\mathrm{D}}^*(q,X) = -\Delta_{\mathrm{D}}^{c*}(-q,X). \tag{A.5e}$$

We also list the following set of useful identities:

$$\Delta(x,y) = \Delta_{>}(x,y) - \Delta_{<}(x,y) = \Delta_{\mathrm{R}}(x,y) - \Delta_{\mathrm{A}}(x,y), \tag{A.6a}$$

$$\Delta_{1}(x,y) = \Delta_{>}(x,y) + \Delta_{<}(x,y) = \Delta_{\mathrm{F}}(x,y) + \Delta_{\mathrm{D}}(x,y), \tag{A.6b}$$

$$\Delta_{\mathrm{R(A)}}(x,y) = \Delta_{\mathrm{F}}(x,y) - \Delta_{<(>)}(x,y) = \Delta^{*}_{\mathrm{F}}(x,y) + \Delta_{>(<)}(x,y), \tag{A.6c}$$

$$\Delta_{\mathcal{P}}(x,y) = \tfrac{1}{2}\varepsilon(x_0 - y_0)\Delta(x,y) = \tfrac{1}{2}\big[\Delta_{\mathrm{R}}(x,y) + \Delta_{\mathrm{A}}(x,y)\big], \tag{A.6d}$$

$$\Delta_{\mathrm{F}}(x,y) = \tfrac{1}{2}\big[\Delta_{\mathrm{R}}(x,y) + \Delta_{\mathrm{A}}(x,y) + \Delta_{>}(x,y) + \Delta_{<}(x,y)\big]. \tag{A.6e}$$

We note that analogous relations hold for the corresponding self-energies and that these identities and relations are true for free and resummed propagators.

B Non-Homogeneous Density Operator

In (B.1), we show the series expansion of the general Gaussian-like density matrix, in which we keep terms linear, bilinear and quadratic in the creation and annihilation operators. Symmetric and asymmetric outer products of multi-particle states are built up by convoluting over all combinations of the W amplitudes. For convenience, the time dependence has been omitted and it is understood that all momenta are integrated with the LIPS measure. Please note that the expansion spans overleaf.

$$
\begin{aligned}
\rho = & \Big(1 + \frac{1}{2} W_{10}(\mathbf{p}_1; 0) W_{01}(0; \mathbf{p}_1) + \frac{1}{4} W_{20}(\mathbf{p}_1, \mathbf{p}_2; 0) W_{02}(0; \mathbf{p}_2, \mathbf{p}_1) + \cdots \Big) \\
& \times \Big\{ |0\rangle\langle 0| \\
& + \Big(- W_{10}(\mathbf{k}_1; 0) + \frac{1}{2} W_{11}(\mathbf{k}_1; \mathbf{q}_1) W_{10}(\mathbf{q}_1; 0) \\
& \qquad + \frac{1}{2} W_{20}(\mathbf{k}_1, \mathbf{q}_1; 0) W_{01}(0; \mathbf{q}_1) + \cdots \Big) |\mathbf{k}_1\rangle\langle 0| \\
& + \Big(- W_{01}(0; \mathbf{k}'_1) + \frac{1}{2} W_{01}(0; \mathbf{q}_1) W_{11}(\mathbf{q}_1; \mathbf{k}'_1) \\
& \qquad + \frac{1}{2} W_{02}(0; \mathbf{k}'_1, \mathbf{q}_1) W_{10}(\mathbf{q}_1; 0) + \cdots \Big) |0\rangle\langle \mathbf{k}'_1| \\
& + \Big((2\pi)^3 2E(\mathbf{k}_1) \delta^{(3)}(\mathbf{k}_1 - \mathbf{k}'_1) - W_{11}(\mathbf{k}_1; \mathbf{k}'_1) + W_{10}(\mathbf{k}_1; 0) W_{01}(0; \mathbf{k}'_1) \\
& \qquad + \frac{1}{2} W_{11}(\mathbf{k}_1; \mathbf{q}_1) W_{11}(\mathbf{q}_1; \mathbf{k}'_1) \\
& \qquad + \frac{1}{4} W_{20}(\mathbf{k}_1, \mathbf{q}_1; 0) W_{02}(0; \mathbf{q}_1, \mathbf{k}'_1) + \cdots \Big) |\mathbf{k}_1\rangle\langle \mathbf{k}'_1|
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{1}{2}\Big(-W_{20}(\mathbf{k}_1,\mathbf{k}_2;0)+W_{10}(\mathbf{k}_1;0)W_{10}(\mathbf{k}_2;0)+\frac{1}{2}W_{11}(\mathbf{k}_1;\mathbf{q}_1)W_{20}(\mathbf{q}_1,\mathbf{k}_2;0)\\
&\qquad+\frac{1}{2}W_{11}(\mathbf{k}_2;\mathbf{q}_1)W_{20}(\mathbf{q}_1,\mathbf{k}_1;0)+\cdots\Big)|\mathbf{k}_1,\mathbf{k}_2\rangle\langle 0|\\
&+\frac{1}{2}\Big(-W_{02}(0;\mathbf{k}_1',\mathbf{k}_2')+W_{01}(0;\mathbf{k}_1')W_{01}(0;\mathbf{k}_2')+\frac{1}{2}W_{02}(0;\mathbf{k}_1',\mathbf{q}_1)W_{11}(\mathbf{q}_1;\mathbf{k}_2')\\
&\qquad+\frac{1}{2}W_{02}(0;\mathbf{k}_2',\mathbf{q}_1)W_{11}(\mathbf{q}_1;\mathbf{k}_1')+\cdots\Big)|0\rangle\langle\mathbf{k}_1',\mathbf{k}_2'|\\
&+\frac{1}{2}\Big(W_{11}(\mathbf{k}_1;\mathbf{k}_1')W_{10}(\mathbf{k}_2;0)+W_{11}(\mathbf{k}_2;\mathbf{k}_1')W_{10}(\mathbf{k}_1;0)\\
&\qquad+W_{20}(\mathbf{k}_1,\mathbf{k}_2;0)W_{01}(0;\mathbf{k}_1')+\cdots\Big)|\mathbf{k}_1,\mathbf{k}_2\rangle\langle\mathbf{k}_1'|\\
&+\frac{1}{2}\Big(W_{11}(\mathbf{k}_1;\mathbf{k}_1')W_{01}(0;\mathbf{k}_2')+W_{11}(\mathbf{k}_1;\mathbf{k}_2')W_{01}(0;\mathbf{k}_1')\\
&\qquad+W_{02}(0;\mathbf{k}_1',\mathbf{k}_2')W_{10}(\mathbf{k}_1;0)+\cdots\Big)|\mathbf{k}_1\rangle\langle\mathbf{k}_1',\mathbf{k}_2'|\\
&+\frac{1}{2}\Big(W_{20}(\mathbf{k}_1,\mathbf{k}_2;0)W_{10}(\mathbf{k}_3;0)+\cdots\Big)|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle\langle 0|\\
&+\frac{1}{2}\Big(W_{02}(0;\mathbf{k}_1',\mathbf{k}_2')W_{01}(0;\mathbf{k}_3')+\cdots\Big)|0\rangle\langle\mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3'|\\
&+\Big[\frac{1}{2}\Big((2\pi)^3 2E(\mathbf{k}_1)\delta^{(3)}(\mathbf{k}_1-\mathbf{k}_1')-W_{11}(\mathbf{k}_1;\mathbf{k}_1')+W_{10}(\mathbf{k}_1;0)W_{01}(0;\mathbf{k}_1')\\
&\qquad\qquad+\frac{1}{2}W_{11}(\mathbf{k}_1;\mathbf{q}_1)W_{11}(\mathbf{q}_1;\mathbf{k}_1')+\frac{1}{4}W_{20}(\mathbf{k}_1,\mathbf{q}_1;0)W_{02}(0;\mathbf{q}_1,\mathbf{k}_1')+\cdots\Big)\\
&\qquad\times\Big((2\pi)^3 2E(\mathbf{k}_2)\delta^{(3)}(\mathbf{k}_2-\mathbf{k}_2')-W_{11}(\mathbf{k}_2;\mathbf{k}_2')+W_{10}(\mathbf{k}_2;0)W_{01}(0;\mathbf{k}_2')\\
&\qquad\qquad+\frac{1}{2}W_{11}(\mathbf{k}_2;\mathbf{q}_2)W_{11}(\mathbf{q}_2;\mathbf{k}_2')+\frac{1}{4}W_{20}(\mathbf{k}_2,\mathbf{q}_2;0)W_{02}(0;\mathbf{q}_2,\mathbf{k}_2')+\cdots\Big)\\
&\quad+\frac{1}{4}\Big(-W_{20}(\mathbf{k}_1,\mathbf{k}_2;0)+W_{10}(\mathbf{k}_1;0)W_{10}(\mathbf{k}_2;0)+\frac{1}{2}W_{11}(\mathbf{k}_1;\mathbf{q}_1)W_{20}(\mathbf{q}_1,\mathbf{k}_2;0)\\
&\qquad\qquad+\frac{1}{2}W_{11}(\mathbf{k}_2;\mathbf{q}_1)W_{20}(\mathbf{q}_1,\mathbf{k}_1;0)+\cdots\Big)\\
&\qquad\times\Big(-W_{02}(0;\mathbf{k}_1',\mathbf{k}_2')+W_{01}(0;\mathbf{k}_1')W_{01}(0;\mathbf{k}_2')+\frac{1}{2}W_{02}(0;\mathbf{k}_1',\mathbf{q}_1)W_{11}(\mathbf{q}_1;\mathbf{k}_2')\\
&\qquad\qquad+\frac{1}{2}W_{02}(0;\mathbf{k}_2',\mathbf{q}_1)W_{11}(\mathbf{q}_1;\mathbf{k}_1')+\cdots\Big)\Big]\,|\mathbf{k}_1,\mathbf{k}_2\rangle\langle\mathbf{k}_1',\mathbf{k}_2'|\\
&+\cdots\Big\}. \qquad\qquad (\text{B.1})
\end{aligned}
$$

C Kadanoff-Baym Equations

In the following appendix, we derive the well-known forms of the Kadanoff-Baym equations [45, 46]. These results are included here for comparison with the perturbative results of the main body.

Inverse Fourier transforming (15.0.4), we obtain the coordinate-space representation of the partially-inverted SD equation

$$-\left[\Box_x^2 + M^2\right]\Delta_{\gtrless}(x,y) + \int_{\Omega_t} \mathrm{d}^4 z \left[\Pi_{\gtrless}(x,z)\Delta_{\mathcal{P}}(z,y) + \Pi_{\mathcal{P}}(x,z)\Delta_{\gtrless}(z,y)\right] = \frac{1}{2}\int_{\Omega_t} \mathrm{d}^4 z \left[\Pi_{<}(x,z)\Delta_{>}(z,y) - \Pi_{>}(x,z)\Delta_{<}(z,y)\right], \quad \text{(C.1)}$$

where we include also the positive-frequency contribution for completeness. Using the fact that

$$\Box_x^2 = \Box_R^2 + \partial_{R,\mu}\partial_X^\mu + \frac{1}{4}\Box_X^2, \quad \text{(C.2)}$$

we may show that the gradient expansion of the Wigner transform of the KB equa-

tions takes the form

$$\begin{aligned}
&\Big[q^2 - M^2 + iq\cdot\partial_X - \frac{1}{4}\Box_X^2\Big]\Delta_{\gtrless}(q,X) \\
&\quad + \int\frac{\mathrm{d}^4Q}{(2\pi)^4}\,(2\pi)^4\delta_t^{(4)}(Q)\exp\big[-i\big(Q\cdot X + \diamondsuit_{q,X}^{-} + 2\diamondsuit_{Q,X}^{+}\big)\big] \\
&\quad \Big[\{\Pi_{\gtrless}(q+Q/2,X)\}\{\Delta_{\mathcal{P}}(q-Q/2,X)\} + \{\Pi_{\mathcal{P}}(q+Q/2,X)\}\{\Delta_{\gtrless}(q-Q/2,X)\}\Big] \\
&\quad = \frac{1}{2}\int\frac{\mathrm{d}^4Q}{(2\pi)^4}\,(2\pi)^4\delta_t^{(4)}(Q)\exp\big[-i\big(Q\cdot X + \diamondsuit_{q,X}^{-} + 2\diamondsuit_{Q,X}^{+}\big)\big] \\
&\quad \Big[\{\Pi_{<}(q+Q/2,X)\}\{\Delta_{>}(q-Q/2,X)\} - \{\Pi_{>}(q+Q/2,X)\}\{\Delta_{<}(q-Q/2,X)\}\Big],
\end{aligned} \tag{C.3}$$

where we recall the definitions of the diamond operators and Poisson brackets in (10.2.10) and (10.2.11) from Section 10.2. Subsequently separating the Hermitian and anti-Hermitian parts of (C.3), we find the constraint and kinetic equations

$$\begin{aligned}
&\Big[q^2 - M^2 - \frac{1}{4}\Box_X^2\Big]\Delta_{\gtrless}(q,X) + \int\frac{\mathrm{d}^4Q}{(2\pi)^4}\,(2\pi)^4\delta_t^{(4)}(Q)\cos\big(Q\cdot X + \diamondsuit_{q,X}^{-} + 2\diamondsuit_{Q,X}^{+}\big) \\
&\qquad \Big[\{\Pi_{\gtrless}(q+\tfrac{Q}{2},X)\}\{\Delta_{\mathcal{P}}(q-\tfrac{Q}{2},X)\} + \{\Pi_{\mathcal{P}}(q+\tfrac{Q}{2},X)\}\{\Delta_{\gtrless}(q-\tfrac{Q}{2},X)\}\Big] \\
&\qquad = \frac{i}{2}\int\frac{\mathrm{d}^4Q}{(2\pi)^4}\,(2\pi)^4\delta_t^{(4)}(Q)\sin\big(Q\cdot X + \diamondsuit_{q,X}^{-} + 2\diamondsuit_{Q,X}^{+}\big) \\
&\qquad \Big[\{\Pi_{>}(q+\tfrac{Q}{2},X)\}\{\Delta_{<}(q-\tfrac{Q}{2},X)\} - \{\Pi_{<}(q+\tfrac{Q}{2},X)\}\{\Delta_{>}(q-\tfrac{Q}{2},X)\}\Big],
\end{aligned} \tag{C.4a}$$

$$\begin{aligned}
&q\cdot\partial_X\Delta_{\gtrless}(q,X) - \int\frac{\mathrm{d}^4Q}{(2\pi)^4}\,(2\pi)^4\delta_t^{(4)}(Q)\sin\big(Q\cdot X + \diamondsuit_{q,X}^{-} + 2\diamondsuit_{Q,X}^{+}\big) \\
&\qquad \Big[\{\Pi_{\gtrless}(q+\tfrac{Q}{2},X)\}\{\Delta_{\mathcal{P}}(q-\tfrac{Q}{2},X)\} + \{\Pi_{\mathcal{P}}(q+\tfrac{Q}{2},X)\}\{\Delta_{\gtrless}(q-\tfrac{Q}{2},X)\}\Big] \\
&\qquad = \frac{i}{2}\int\frac{\mathrm{d}^4Q}{(2\pi)^4}\,(2\pi)^4\delta_t^{(4)}(Q)\cos\big(Q\cdot X + \diamondsuit_{q,X}^{-} + 2\diamondsuit_{Q,X}^{+}\big) \\
&\qquad \Big[\{\Pi_{>}(q+\tfrac{Q}{2},X)\}\{\Delta_{<}(q-\tfrac{Q}{2},X)\} - \{\Pi_{<}(q+\tfrac{Q}{2},X)\}\{\Delta_{>}(q-\tfrac{Q}{2},X)\}\Big],
\end{aligned} \tag{C.4b}$$

respectively.

In the late-time limit, $t\to\infty$, the Q dependence is removed and we neglect the effects of the uncertainty principle (important for the early-time behaviour).

Subsequently keeping terms to zeroth order in the gradient expansion, the above expressions reduce to the compact form of the Kadanoff-Baym (KB) equations (cf. [1, 36, 37, 45, 46])

$$\big[q^2 - M^2\big]\Delta_{\gtrless}(q,X) = -\Big[\Pi_{\gtrless}(q,X)\Delta_{\mathcal{P}}(q,X) + \Pi_{\mathcal{P}}(q,X)\Delta_{\gtrless}(q,X)\Big], \tag{C.5a}$$

$$q\cdot\partial_X\Delta_{\gtrless}(q,X) = \frac{i}{2}\Big[\Pi_{>}(q,X)\Delta_{<}(q,X) - \Pi_{<}(q,X)\Delta_{>}(q,X)\Big]. \tag{C.5b}$$

The kinetic equation is then reminiscent of the classical Boltzmann equation.

D Monte Carlo Integration

This appendix is based on the concise introduction to Monte Carlo integration provided in [111]. We include this brief outline for completeness.

Let us consider the integral

$$\langle f \rangle = \int_0^1 \mathrm{d}x\, f(x), \tag{D.1}$$

which is just the mean of the function $f(x)$ over the interval $(0, 1)$. The variance of this mean is

$$\sigma^2 = \langle f^2 \rangle - \langle f \rangle^2 = \int_0^1 \mathrm{d}x \big[f(x) - \langle f \rangle \big]^2. \tag{D.2}$$

In order to estimate the value of this integral by generating N random numbers r_k uniformly distributed over the interval $(0, 1)$. We may then sample the integral above at N points and approximate it by the arithmetic mean

$$\langle \bar{f} \rangle = \frac{1}{N} \sum_{k=1}^{N} f(r_k). \tag{D.3}$$

This is in itself a random variable with expectation value $\langle f \rangle$. The approximation to the variance is therefore

$$\bar{\sigma}^2 = \frac{1}{N-1} \sum_{k=1}^{N} \big[f(r_k) - \langle \bar{f} \rangle \big]^2. \tag{D.4}$$

The factor of $N - 1$ arises because this variance is calculated from the arithmetic mean and not the true value.

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