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FAITHFUL REALIZATIONS AND SEMICLASSICAL PHYSICS

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Abstract

The method of faithful realizations is defined and explored within the context of several physical problems. We constructed a general procedure for deriving faithful realizations from arbitrary semi-classical truncations, as well as applying this procedure to several explicit examples. This method is useful in systems which have a strong time dependence or which lack a ground state, because in these situations one cannot use the standard tools, such as the effective action.

Using the faithful canonical realizations we developed, as well as an all orders closure, we studied the problem of tunneling times, which has been recently debated in the literature. Our definition of tunneling times, based on the canonical realizations, always gives a time delay. The usage of a canonical coordinate system also allowed us to use the moments as a tool to study the purity of a quantum state. That is, given a set of moments, a faithful canonical realization will have some parameters that correspond to the purity of the state. Moreover, canonical realizations facilitate the usages of methods from statistical mechanics in the realm of canonical effective methods, allowing one to consider ensemble averages of semi-classical quantities. They also facilitate the usage of the powerful techniques of canonical transformations in semi-classical physics. Using the framework of realization equivalence, we were also able to explore a link between the model of loop quantum cosmology as well as a model of group field cosmology. This link has led to several implications on the group field side of the equivalence, with regards to the formations of singularities and of quantization ambiguities.

Table of Contents

List of Figures

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Chapter 1
Introduction

1.1 Motivations

Most problems in physics are too difficult to be solved exactly. In practice one has to find a solvable problem that is "close" to the actual problem and implement some form of perturbation theory to extract predictions. In settings close to classical mechanics, where quantum effects are nevertheless relevant, one can do semi-classical perturbation theory in order to study the problem at hand. A powerful tool for accomplishing this is the effective action [1]. However, this tool is most useful only close to the adiabatic vacuum state. Such a state will not exist in certain cosmological systems, or in systems without ground states. Furthermore, in systems with instabilities, one might not be interested in the evolution close to the vacuum state, but rather close to an unstable state. Nevertheless, one might want to perform semi-classical analysis for these types of systems. Canonical effective methods provides a pathway for one to perform a semi-classical analysis in cases where adiabatic vacuum states don't exist or aren't of interest. This approach is technically more involved though, owing to a non-linear Poisson bracket and constraints stemming from the Cauchy-Schwartz inequality. A way past these technicalities is to use a set of coordinates that renders the Poisson bracket canonical. This can simplify problems, aid one's intuition and render the constraints trivial to implement in many cases.

A powerful tool for extracting semiclassical physics from a system is the effective action. One famous example is Coleman's use of the effective action in order to show that spontaneous symmetry breaking can arise from radiative corrections [2].

It has also been used in a myriad of other applications in particle physics. For an historical review see [3]. The effective action, Γ, mimics the classical action, S, because we have the correspondence;

$$\frac{\delta S[q]}{\delta q} = -J \leftrightarrow \frac{\delta \Gamma[\phi]}{\delta \phi} = -J. \tag{1.1}$$

Where now $\Gamma[\phi]$ has $\hbar$ dependent corrections that can effect the evolution of the system. The hope is that one can use this quantum effective action to study the behavior of the system in the presence of quantum effects. If the system is close to the ground state one can use the typical ansatz for the effective action,

$$\Gamma[\phi] = \int d^4x \left[-V_{\text{eff}}(\phi) - \frac{1}{2}\mathcal{K}(\phi)\partial_\mu\phi\partial^\mu\phi + ... \right]. \tag{1.2}$$

Where the ellipsis stands for a derivative expansion. If the field is slowly varying one can ignore the higher order derivatives, and then derive the equations of motion for the field to be $\partial_\mu\partial^\mu\phi = -V'_{\text{eff}}(\phi)$. This is the local potential approximation [4]. The form of this equation suggests that we can use V_{eff} for the effective potential, and that we can use this potential to study the dynamics near equilibrium. For example, in simple quantum mechanics in one dimension, the adiabatic effective potential can be derived either canonically or by path integral methods [5, 19], and is found to be;

$$V_{\text{eff}}(q) = V_{\text{class}}(q) + \frac{\hbar}{2}\sqrt{V''_{\text{class}}(q)} + \frac{9\hbar^2}{224}\left(V''_{\text{class}}(q)\right)^{-7/9}\frac{d^2}{dq^2}\left[\left(V''_{\text{class}}(q)\right)^{7/9}\right] + \mathcal{O}(\hbar^3). \tag{1.3}$$

This shows explicitly how $\hbar$ dependent corrections can enter the equations of motion and affect the dynamics.

The limits of the effective action can be found if one tries to access the full dynamical content of a theory. Γ can be used to track the semiclassical dynamics of a quantum system, however if there is strong space or time dependence in the problem, the derivative expansion in the action won't exist. Just as with most other divergent asymptotic expansions, one might try to employ some resummation or approximant procedure. This can be done in many cases, but not generally. For example, the derivative expansion for QED is divergent always because the theory is unstable for negative fine structure constant [6], however for simple cases the

expansion is alternating in sign and is Borel summable. Generally however, if non perturbative instabilities are introduced into the theory the derivative expansion is non-alternating and not Borel summable, signaling a breakdown of the effective action [7].

Furthermore, when one computes the effective action from (1.2), one is implicitly perturbing around the ground state. In particular, this is an issue for quantum gravity because it's not expected that the gravitational field will have a non-perturbative ground state [11]. Attempts have been made to circumvent these problems of states or divergent expansions in [8–10]. However these attempts usually involve some type of time dependent variational principle, which requires one to promote some state to a privileged status when there may be no physical reason to do so. With this loss of generality, one might worry that some physical effects may be missed.

Lastly, the effective action is possibly hard to interpret. Close to the adiabatic vacuum state, the interpretation that Γ is the action for the expectation value of the field is fine. However, pushing towards non adiabatic problems this interpretation is not so clear. For example, Γ is generally imaginary, unlike the classical action. This can be seen by examining (1.3). If the particle enters a region where the concavity is negative one finds imaginary quantum corrections. This is because, the quantum q variable in (1.1) is not the expectation value of $\hat{q}$, but is related to non-diagonal matrix elements of $\hat{q}$ [4]. The unclear connection between the classical dynamics and the quantum action in these circumstances can be troublesome if one wants to study problems in regimes away from a ground state, or when the state is non-adiabatic.

These issues outlined above are particularly relevant in quantum cosmology. Euclidean path-integral and effective action techniques have been useful for certain problems in quantum cosmology [11]. However, at a broader level most quantum cosmological models do not have ground states [12]. Furthermore, states with adiabatic fluctuations are hard to find in quantum cosmology [13]. Therefore, a general toolkit that circumvents these issues is needed.

Canonical effective methods provides a scheme that circumvents the issues outlined above, at the price of being more technically involved. To begin, one can start with the Ehrenfest Theorem;

$$\begin{aligned}\langle \hat{F} \rangle &= -\langle V'_{\text{class}}(\hat{q}) \rangle \\ &= -\underbrace{V'_{\text{class}}(\langle \hat{q} \rangle)}_{\text{Classical Force}} \underbrace{-\sum_{n=2}^{\infty} \frac{1}{n!} V^{(n)}_{\text{class}}(\langle \hat{q} \rangle) \langle (\hat{q} - \langle \hat{q} \rangle)^n \rangle}_{\text{Quantum Corrections}} .\end{aligned} \tag{1.4}$$

This shows explicitly how quantum corrections can affect the classical dynamics by way of moments of the state: $\langle (\hat{q} - \langle \hat{q} \rangle)^n \rangle$. The full state is then specified by the coordinates $\Big(q, p, \Delta(q^a p^b)\Big)$. Where a and b are positive integers such that $a + b \geq 2$, and for simplicity, we have the notations: $q = \langle \hat{q} \rangle,\ p = \langle \hat{p} \rangle,\ \Delta(q^a p^b) = \langle (\hat{q} - \langle \hat{q} \rangle)^a (\hat{p} - \langle \hat{p} \rangle)^b \rangle_{weyl}$. Weyl ordering is used in order to avoid over-counting the moments and to ensure that the moments are real valued, which is necessary because they are observables. In order to track the exact dynamics of the state one will need the dynamics of the moments as well. The Hamiltonian generating the dynamics of the moments is simply $H_Q\Big(q, p, \Delta(q^a p^b)\Big) = \langle \hat{H}_{weyl} \rangle$. This can be expanded in terms of moments:

$$H_Q = \Big(q, p, \Delta(q^a p^b)\Big) = H_{\text{class}}(q, p) + \sum_{a=0}^{\infty} \sum_{b=0}^{\infty} \frac{1}{a! b!} \frac{\partial^{a+b} H_{\text{class}}(q, p)}{\partial p^a \partial q^b} \Delta(p^a q^b). \tag{1.5}$$

We also have the bilinear skew-symmetric bracket: $\Big\{\langle \hat{A} \rangle, \langle \hat{B} \rangle\Big\} = \frac{1}{i\hbar} \langle \Big[\hat{A}, \hat{B}\Big] \rangle$. This bracket needs to be augmented by the Leibniz rule in order to define a Poisson bracket for all moments. So by definition, one has to enforce: $\Big\{\langle \hat{A} \rangle, \langle \hat{B} \rangle \langle \hat{C} \rangle\Big\} = \Big\{\langle \hat{A} \rangle, \langle \hat{B} \rangle\Big\} \langle \hat{C} \rangle + \Big\{\langle \hat{A} \rangle, \langle \hat{C} \rangle\Big\} \langle \hat{B} \rangle$. For example, this can be used to calculate the Poisson bracket between products of moments:

$$\begin{aligned}\Big\{\Delta(q^2), \Delta(qp)\Delta(p^2)\Big\} &= \Big\{\Delta(q^2), \Delta(qp)\Big\} \Delta(p^2) + \Big\{\Delta(q^2), \Delta(p^2)\Big\} \Delta(qp) \\ &= 2\Delta(q^2)\Delta(p^2) + 4\Delta(qp)^2\end{aligned} \tag{1.6}$$

With these tools in hand, we can write down the equations of motion for a function of the coordinates,

$$\dot{K}\Big(q, p, \Delta(q^a p^b)\Big) = \{K, H_Q\}. \tag{1.7}$$

In this way, the quantum evolution of the system can be tracked exactly by studying the dynamics of q, p, and $\Delta(q^a p^b)$. For brevity, a system with a single degree of freedom has been focused on, however this prescription generalizes easily to systems with many degrees of freedom.

The dynamics given by (1.7) are equivalent to the dynamics one obtains from the Schrödinger evolution. However, doing exact calculations in this scheme can be cumbersome in all but the simplest problems because (1.7) corresponds to an infinte dimensional system of non linear differential equations. To make progress, the state is assumed to be semi-classical: $\Delta(q^a p^b) \sim \mathcal{O}(\hbar^{(a+b)/2})$. This property is motivated by the Gaussian states, who are the prodigal semi-classical states. Once this property is assumed, moments that are above a given order in $\sqrt{\hbar}$ can be truncated to give a system that is finite, and in principle solvable. In the language of statistics, this amounts to choosing the stochastic closure [101]. For situations where the semi-classical approximation is not valid, one can choose another more appropriate closure.

While numerically tractable, the system will generally be non linear, due to a non linear Poisson bracket, and subject to non-holonomic constraints due to the Cauchy-Schwartz inequality. Therefore performing calculations with this approach can still be cumbersome and non intuitive. In physics, one usually puts some thought into choosing a coordinate system that is optimal for the problem one is solving. In the current situation, a natural coordinate system would be one that brings the Poisson tensor into canonical form. In the examples studied in this dissertation, these canonical coordinate systems, generally allow one much more intuition. Furthermore, usage of a canonical coordinate system can trivialize these non-holonomic constraints, or transform them into reality conditions, which are much easier to implement. These properties allow one to more quickly move through calculations. Furthermore, since the Poisson tensor is independent of the Hamiltonian, the work spent on putting it into a canonical form can be used in many problems.

1.2 Organization

In this thesis the construction, properties, and applications of the canonical coordinate systems are explored. The contents of each chapter are summarized below.

- **Chapter 2**:

  Here the notions traced in the motivation section regarding canonical coordinate systems are made rigorous. The semi-classical phase space is defined as a semi-classical truncation. This is a manifold with a boundary, the coordinates on this manifold are: $\Big(q, p, \Delta(q^a p^b)\Big)$, where $a + b \leq N$. Hence the notion of truncation. The semiclassical truncation is equipped with a non-linear Poisson bracket: $\{\Delta^i, \Delta^j\} = \mathcal{P}^{ij}(\Delta)$. A general method to transform $\mathcal{P}$ into the canonical bracket is developed and applied to several specific examples. An invertible transformation that puts $\mathcal{P}$ in canonical form is called a faithful realization of the Poisson algebra. For a system with N degrees of freedom, the algebra of moments at the second order is identified as the Lie algebra $sp(2N, \mathbb{R})$. A consequence of this is that the Casimirs of $sp(2N, \mathbb{R})$ are approximate constants of motion for semiclassical systems.

- **Chapter 3**: Canonical semiclassical methods can be used to develop an intuitive definition of tunneling time through potential barriers. An application to atomic ionization is given here, considering both static and time-dependent electric fields. The results allow one to analyze different theoretical constructions proposed recently to evaluate ionization experiments based on attoclocks. They also suggest new proposals of determining tunneling times, for instance through the behavior of fluctuations.

- **Chapter 4**: New canonical realizations for up to fourth order in moments for a single classical degree of freedom and to second order for a pair of classical degrees of freedom are derived and applied to several model systems. It is shown that these new canonical variables facilitate the derivation of quantum-statistical quantities and effective potentials. Moreover, by formulating quantum dynamics in classical language, these methods result in new heuristic pictures, for instance of tunneling, that can guide further investigations.

- **Chapter 5**: The paradigmatic models often used to highlight cosmological features of loop quantum gravity and group field theory are shown to be equivalent, in the sense that they are different realizations of the same model given by harmonic cosmology. The loop version of harmonic cosmology is a canonical realization, while the group-field version is a bosonic realization. The existence of a large number of bosonic realizations suggests generalizations of models in group field cosmology.

- **Chapter 6**: All contributions of this thesis are summarized here. The outlook for the methods for applications in Cosmology and quantum mechanics are discussed.

Chapter 2
Faithful Realizations of Semiclassical Truncations

2.1 Introduction

In this chapter, we lay the groundwork for the method of faithful realizations that we will use in the following chapters. We begin by reviewing canonical effective methods. From there, we introduce the concept of a faithful realization, which can be used to simplify canonical effective calculations. We present a method for finding faithful canonical realizations in general case. We then apply this method to several example cases. As an example, we study the phenomenon of parametric resonance in two coupled harmonic oscillators.

Semiclassical truncations approximate quantum dynamics by dynamical systems in which expectation values are coupled to moments of a state. The classical phase space is thereby extended to an enlarged manifold with a Poisson bracket of expectation values and moments derived from the commutator of basic operators. These canonical effective methods have been used in various contexts, such as quantum chemistry [100] and quantum cosmology [107], and they reproduce well-known results including tunneling phenomena [16], the low-energy effective action [92, 93], or the Coleman–Weinberg potential [19]. However, the enlargement of the classical phase space tends to complicate qualitative interpretations as well as computations, in particular because moments, unlike expectation values, do not form canonically conjugate pairs. In this paper, we therefore analyze the problem of constructing canonical realizations of Poisson systems, or their Casimir–Darboux

coordinates. To second moment order for a single pair of classical degrees of freedom, an interesting canonical realization has been known for some time [99, 100]. Our main goal is to extend these results to multiple degrees of freedom and to higher orders in a semiclassical expansion.

At leading order, semiclassical truncations turn out to be closely related to the Lie algebras $\mathrm{sp}(2N, \mathbb{R})$. Our methods and examples can therefore be extended directly to finding canonical realizations for these algebras. Moreover, once a canonical realization is found, one automatically obtains a bosonic realization using the standard Poisson structure on the complex numbers. (Canonical pairs are thereby replaced by classical analogs of annihilation and creation operators.)

We put special emphasis on the construction of faithful realizations, in which the number of independent variables is equal to the dimension of the original system, and the co-rank of the Poisson tensor agrees with the number of Casimir functions. Canonical and bosonic realizations of systems of the type studied here have been used for several decades, but achieving faithfulness often presented a problem. Bosonic realizations go back to theoretical work on magnetic systems [21]. Interest in particular in bosonic realizations of $\mathrm{sp}(6, \mathbb{R})$ grew after the introduction of a symplectic model of nuclear shells and vibrations [22]. Non-faithful bosonic realizations have been used in several papers mainly to compute matrix elements in irreducible representations [23, 25, 118–120]. Some of these studies noted difficulties in finding faithful realizations, starting with $\mathrm{sp}(4, \mathbb{R})$ [119, 120]. Bosonic and canonical realizations of Lie algebras other than $\mathrm{sp}(2N, \mathbb{R})$ have been analyzed and formalized in [28–32], which in most cases were not faithful.

Our results lead to an extension of some of the results of [119] to a faithful bosonic realization, but we expect the main applications of our methods to be in semiclassical discussions of quantum mechanics. Even though we address quantum systems, the use of semiclassical truncations means that we are interested here in *classical* realizations of a system with Poisson brackets. We do not consider the more complicated question of constructing bosonic realizations of operator algebras — the main topic of [119] — in which factor ordering questions are relevant.

2.2 Canonical Effective Methods

Canonical effective equations [92, 93] describe quantum effects through interactions between expectation values and moments of a state with respect to a fixed set of basic observables. The commutator of operators induces a Poisson bracket on the space of expectation values and moments, leading to an infinite-dimensional extension of the classical phase space. In semiclassical approximations of varying degrees, finite-dimensional truncations are used for each canonical pair. The Hamiltonian operator then implies an effective Hamiltonian on the extended phase space for each of its finite-dimensinal truncations, and quantum dynamics can be analyzed much like a classical dynamical system. Mathematically, canonical effective methods replace partial differential equations for wave functions by a system of coupled ordinary differential equations for an enlarged set of variables

We assume that the unital $*$-algebra $\mathcal{A}$ of observables defining the quantum system is canonical, that is, generated by the unit operator together with a finite set of self-adjoint position and momentum operators Q_j and Π_k, $1 \leq j, k \leq N$, with canonical commutation relations

$$[Q_j, \Pi_k] = i\hbar\delta_{jk}\,. \tag{2.1}$$

States are positive linear functionals ω from the algebra to the complex numbers, such that $\omega(a^*a) \geq 0$ for all $a \in \mathcal{A}$ [33]. They may (but need not) be obtained from wave functions or density matrices in or acting on a Hilbert space $\mathcal{H}$ on which $\mathcal{A}$ may be represented by $a \mapsto \hat{a}$: In such a case, every $\psi \in \mathcal{H}$ defines a state $\omega_\psi \colon a \mapsto \langle\hat{a}\rangle_\psi$, and every density matrix $\hat{\rho}$ defines a state $\omega_\rho \colon a \mapsto \mathrm{tr}(\hat{a}\hat{\rho})$. To be specific, and for easier comparison with the physics literature on the subject, we will use the notation $\langle\hat{a}\rangle$ to denote $\omega(a)$, but expectation values could as well be defined using mixed states or algebraic states.

We introduce a set of basic variables taking real values:

Definition 1 *Given a state on a canonical algebra $\mathcal{A}$ generated by self-adjoint Q_j and Π_k, in addition to the unit, the* basic expectation values *are $q_j = \langle\hat{Q}_j\rangle \in \mathbb{R}$ and $\pi_k = \langle\hat{\Pi}_k\rangle \in \mathbb{R}$.*

For positive integers k_i and l_i such that $\sum_{i=1}^N (k_i + l_i) \geq 2$, the moments *of the*

state are given by

$$\Delta\left(q_1^{k_1}\cdots q_N^{k_N}\pi_1^{l_1}\cdots\pi_N^{l_N}\right) = \langle(\hat{Q}_1-q_1)^{k_1}\cdots(\hat{Q}_N-q_N)^{k_N}(\hat{\Pi}_1-\pi_1)^{l_1}\cdots(\hat{\Pi}_N-\pi_N)^{l_N}\rangle_{\mathrm{Weyl}}\,, \tag{2.2}$$

where the product of operators is Weyl (totally symmetrically) ordered.

If the state is a Gaussian wave function in the standard Hilbert space on which $\mathcal{A}$ can be represented, the moments obey the hierarchy

$$\Delta\left(q_1^{k_1}\cdots q_N^{k_N}\pi_1^{l_1}\cdots\pi_N^{l_N}\right) = O\left(\hbar^{\frac{1}{2}\sum_n(l_n+k_n)}\right)\,. \tag{2.3}$$

This property motivates

Definition 2 *A state on a canonical algebra $\mathcal{A}$ is* semiclassical *if its moments obey the hierarchy (4.5).*

A semiclassical state is much more general than the Gaussian family, which has two free parameters per canonical pair of degrees of freedom. A general semiclassical state, by contrast, allows for infinitely many free parameters per canonical pair of degrees of freedom.

We will use the semiclassical hierarchy mainly in order to truncate the infinite-dimensional space of expectation values and moments:

Definition 3 *The* semiclassical truncation of order $s \geq 2$ *of a quantum system with canonical algebra $\mathcal{A}$ is a finite-dimensional manifold $\mathcal{P}_s$ with boundary, determined by global coordinates q_j, π_k and all moments (4.2) such that $\sum_n(l_n+k_n)\leq s$. Its boundary components are obtained from the Cauchy–Schwarz inequality.*

A semiclassical truncation of order s therefore includes variables up to order $\frac{1}{2}s$ in $\hbar$ when evaluated on a Gaussian state. Well-known components of the boundary are given by Heisenberg's uncertainty principle

$$\Delta(q_j^2)\Delta(\pi_k^2) - \Delta(q_j\pi_k)^2 \geq \frac{\hbar^2}{4}\delta_{jk}\,, \tag{2.4}$$

but there are higher-order versions relevant for $s > 2$.

Basic expectation values and moments are equipped with a Poisson bracket defined by

$$\{\langle\hat{A}\rangle,\langle\hat{B}\rangle\} = \frac{1}{i\hbar}\langle[\hat{A},\hat{B}]\rangle\,, \tag{2.5}$$

extended to all moments by using linearity and the Leibniz rule. The Poisson bracket turns any semiclassical truncation into a phase space by ignoring in $\{\Delta_1, \Delta_2\}$ all terms of order higher than s in moments. This condition includes the convention that the product of a moment of order s_1 and a moment of order s_2 is of semiclassical order $s_1 + s_2$. Moreover, the product of a moment of order s_1 with $\hbar^{s_2}$ is of order $s_1 + 2s_2$. The consistency of this notion of order and the resulting truncation has been shown in [96].

In general, the Poisson tensor on a semiclassical truncation is not invertible, such that there is no natural symplectic structure on a semiclassical phase space. For instance, for $N = 1$ the phase space of a semiclassical truncation of order $s = 1$ is five-dimensional with coordinates $(q, \pi, \Delta(q^2), \Delta(q\pi), \Delta(\pi^2))$, and cannot be symplectic. The non-zero basic brackets are

$$\{q, \pi\} = 1 \tag{2.6}$$

and

$$\{\Delta(q^2), \Delta(q\pi)\} = 2\Delta(q^2) \quad , \quad \{\Delta(q\pi), \Delta(\pi^2)\} = 2\Delta(\pi^2) \quad , \quad \{\Delta(q^2), \Delta(\pi^2)\} = 4\Delta(q\pi)\,. \tag{2.7}$$

Quantum dynamics is determined by a Hamiltonian element $H \in \mathcal{A}$. We assume that the Hamiltonian element is given by a sum of Weyl-ordered products of the canonical generators. It defines the quantum Hamiltonian $H_Q(\langle\cdot\rangle, \Delta) = \langle\hat{H}\rangle_{\langle\cdot\rangle,\Delta}$, identified as a function of basic expectation values and moments through the state used in $\langle\hat{H}\rangle$. On a semiclassical truncation of order s, the quantum Hamiltonian leads to the effective Hamiltonian of order s,

$$\begin{aligned} H_{\mathrm{eff},s} &= \langle H(\hat{Q}_j + (\hat{Q}_j - q_j), \hat{\Pi}_k + (\hat{\Pi}_k - \pi_k))\rangle \qquad (2.8)\\ &= H(q,\pi) + \sum_{\sum_n (j_n+k_n)=2}^{s} \frac{\partial^n H(q,\pi)}{\partial q_1^{j_1}\cdots\partial q_N^{j_N}\partial\pi_1^{k_1}\cdots\partial\pi_N^{k_N}} \frac{\Delta\left(q_1^{j_1}\cdots q_N^{j_N}\pi_1^{k_1}\cdots\pi^{k_N}\right)}{j_1!\cdots j_N! k_1!\cdots k_N!}\,, \end{aligned}$$

obtained by a formal Taylor expansion in $\hat{Q}_j - q_j$ and $\hat{\Pi}_k - \pi_k$, where $H(q,\pi)$ is the classical Hamiltonian corresponding to $H \in \mathcal{A}$. If the Hamiltonian is a polynomial in basic operators, the expansion in (4.6) is a finite sum and exact, and merely rearranges the monomial contributions to $\hat{H}$ in terms of central moments. By

definition of the Poisson bracket from the commutator, Hamiltonian equations of motion

$$\dot{f}(\langle\cdot\rangle,\Delta) = \{f(\langle\cdot\rangle,\Delta), H_{\mathrm{eff},s}\} \tag{2.9}$$

generated by an effective Hamiltonian are truncations of Heisenberg's equations of motion evaluated in a state.

2.3 Faithful realizations of semiclassical truncations

While the Poisson brackets $\{q_j,\pi_k\}=1$, $\{q_j,\Delta\}=0=\{\pi_k,\Delta\}$ involving basic expectation values are simple, the brackets between two moments are non-canonical and, in general, non-linear [92, 97]:

$$\begin{aligned}\{\Delta(q^b\pi^a),\Delta(q^d\pi^c)\} &= a\,d\,\Delta(q^b\pi^{a-1})\Delta(q^{d-1}\pi^c) - bc\Delta(q^{b-1}\pi^a)\Delta(q^d\pi^{c-1}) \\ &\quad + \sum_{\text{odd } n=1}^{M}\left(\frac{i\hbar}{2}\right)^{n-1} K^n_{abcd}\,\Delta(q^{b+d-n}\pi^{a+c-n})\end{aligned} \tag{2.10}$$

with $M=\min(a+c,b+d,a+b,c+d)$ and

$$K^n_{abcd} = \sum_{m=0}^{n}(-1)^m m!(n-m)!\binom{a}{m}\binom{b}{n-m}\binom{c}{n-m}\binom{d}{m}\,. \tag{2.11}$$

Since only odd n are included in the sum in (4.13), all coefficients are real. Whenever a term $\Delta(q)$ or $\Delta(\pi)$ appears on the right, it is understood to be zero, which is consistent with an extension of (4.2) to $\sum(k_i+l_i)=1$ because $\langle\hat{a}-a\rangle=0$ for any operator $\hat{a}$. The brackets (4.13) are therefore linear in moments if and only if $a+b=2$ or $c+d=2$.

We will look for mappings of the moments to new variables such that the Poisson brackets can be simplified. In particular, we will derive canonical realizations of semiclassical truncations.

Definition 4 *A* canonical realization *of an algebra $(C^\infty(M),\{\cdot,\cdot\})$ on an open submanifold $\mathcal{U}\subset M$ is a homomorphism $(C^\infty(\mathcal{U}),\{\cdot,\cdot\})\to(C^\infty(\mathbb{R}^{2p}\times\mathbb{R}^I),\{\cdot,\cdot\}_{\mathrm{can}})$ to the algebra of functions on the Poisson manifold $\mathbb{R}^{2p+I}$ equipped with the canonical Poisson bracket on $\mathbb{R}^{2p}$, while $\{f,C\}_{\mathrm{can}}=0$ for all $f\in C^\infty(\mathbb{R}^{2p}\times\mathbb{R}^I)$ and $C\in\mathbb{R}^I$.*

A canonical realization of $(C^\infty(M), \{\cdot,\cdot\})$ *is* faithful *if* $\dim M = 2p + I$ *and* $2p$ *is equal to the rank of the Poisson tensor on* M*.*

Our examples of M will be given by open submanifolds of the phase space of a given semiclassical truncation. A closely related concept is that of a bosonic realization:

Definition 5 *A* bosonic realization *of an algebra* $(C^\infty(M), \{\cdot,\cdot\})$ *on an open submanifold* $\mathcal{U} \subset M$ *is a homomorphism* $(C^\infty(\mathcal{U}), \{\cdot,\cdot\}) \to (C^\infty(\mathbb{C}^p \times \mathbb{R}^I), \{\cdot,\cdot\}_{\mathrm{bos}})$ *to the algebra of functions on the Poisson manifold* $\mathbb{C}^p \times \mathbb{R}^I$*, where* $\mathbb{C}$ *is equipped with the Poisson bracket* $\{z^*, z\}_{\mathrm{bos}} = i$*, while* $\{f, C\}_{\mathrm{bos}} = 0$ *for all* $f \in C^\infty(\mathbb{C}^p \times \mathbb{R}^I)$ *and* $C \in \mathbb{R}^I$*.*

A bosonic realization of $(C^\infty(M), \{\cdot,\cdot\})$ *is* faithful *if* $\dim M = 2p + I$ *and* $2p$ *is equal to the rank of the Poisson tensor on* M*.*

Pullbacks by the local symplectomorphisms

$$\Phi\colon \mathbb{R}^{2p} \to \mathbb{C}^p, (q_j, p_k) \mapsto \left(\tfrac{1}{\sqrt{2}}(q_l + ip_l)\right) \tag{2.12}$$

define a bijection between canonical realizations and bosonic realizations which preserves faithfulness.

We note that the definitions impose reality conditions on the canonical or bosonic variables. In particular, all q_j and p_k must be real, and a bosonic pair (z, z') with $\{z', z\} = i$ must be such that $z' = z^*$.

2.3.1 Poisson structure of semiclassical truncations

Since basic expectation values have canonical Poisson brackets with one another and zero Poisson brackets with any moment, the non-trivial task is to construct a canonical realization of the space of moments for a given semiclassical truncation, at fixed basic expectation values.

A canonical realization of a semiclassical truncation of order s induces a map

$$\mathcal{X}^{(s)}\colon \mathcal{U} \subset \mathcal{P}_s \to \mathbb{R}^{2p} \times \mathbb{R}^I, (\Delta) \mapsto (s_\alpha, p_\beta, U_\gamma) \tag{2.13}$$

such that the variables (s_α, p_β), $\{s_\alpha, p_\beta\} = \delta_{\alpha\beta}$, can be used as coordinates on symplectic leaves defined by constant U_γ. The coordinates U_γ are therefore local expressions of Casimir functions of the Poisson manifold [85].

A faithful realization requires a bijective map between the moments and canonical variables. For a single degree of freedom and a semiclassical truncation of order s, the dimension D of the phase space is the number of moments up to order s, or

$$D = \sum_{j=2}^{s} (j+1) = \frac{1}{2}(s^2 + 3s - 4)\,. \tag{2.14}$$

Note again that this dimension D may be even or odd, depending on s. Even if D is even, the Poisson tensor is not guaranteed to be invertible.

Every function on a Poisson manifold we are considering can be expressed as a function of finitely many moments Δ_i in some ordering. We introduce the Poisson tensor

$$\mathbb{P}_{ij}^{(s)}(\Delta) = \{\Delta_i, \Delta_j\}\,, \tag{2.15}$$

such that the Poisson brackets of the set of coordinates $\mathcal{X}^{(s)}(\Delta)$ are

$$\{\mathcal{X}_\alpha^{(s)}(\Delta), \mathcal{X}_\beta^{(s)}(\Delta)\} = \sum_{i,j=1}^{D} \frac{\partial \mathcal{X}_\alpha^{(s)}(\Delta)}{\partial \Delta_i}\, \mathbb{P}_{ij}^{(s)}(\Delta)\, \frac{\partial \mathcal{X}_\beta^{(s)}(\Delta)}{\partial \Delta_j}\,. \tag{2.16}$$

The dimension of the nullspace of the Poisson tensor is equal to the number of Casimir functions in a neighborhood of a given set of Δ_i.

If the co-rank of the Poisson tensor is equal to I, at each point of phase space there exist I linearly independent vectors $\mathbf{w}_k$, $k = 1, \ldots, I$ with components $w_k^i, i = 1, \ldots, D$, such that

$$\sum_{j=1}^{D} \mathbb{P}_{ij}^{(s)} w_k^j = 0, \;\; k = 1, \ldots, I\,. \tag{2.17}$$

The vectors $\mathbf{w}_k = (w_k^j)$ are the eigenvectors of the Poisson tensor with zero eigenvalue. Since this eigenspace has I-fold degeneracy, the $\mathbf{w}_k$ are not unique if $I > 1$. They can be rearranged in linear combinations with coefficients depending on Δ_i.

Suppose one of the eigenvectors, $\mathbf{w}_k$, can be expressed as

$$w_k^i = \frac{\partial C_k(\Delta)}{\partial \Delta_i}\,. \tag{2.18}$$

Then $C_k(\Delta)$ is a Casimir function which commutes with any function on the

Poisson manifold. At a given point, each 1-form $\mathrm{d}C_k$ defines a smooth submanifold of codimension one in the Poisson manifold through $\mathrm{d}C_k = 0$. As the eigenvectors $\mathbf{w}_k$, and therefore the $\mathrm{d}C_k$, are linearly independent, the intersections of all I $(D-1)$-dimensional submanifolds is a $(D-I)$-dimensional submanifold, called a symplectic leaf. If we choose local coordinates $(v_1, \ldots, v_{D-I})$ on a symplectic leaf, we have $(v_1, \cdots, v_{2n}, C_1, \cdots, C_I)$ as a coordinate system on phase space, where $n = \frac{1}{2}(D-I)$. The Poisson tensor in these coordinates takes the form

$$\mathbb{P}_{ij}^{(s)} = \left(\begin{array}{c|c} \tilde{\mathbb{P}}_{\alpha\beta}^{(s)} & 0 \\ \hline 0 & 0 \end{array}\right), \tag{2.19}$$

where $\tilde{\mathbb{P}}_{\alpha\beta}^{(s)} = \{v_\alpha, v_\beta\}$ and $\det(\tilde{\mathbb{P}}_{\alpha\beta}^{(s)}) \neq 0$. A faithful canonical realization provides a map

$$(v_1, \cdots, v_{2n}, C_1, \cdots, C_I) \to (s_1, \cdots, s_n, p_1, \cdots, p_n, U_1, \cdots, U_I) \tag{2.20}$$

of the local coordinates. After applying this map, the Poisson tensor has the form (2.19) with

$$\tilde{\mathbb{P}}_{\alpha\beta}^{(s)} = \begin{pmatrix} 0 & \mathbb{I}_n \\ -\mathbb{I}_n & 0 \end{pmatrix}. \tag{2.21}$$

Darboux' theorem shows that local canonical coordinates s_α and p_β exist.

As $\dot{C}_I = \{C_I, H\} = 0$ for any Hamiltonian H, motion is always confined to a symplectic leaf $C_I = \text{const}$. Moreover, the existence of a Casimir function implies that the Hamiltonian is not unique because $\{f, H\} = \{f, H + \lambda^I C_I\}$ for any phase-space function f and $\lambda^I \in \mathbb{R}$.

2.3.2 Algebraic structure of second-order semiclassical truncations

For a system with N classical degrees of freedom, we collectively refer to q_j and π_k as x_i, $i = 1, \ldots, 2N$. As can be seen from (4.13) or directly from commutators, the Poisson brackets of second-order semiclassical truncations are then of the form

$$\{\Delta(x_i x_j), \Delta(x_k x_l)\} = \sum_{m \leq n} f_{ij;kl}^{mn} \Delta(x_m x_n)\,. \tag{2.22}$$

The $\Delta(x_i x_j)$ form an independent set of moments if we require that $i \leq j$.

The brackets are linear and form a Lie algebra with structure constants

$$f^{mn}_{ij;kl} = \tau_{ik}\delta^m_j\delta^n_l + \tau_{il}\delta^m_j\delta^n_k + \tau_{jk}\delta^m_i\delta^n_l + \tau_{jl}\delta^m_i\delta^n_k\,, \tag{2.23}$$

using $\tau_{ij} = \{x_i, x_j\}$. For τ_{ij}, we have the identity

$$\sum_j \tau_{ij}\tau_{jk} = \sum_j \{x_i, x_j\}\{x_j, x_k\} = -\delta_{ik} \tag{2.24}$$

because both brackets are non-zero if and only if x_j is canonically conjugate to both x_i and x_k, which implies $x_i = x_k$ for basic variables. We note that the $f^{mn}_{ij;kl}$ are manifestly symmetric in the index pairs (i, j) and (k, l), but not in (m, n).

Instead of summing over restricted double indices, it is more convenient to symmetrize all of them explicitly, in particular

$$f^{(mn)}_{ij;kl} = \frac{1}{2}\left(\tau_{ik}\delta^m_j\delta^n_l + \tau_{il}\delta^m_j\delta^n_k + \tau_{jk}\delta^m_i\delta^n_l + \tau_{jl}\delta^m_i\delta^n_k + \tau_{ik}\delta^n_j\delta^m_l + \tau_{il}\delta^n_j\delta^m_k + \tau_{jk}\delta^n_i\delta^m_l + \tau_{jl}\delta^n_i\delta^m_k\right)\,, \tag{2.25}$$

and include all $\Delta(x_m x_n)$ in (2.22) using $\Delta(x_m x_n) = \Delta(x_n x_m)$. Summations over restricted double indices (m, n) such that $m \leq n$ can then be replaced by two full summations over m and n. For instance,

$$\{\Delta(x_i x_j), \Delta(x_k x_l)\} = \sum_{m\leq n} f^{mn}_{ij;kl}\Delta(x_m x_n) = \sum_{m,n} f^{(mn)}_{ij;kl}\Delta(x_m x_n)\,. \tag{2.26}$$

2.3.2.1 Cartan metric and root vectors

We compute the Cartan metric

$$g_{ij;kl} = \sum_{m,n,o,p} f^{(op)}_{ij;mn} f^{(mn)}_{kl;op} = 4(N+1)\left(\tau_{il}\tau_{kj} + \tau_{ik}\tau_{lj}\right)\,. \tag{2.27}$$

Lemma 1 *The Cartan metric (2.27) is non-degenerate.*

Proof: The metric acts on objects of the form $V = \sum_{i,j} V^{ij}\Delta(x_i x_j)$ via

$$g(V_1, V_2) = \sum_{i,j,k,l} g_{ij;kl} V_1^{ij} V_2^{kl}\,. \tag{2.28}$$

For V to be non-zero we need $\mathrm{Sym}(V^{ij}) = \frac{1}{2}(V^{ij} + V^{ji}) \neq 0$ because $\Delta(x_i x_j) = \Delta(x_j x_i)$. Suppose there is a non zero object V in the null space of g, such that $g(V, \cdot) = 0$ or $\sum_{i,j} V^{ij} g_{ij;kl} = 0$. Using (2.27) and rearranging, we find

$$0 = 8(N+1) \sum_{i,j} \tau_{li} \,\mathrm{Sym}(V^{ij})\, \tau_{jk} \,. \tag{2.29}$$

Because τ is invertible, (2.29) implies that V^{ij} is antisymmetric, but then $V = 0$. We conclude that g is non-degenerate. □

The algebra of second-order moments is therefore a semi-simple Lie algebra. We can show that it is actually simple, and identify it, by examining its Dynkin diagram. We should first find the Cartan subalgebra.

Lemma 2 *The adjoint action of any moment of the form $\Delta(q_i q_j)$, $\Delta(\pi_i \pi_j)$, or $\Delta(q_k \pi_l)$ with $k \neq l$ is nilpotent.*

Proof: The claim is easy to see for $\Delta(q_i q_j)$ and $\Delta(\pi_i \pi_j)$: The adjoint action of $\Delta(q_i q_j)$ on a moment Δ is a sum of moments in which any π_k that may appear in Δ is replaced by q_k, if $k = i$ or $k = j$. After applying this action twice, no π_k is left and the third application gives zero. Analogous arguments hold for $\Delta(\pi_i \pi_j)$.

For $\Delta(q_k \pi_l)$ with $k \neq l$, the adjoint action is non-zero only on moments of the form $\Delta(x \pi_k)$ or $\Delta(y q_l)$, where x and y can be any position or momentum component. In the first case, we compute

$$\begin{aligned} \{\Delta(q_k \pi_l), \Delta(x \pi_k)\} &= \Delta(x \pi_l) + \{\pi_l, x\} \Delta(q_k \pi_k) \\ &= \begin{cases} \Delta(q_l \pi_l) - \Delta(q_k \pi_k) & \text{if } x = q_l \\ \Delta(x \pi_l) & \text{if } x \neq q_l \end{cases} \end{aligned}$$

Therefore,

$$\begin{aligned} \{\Delta(q_k \pi_l), \{\Delta(q_k \pi_l), \Delta(x \pi_k)\}\} &= \begin{cases} -\Delta(q_k \pi_l) & \text{if } x = q_l \\ \{q_k, x\} \Delta(\pi_l^2) & \text{if } x \neq q_l \end{cases} \\ &= \begin{cases} -\Delta(q_k \pi_l) & \text{if } x = q_l \\ \Delta(\pi_l^2) & \text{if } x = \pi_k \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

The next adjoint action of $\Delta(q_k\pi_l)$ gives zero, and similarly on $\Delta(yq_l)$. □

Since nilpotent actions are non-diagonalizable, we construct the Cartan subalgebra from moments of the form $\Delta(q_i\pi_i)$. Since they Poisson commute with one another, they span the Cartan subalgebra

$$H = \langle \Delta(q_i\pi_i) \rangle_{1\leq i\leq N} \ . \tag{2.30}$$

The moments $\Delta(q_i\pi_i)$ are orthogonal to one another and have the same norm with respect to the Cartan metric.

The entire set of moments forms a Cartan–Weyl basis. For any $\Delta(q_i\pi_i)$, the set of basic moments $\Delta(x_kx_l)$ with $k \leq l$ is an eigenbasis of the adjoint action with eigenvalues 2 if $x_k = x_l = \pi_i$, 1 if $x_l = \pi_i$ and $q_i \neq x_k \neq \pi_i$, -1 if $x_k = q_i$ and $q_i \neq x_l \neq \pi_i$, -2 if $x_k = x_l = q_i$, and zero otherwise. The eigenvectors with eigenvalues ± 2 have eigenvalue 0 with any other $\Delta(q_i\pi_i)$, while the eigenvectors with eigenvalues ± 1 are shared by two moments of the form $\Delta(q_i\pi_i)$. The root system is therefore given by all vectors with only two non-zero components of opposite sign and absolute value one, and vectors with a single non-zero component equal to ± 2. A suitable subset of eigenmoments with the smallest possible positive eigenvalues for the adjoint action of all $\Delta(q_i\pi_i)$ gives the simple root vectors

$$\Big\{ \Delta(q_2\pi_1), \Delta(q_3\pi_2), \ldots, \Delta(q_N\pi_{N-1}), \Delta(\pi_N^2) \Big\} \ , \tag{2.31}$$

with simple roots

$$\begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \end{pmatrix} \ , \quad \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \end{pmatrix} \ , \ \cdots \ , \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ -1 \end{pmatrix} \ , \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 2 \end{pmatrix} \ . \tag{2.32}$$

The resulting Dynkin diagram, shown in Fig. 2.1, belongs to $\mathrm{sp}(2N, \mathbb{R})$.

The Casimir functions of $\mathrm{sp}(2N, \mathbb{R})$ can therefore be thought of as approximate

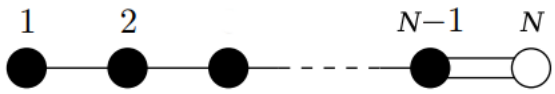

Figure 2.1. The Dynkin diagram for a second-order semiclassical truncation. We adopt the convention that the filled circles correspond to shorter roots and the empty circles correspond to longer roots.

constants of motion in quantum mechanics: At the second semiclassical order, the Hamiltonian is a function of basic expectation values and second-order moments, and the $\mathrm{sp}(2N, \mathbb{R})$ Casimir functions commute with any such function. These constants of motion can be written as

$$U_{2m} \propto \mathrm{tr}\left[(\tau\Delta)^{2m}\right] \ , \ m \leq N \tag{2.33}$$

where Δ is a matrix with components $\Delta_{ij} = \Delta(x_i x_j)$, and $\tau_{ij} = \{x_i, x_j\}$ as before. There is one approximate constant of motion per classical degree of freedom.

2.3.2.2 Example of $\mathrm{sp}(4, \mathbb{R})$

For two classical degrees of freedom, we show the Cartan metric ordering the moments as

$$\left\{\Delta(\pi_1^2), \Delta(\pi_1 q_1), \Delta(q_1^2), \Delta(\pi_2^2), \Delta(\pi_2 q_2), \Delta(q_2^2), \Delta(\pi_1\pi_2), \Delta(\pi_1 q_2), \Delta(\pi_2 q_1), \Delta(q_1 q_2)\right\} . \tag{2.34}$$

The result,

$$g = \begin{pmatrix} 0 & 0 & -24 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 12 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -24 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -24 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 12 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -24 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -12 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & & 12 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -12 & 0 & 0 & 0 \end{pmatrix} , \tag{2.35}$$

is easily seen to be non-degenerate. The Cartan subalgebra is

$$H = \langle \Delta(q_1\pi_1), \Delta(q_2\pi_2) \rangle \ , \tag{2.36}$$

and the simple root vectors

$$\left\{ \Delta(q_2\pi_1), \Delta(\pi_2^2) \right\} \tag{2.37}$$

imply simple roots

$$\alpha_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad , \quad \alpha_2 = \begin{pmatrix} 0 \\ 2 \end{pmatrix} \tag{2.38}$$

corresponding to the Cartan matrix

$$K = \begin{pmatrix} 2 & -1 \\ -2 & 2 \end{pmatrix} \tag{2.39}$$

of $\mathrm{sp}(4, \mathbb{R})$ (or C_2).

2.3.3 Examples

We present standard examples of faithful realizations before we proceed with the general theory.

2.3.3.1 The Lie algebra su(2)

The Poisson bracket for su(2) with generators S_i, $i = 1, 2, 3$, is given by

$$\{S_i, S_j\} = \sum_{k=1}^{3} \epsilon_{ijk} S_k \,. \tag{2.40}$$

It is well known that $S^2 = \sum_{i=1}^{3} S_i^2$ is a Casimir function of this algebra. The task is to find a pair of functions of the generators that are canonically conjugate with respect to the original Poisson tensor. These variables can be defined implicitly by

$$S_x = \sqrt{S^2 - S_z^2}\,\cos(\phi) \quad , \quad S_y = \sqrt{S^2 - S_z^2}\,\sin(\phi)\,, \tag{2.41}$$

such that $\{\phi, S_z\} = 1$. Solving for ϕ and inserting it into the Poisson bracket, we indeed have

$$\{\phi, S_z\} = \{\arctan\left(S_y/S_x\right), S_z\} = \frac{\partial \arctan(S_y/S_x)}{\partial S_x}\{S_x, S_z\} + \frac{\partial \arctan(S_y/S_x)}{\partial S_y}\{S_y, S_z\} = 1\,. \tag{2.42}$$

2.3.3.2 The Lie algebra su(1,1)

The Lie algebra su$(1,1)$ is defined by the relations

$$[\mathcal{K}_0, \mathcal{K}_1] = -\mathcal{K}_2 \quad , \quad [\mathcal{K}_1, \mathcal{K}_2] = \mathcal{K}_0 \quad , \quad [\mathcal{K}_0, \mathcal{K}_2] = \mathcal{K}_1\,. \tag{2.43}$$

For this bracket, a faithful canonical realization is given by

$$\mathcal{K}_0 = k + \frac{1}{2}\left(s^2 + p_s^2\right) \quad , \quad \mathcal{K}_1 = \frac{s}{2}\sqrt{4k + s^2 + p_s^2} \quad , \quad \mathcal{K}_2 = \frac{p_s}{2}\sqrt{4k + s^2 + p_s^2}\,, \tag{2.44}$$

where $K_1^2 + K_2^2 - K_0^2 = -k^2$ is the Casimir function and s and p_s are canonically conjugate variables.

2.3.3.3 The Lie algebra $\mathrm{sp}(2,\mathbb{R})$

The Lie algebra $\mathrm{sp}(2,\mathbb{R})$ can be expressed as the set of matrices of the form $\begin{pmatrix} c & a \\ b & -c \end{pmatrix}$, with generators

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad , \quad B = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad , \quad C = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.45}$$

and relations

$$[A,B] = C \quad , \quad [A,C] = -2A \quad , \quad [B,C] = 2B\,. \tag{2.46}$$

Over the complex numbers, this Lie algebra is isomorphic to $\mathrm{su}(1,1)$ via

$$A = K_2 + iK_1 \quad , \quad B = K_2 - iK_1 \quad , \quad C = 2iK_0\,. \tag{2.47}$$

The canonical realization (2.44) can therefore be mapped to this case:

$$A = \frac{1}{2}(p_s{+}is)\sqrt{4k+s^2+p_s^2} \quad , \quad B = \frac{1}{2}(p_s{-}is)\sqrt{4k+s^2+p_s^2} \quad , \quad C = i(2k{+}s^2{+}p_s^2)\,. \tag{2.48}$$

However, because $\mathrm{sp}(2,\mathbb{R})$ and $\mathrm{su}(1,1)$ are different real forms, these generators are not real. The generators (5.31) therefore do not present a suitable canonical realization for our purposes.

Similarly, using $b = 2^{-1/2}(s + ip_s)$, we obtain generators

$$A = ib^*\sqrt{b^*b + 2k} \quad , \quad B = -ib\sqrt{b^*b+2k} \quad , \quad C = 2i(b^*b + k) \tag{2.49}$$

of Holstein–Primakoff type [21] in which A and $B = A^*$ can be quantized to raising and lowering operators. However, these generators are not real either, and do not present a suitable bosonic realization.

2.3.3.4 Second-order semiclassical truncation for a single pair of classical degrees of freedom

The constructions used in [99, 100] can be interpreted as a faithful canonical realization

$$\Delta(q^2) = s^2 \quad , \quad \Delta(q\pi) = sp_s \quad , \quad \Delta(\pi^2) = p_s^2 + \frac{U}{s^2} \tag{2.50}$$

of a semiclassical truncation with $N = 1$, $s = 2$, and Casimir function U.

The mapping

$$A = -\frac{1}{2}\Delta(\pi^2) \quad , \quad B = \frac{1}{2}\Delta(q^2) \quad , \quad C = \Delta(q\pi) \tag{2.51}$$

generates an isomorphism to $\mathrm{sp}(2,\mathbb{R})$, giving a simple example of the results of Section 2.3.2, and a corresponding faithful canonical realization of $\mathrm{sp}(2,\mathbb{R})$. If we use the canonical realization (2.44) of $\mathrm{su}(1,1)$, on the other hand, we obtain complex expressions for the moments and therefore violate the reality conditions imposed on faithful canonical realizations.

Using (2.51), the canonical realization (2.50) can be related to (2.49) if we define

$$b' = \frac{-\sqrt{2}iA}{\sqrt{-iC+2k}} = \frac{i}{\sqrt{2}}\frac{p_s^2 + U/s^2}{\sqrt{\sqrt{U} - isp_s}} \quad , \quad b = \frac{\sqrt{2}iB}{\sqrt{-iC+2k}} = \frac{i}{\sqrt{2}}\frac{s^2}{\sqrt{\sqrt{U} - isp_s}} \tag{2.52}$$

with $U = 4k^2$, such that $\{b', b\} = i$. However, reality conditions are again violated because $b' \neq b^*$.

2.3.3.5 Non-faithful bosonic realization of $\mathrm{sp}(2N,\mathbb{R})$

The Lie algebra $\mathrm{sp}(2N,\mathbb{R})$ can be written with $N(2N+1)$ generators A_{ij} $(i \leq j)$, B_{ij} $(i \leq j)$ and C_{ij} where $i, j = 1, \ldots, N$ and relations [118]

$$[A_{ij}, A_{i'j'}] = 0 = [B_{ij}, B_{i'j'}] \tag{2.53}$$

$$[B_{ij}, A_{i'j'}] = C_{j'j}\delta_{ii'} + C_{i'j}\delta_{ij'} + C_{j'i}\delta_{ji'} + C_{ii'}\delta_{jj'} \tag{2.54}$$

$$[C_{ij}, A_{i'j'}] = A_{ij'}\delta_{ji'} + A_{ii'}\delta_{jj'} \tag{2.55}$$

$$[C_{ij}, B_{i'j'}] = -B_{jj'}\delta_{ii'} - B_{ji'}\delta_{ij'} \tag{2.56}$$

$$[C_{ij}, C_{i'j'}] = C_{ij'}\delta_{i'j} - C_{i'j}\delta_{ij'} \, . \tag{2.57}$$

It has a bosonic realization [117–120]

$$A_{ij} = \sum_{\alpha=1}^{n} b^*_{i\alpha} b^*_{j\alpha} \quad , \quad B_{ij} = \sum_{\alpha=1}^{n} b_{i\alpha} b_{j\alpha} \quad , \quad C_{ij} = \frac{1}{2} \sum_{\alpha=1}^{n} (b^*_{i\alpha} b_{j\alpha} + b_{j\alpha} b^*_{i\alpha}) \tag{2.58}$$

for every integer $n \geq 1$, with nN boson variables $b_{i\alpha}$ (implying $2nN$ degrees of freedom).

For our purposes, this realization violates reality conditions. Moreover, it is not faithful: Since $2N + 1$ is odd, the number of degrees of freedom cannot match the dimension $N(2N + 1)$ of $\mathrm{sp}(2N, \mathbb{R})$, and since $\mathrm{sp}(2N, \mathbb{R})$ has rank N, it has N Casimirs. For a faithful bosonic realization, one therefore needs N^2 boson variables $b_{i\alpha}$ (that is, $n = N$) and N Casimir variables. Finding an explicit realization of this form has proven to be difficult even for $\mathrm{sp}(4, \mathbb{R})$. For instance, possible expressions have been given up to solving complicated partial differential equations [119] or diagonalizing large matrices [120]. In the next section, we will solve this problem for the analogous question of finding a faithful canonical realization of a second-order semiclassical truncation with two classical degrees of freedom, which is algebraically equivalent to $\mathrm{sp}(4, \mathbb{R})$.

2.4 Constructing Casimir–Darboux coordinates

A partially constructive proof of Darboux' theorem for symplectic manifolds is presented in [98]: Given a symplectic manifold (M, ω), the following steps demonstrate the existence of Darboux coordinates (q_j, π_k) in a neighborhood $\mathcal{U} \subset M$ around a given point $x \in M$, such that $\omega = \sum_j \mathrm{d}q_j \wedge \mathrm{d}\pi_j$. We first choose some function on M, calling it q_1, such that $\mathrm{d}q_1 \neq 0$ at x. Its Hamiltonian vector field X_{q_1} is then non-zero and generates a non-trivial flow $F_{q_1}(t) = \exp(tX_{q_1})$ in a neighborhood of x. Choosing a hypersurface transverse to X_{q_1}, we can endow the whole neighborhood with a pair of coordinates given by q_1 and $\pi_1 = -t$, defined by the parameter t of the Hamiltonian flow such that $t = 0$ on the hypersurface. These two coordinates are canonically conjugate because

$$\{q_1, \pi_1\} = X_{q_1} t = \frac{\partial}{\partial t} t = 1 \,. \tag{2.59}$$

We then move on to the hypersurface defined by $q_1 = 0 = \pi_1$, apply the previous

steps, and iterate until we have the required number of coordinates q_j and π_k defined on a family of hypersurfaces of decreasing dimension. Starting with the last hypersurface of dimension two, we iteratively transport the coordinates into a neighborhood within the next higher hypersurface by declaring that they take constant values on all lines of the flows $F_{q_i}(s)F_{\pi_i}(t)$, if q_i and π_j have already been transported in this way. The proof concludes by showing that the coordinates transported to the neighborhood $\mathcal{U}$ of x in M are indeed canonical.

The steps used to prove Darboux' theorem for symplectic manifolds can be simplified and extended to a systematic procedure to derive Casimir–Darboux coordinates on Poisson manifolds. We keep the first step, but instead of using hypersurfaces of constant canonical coordinates we construct hypersurfaces which are Poisson orthogonal to the already constructed canonical pairs. This modification eliminates the need to transport coordinates from hypersurfaces to the full manifold. We first illustrate the method for the second-order semiclassical truncation of a single pair of classical degrees of freedom.

2.4.1 Canonical realization for a single pair of degrees of freedom at second order

The Poisson brackets of our non-canonical coordinates $\Delta(q^2)$, $\Delta(q\pi)$ and $\Delta(\pi^2)$ are given in (4.8):

$$\{\Delta(q^2),\Delta(q\pi)\}=2\Delta(q^2)\quad,\quad\{\Delta(q\pi),\Delta(\pi^2)\}=2\Delta(\pi^2)\quad,\quad\{\Delta(q^2),\Delta(\pi^2)\}=4\Delta(q\pi)\,. \tag{2.60}$$

As our first canonical coordinate we choose $s=\sqrt{\Delta(q^2)}$. Identifying the (negative) parameter along its Hamiltonian flow with the new momentum p_s, we have the differential equations

$$\frac{\partial\Delta(q^2)}{\partial p_s} = -\{\Delta(q^2),\sqrt{\Delta(q^2)}\}=0 \tag{2.61}$$

$$\frac{\partial\Delta(q\pi)}{\partial p_s} = -\{\Delta(q\pi),\sqrt{\Delta(q^2)}\}=\sqrt{\Delta(q^2)}=s \tag{2.62}$$

$$\frac{\partial\Delta(\pi^2)}{\partial p_s} = -\{\Delta(\pi^2),\sqrt{\Delta(q^2)}\}=2\frac{\Delta(q\pi)}{\sqrt{\Delta(q^2)}}=2\frac{\Delta(q\pi)}{s}\,. \tag{2.63}$$

Since s is held constant in these equations, we can first solve (4.27) by a simple integration,

$$\Delta(q\pi) = sp_s + f_1(s)\,, \tag{2.64}$$

insert the result in (4.28) and integrate once more:

$$\Delta(\pi^2) = p_s^2 + 2\frac{f_1(s)}{s}p_s + f_2(s)\,. \tag{2.65}$$

Computing $\{\Delta(q\pi), \Delta(\pi^2)\}$ using the canonical nature of the variables s and p_s, and requiring that it equal $2\Delta(\pi^2)$ implies two equations:

$$\frac{\mathrm{d}f_1}{\mathrm{d}s} = \frac{f_1}{s} \quad , \quad \frac{\mathrm{d}f_2}{\mathrm{d}s} = 2\frac{f_1}{s^2}\frac{\mathrm{d}f_1}{\mathrm{d}s} - 2\frac{f_2}{s}\,. \tag{2.66}$$

They are solved by

$$f_1(s) = U_2 s \quad , \quad f_2(s) = \frac{U_1}{s^2} + U_2^2 \tag{2.67}$$

with constants U_1 and U_2. We can eliminate U_2 by a canonical transformation replacing p_s with $p_s + U_2$. The constant U_1 is the Casimir coordinate. The resulting moments in terms of Casimir–Darboux variables are

$$\Delta(q^2) = s^2 \quad , \quad \Delta(q\pi) = sp_s \quad , \quad \Delta(\pi^2) = p_s^2 + \frac{U_1}{s^2} \tag{2.68}$$

as in (2.50) or [99, 100]. The Casimir coordinate U_1 can be interpreted as the left-hand side of Heisenberg's uncertainty relation,

$$\Delta(q^2)\Delta(\pi^2) - \Delta(q\pi)^2 = U_1 \geq \frac{\hbar^2}{4}\,, \tag{2.69}$$

which is a constant of motion at second semiclassical order.

2.4.2 Poisson tensors of rank greater than two

If we have a Poisson tensor of rank greater than two, we have to iterate the procedure used in our example in order to find additional canonical pairs. In general, it may be difficult to solve some of the differential equations explicitly.

Instead of using general solutions and eliminating surplus parameters through canonical transformations, in practice it is more useful to make suitable choices

for functions such as f_1 and f_2 in the preceding example. There are wrong choices in the sense that the procedure may terminate before the required number of coordinates has been found, in which case one obtains a non-faithful canonical realization. Usually, it is not difficult to see which choices lead to a loss of degrees of freedom.

In order to iterate the procedure, we use the following method related to the notion of Dirac observables in canonical relativistic systems [39–41]. Having found a canonical pair (s, p_s) on a (sub)manifold of dimension d, we construct $d-2$ independent functions f_i such that $\{f_i, s\} = 0 = \{f_i, p_s\}$ for all i. These functions are then Dirac observables with respect to s and p_s. The construction of Dirac observables is, in general, a very difficult task, and in fact presents one of the main problems of canonical quantum gravity. Here, however, the structure of already-constructed canonical coordinates helps to make the construction of suitable f_i feasible. In particular, the free functions that remain after constructing s and p_s, such as f_1 and f_2 in the example, are, by construction, independent of s, and therefore already fulfill $\{f_i, p_s\} = 0$.

Only a single set of conditions, $\{f_i, s\} = 0$, then remains to be implemented by suitable combinations of the original f_i, which can be done by eliminating integration parameters in the flow $F_s(t)$. For instance, had we not already known that U_1 in (2.69) is a Casimir function, we could have derived it as follows: The flow generated by $s^2 = \Delta(q^2)$ on the remaining moments is determined by the differential equations

$$\frac{\mathrm{d}\Delta(q\pi)}{\mathrm{d}t} = -2\Delta(q^2) \quad , \quad \frac{\mathrm{d}\Delta(\pi^2)}{\mathrm{d}t} = -4\Delta(q\pi)\,. \tag{2.70}$$

The first equation implies that $\Delta(q\pi)[t] = -2\Delta(q^2)t + d$ with t-independent d. Inserting this solution in the second equation, we find $\Delta(\pi^2)[t] = 4\Delta(q^2)t^2 - 4dt + e$ with another constant e. We now eliminate t by inserting $t = \frac{1}{2}(d - \Delta(q\pi)[t])/s^2$ in $\Delta(\pi^2)[t]$:

$$\Delta(\pi^2)[t] = \frac{\Delta(q\pi)[t]^2}{\Delta(q^2)} - 3\frac{d^2}{\Delta(q^2)} + e\,. \tag{2.71}$$

Therefore, $U_1 = \Delta(q^2)\Delta(\pi^2)[t] - \Delta(q\pi)[t]^2 = -3d^2 + es^2$ is independent of t, which implies $\mathrm{d}U_1/\mathrm{d}t = \{U_1, \Delta(q^2)\} = 0$, and U_1 is a Dirac observable with respect to $\Delta(q^2)$ which can be used as a coordinate Poisson orthogonal to s.

The Poisson bracket of two Dirac observables is also a Dirac observable. (This property may be useful for calculating further Dirac observables once more than two have been found.) Given a complete set of Dirac observables, they form coordinates on a Poisson manifold, and we can compute their Poisson brackets from their expressions in terms of the original variables. On this new Poisson manifold, we proceed as in the first step, and then iterate. The procedure terminates when we reach the full dimension, in which case the Poisson manifold is symplectic, or when we obtain a complete set of Poisson commuting Dirac observables. The commuting Dirac observables are the Casimir functions. Because all coordinates constructed in this way are functions of the original variables (the moments in our case of interest), there is no need to transport coordinates to successive hypersurfaces.

2.4.3 Second-order canonical realization for two classical degrees of freedom

A non-trivial example of our general procedure is given by the second-order semi-classical truncation of a system with two pairs of classical degrees of freedom, (q_1, π_1) and (q_2, π_2). We obtain ten moments: two fluctuations and one covariance for each pair, as well as four cross-covariance such as $\Delta(q_1 q_2)$. The rank of the resulting Poisson tensor is eight, so that we should construct four canonical pairs and two Casimir functions.

Since we already discussed the case of a single canonical pair, we can speed up the first step and construct two canonical pairs at the same time by defining $s_1 = \sqrt{\Delta(q_1^2)}$ and $s_2 = \sqrt{\Delta(q_2^2)}$. Their canonical momenta can be generated as in the case of a single degree of freedom, but analogs of the functions f_i could now depend on all the remaining canonical variables: We have

$$\Delta(q_1\pi_1) = s_1 p_1 + f_{q_1\pi_1} \quad , \quad \Delta(\pi_1^2) = p_1^2 + 2\frac{p_1}{s_1} f_{q_1\pi_1} + f_{q_1\pi_1}^2 + \frac{f_{\pi_1^2}}{s_1^2} \tag{2.72}$$

and

$$\Delta(q_2\pi_2) = s_2 p_2 + f_{q_2\pi_2} \quad , \quad \Delta(\pi_2^2) = p_2^2 + 2\frac{p_2}{s_2} f_{q_2\pi_2} + f_{q_2\pi_2}^2 + \frac{f_{\pi_2^2}}{s_2^2} \tag{2.73}$$

with four functions $f_{q_1\pi_1}$, $f_{\pi_1^2}$, $f_{q_2\pi_2}$ and $f_{\pi_2^2}$ independent of s_1, p_1, s_2 and p_2.

We now have to find spaces which are Poisson orthogonal to (s_1, p_1, s_2, p_2), or functions of the moments which Poisson commute with all four canonical coordinates. If we choose $f_{q_1\pi_1} = 0 = f_{q_2\pi_2}$, this condition is equivalent to having moments which Poisson commute with $\Delta(q_1^2)$, $\Delta(q_1p_1)$, $\Delta(q_2^2)$ and $\Delta(q_2p_2)$. Two such functions are

$$f_{\pi_1^2} = s_1^2\Delta(\pi_1^2) - s_1^2p_1^2 = \Delta(q_1^2)\Delta(\pi_1^2) - \Delta(q_1\pi_1)^2 =: f_1 \tag{2.74}$$

and

$$f_{\pi_2^2} = s_2^2\Delta(\pi_2^2) - s_2^2p_2^2 = \Delta(q_2^2)\Delta(\pi_2^2) - \Delta(q_2\pi_2)^2 =: f_2 \tag{2.75}$$

obtained simply by solving (4.92) and (4.93) for $f_{\pi_1^2}$ and $f_{\pi_2^2}$. After computing the Poisson brackets between all the cross-covariances and $\Delta(q_1^2) = s_1^2$, $\Delta(q_1\pi_1) = s_1p_1$, $\Delta(q_2^2) = s_2^2$ and $\Delta(q_2\pi_2) = s_2p_2$, we can construct a complete set of other Poisson commuting functions by integrating flow equations generated by $\Delta(q_1^2)$, $\Delta(q_1\pi_1)$, $\Delta(q_2^2)$ and $\Delta(q_2\pi_2)$. The resulting combinations are

$$f_3 = \Delta(q_1\pi_2)\Delta(q_2\pi_1) - \Delta(q_1q_2)\Delta(\pi_1\pi_2) \tag{2.76}$$

$$f_4 = \Delta(q_1^2)\frac{\Delta(q_2\pi_1)}{\Delta(q_1q_2)} - \Delta(q_1\pi_1) \tag{2.77}$$

$$f_5 = \Delta(q_2^2)\frac{\Delta(q_1\pi_2)}{\Delta(q_1q_2)} - \Delta(q_2\pi_2) \tag{2.78}$$

$$f_6 = \frac{\Delta(q_1^2)\Delta(q_2^2)}{\Delta(q_1q_2)^2}\,, \tag{2.79}$$

as can be checked explicitly. The Poisson brackets between these six functions are closed, so that we can iterate the procedure.

We start the next step by defining $s_3 = f_6$, which is the inverse of the squared correlation between the two particle positions. Its flow equations impose conditions on derivatives of functions Poisson-commuting with p_3, which can again be integrated. Solving some of the integrals, we obtain p_3 as a function of the f_i and s_3, explicitly

$$p_3 = \frac{f_4 + f_5}{4s_3(1 - s_3)}\,. \tag{2.80}$$

Moreover, the four combinations

$$g_1 = f_1 + \frac{(f_4 + f_5)^2}{4(1 - f_6)} + \frac{1}{2}\frac{(f_4 + f_5)(f_4 - f_5)}{1 - f_6} \tag{2.81}$$

$$g_2 = f_2 + \frac{(f_4+f_5)^2}{4(1-f_6)} - \frac{1}{2}\frac{(f_4+f_5)(f_4-f_5)}{1-f_6} \tag{2.82}$$

$$g_3 = f_3 + \frac{(f_4+f_5)^2}{4(1-f_6)} \tag{2.83}$$

$$g_4 = \frac{1}{2}(f_4-f_5) \tag{2.84}$$

Poisson commute with s_3 and p_3, as can again be checked explicitly. It turns out that

$$g_1 + g_2 - 2g_3 = U_1 \tag{2.85}$$

is the quadratic Casimir of the full moment system. Using U_1, we have three remaining variables, which can conveniently be chosen to be $g_1 \pm g_2$ and g_4. Their mutual Poisson brackets are again closed.

The next step of the procedure leads to the combinations

$$h_1 = \frac{g_4}{\sqrt{s_3-1}} \tag{2.86}$$

$$h_2 = (g_1-g_2)\sqrt{\frac{s_3-1}{s_3}} \tag{2.87}$$

$$h_3 = \frac{(1-s_3)(g_1+g_2) + s_3U_1 + 2(1+s_3)(1-s_3)^{-1}g_4^2}{\sqrt{s_3}} \tag{2.88}$$

Poisson-commuting with s_3 and p_3, in addition to U_1. We choose $p_4 = h_1$ as our final canonical momentum, such that invariance under its flow implies

$$h_2 = A(p_4)\cos(s_4) \tag{2.89}$$

$$h_3 = A(p_4)\sin(s_4) \tag{2.90}$$

with some function $A(p_4)$. From the remaining Poisson brackets of h_i, it follows that

$$A(p_4)\frac{\mathrm{d}A(p_4)}{\mathrm{d}p_4} = -8p_4U_1 + 32p_4^3\,. \tag{2.91}$$

The general solution of this equation is

$$A(p_4) = \sqrt{U_2 - 8p_4^2U_1 + 16p_4^4} \tag{2.92}$$

with a constant of integration U_2 which can be interpreted as the second Casimir.

(At this point, it could be any function of the quadratic and quartic Casimirs).

To summarize, we express the original moments in terms of Casimir–Darboux variables. For moments of the first classical pair of degrees of freedom, we find

$$\Delta(q_1^2) = s_1^2 \quad , \quad \Delta(q_1\pi_1) = s_1 p_1 \tag{2.93}$$

$$\Delta(\pi_1^2) = p_1^2 + \frac{\Phi(s_3,p_3,s_4,p_4)}{s_1^2} \tag{2.94}$$

with

$$\begin{aligned}\Phi(s_3,p_3,s_4,p_4) = & -\frac{s_3+1}{s_3-1}p_4^2 - 4s_3\sqrt{s_3-1}p_3p_4 + 4s_3^2(s_3-1)p_3^2 + \frac{1}{2}\frac{s_3}{s_3-1} \\ & -\frac{1}{2}\frac{\sqrt{s_3}}{s_3-1}\sqrt{U_2 - 8p_4^2U_1 + 16p_4^4}\left(\sqrt{s_3-1}\cos(s_4) + \sin(s_4)\right).\end{aligned} \tag{2.95}$$

For moments of the second classical pair of degrees of freedom,

$$\Delta(q_2^2) = s_2^2 \quad , \quad \Delta(q_2\pi_2) = s_2 p_2 \tag{2.96}$$

$$\Delta(\pi_2^2) = p_2^2 + \frac{\Gamma(s_3,p_3,s_4,p_4)}{s_2^2} \tag{2.97}$$

with

$$\begin{aligned}\Gamma(s_3,p_3,s_4,p_4) = & -\frac{s_3+1}{s_3-1}p_4^2 + 4s_3\sqrt{s_3-1}p_3p_4 + 4s_3^2(s_3-1)p_3^2 + \frac{1}{2}\frac{s_3}{s_3-1} \\ & -\frac{1}{2}\frac{\sqrt{s_3}}{s_3-1}\sqrt{U_2 - 8p_4^2U_1 + 16p_4^4}\left(-\sqrt{s_3-1}\cos(s_4) + \sin(s_4)\right).\end{aligned} \tag{2.98}$$

Finally, we have

$$\begin{aligned}\Delta(\pi_1\pi_2) = & \frac{p_1p_2}{\sqrt{s_3}} + \sqrt{\frac{s_3-1}{s_3}}\left(\frac{p_2}{s_1} - \frac{p_1}{s_2}\right)p_4 \\ & -2\sqrt{s_3}(s_3-1)\left(\frac{p_1}{s_2} + \frac{p_2}{s_1}\right)p_3 + \frac{(3s_3-1)}{s_1s_2\sqrt{s_3}(s_3-1)}p_4^2 \\ & -4\frac{(s_3-1)s_3^{3/2}}{s_1s_2}p_3^2 - \frac{\sqrt{s_3}}{2s_1s_2(s_3-1)}U_1 \\ & +\frac{s_3}{2s_1s_2(s_3-1)}\sin(s_4)\sqrt{U_2 - 8p_4^2U_1 + 16p_4^4}\end{aligned} \tag{2.99}$$

$$\Delta(q_1\pi_2) = \frac{p_2s_1}{\sqrt{s_3}} - \sqrt{\frac{s_3-1}{s_3}}\frac{s_1}{s_2}p_4 - 2(s_3-1)\sqrt{s_3}\frac{s_1}{s_2}p_3 \tag{2.100}$$

$$\Delta(q_2\pi_1) = \frac{p_1 s_2}{\sqrt{s_3}} + \sqrt{\frac{s_3-1}{s_3}}\frac{s_2}{s_1}p_4 - 2\,(s_3-1)\,\sqrt{s_3}\frac{s_2}{s_1}p_3 \tag{2.101}$$

$$\Delta(q_1 q_2) = \frac{s_1 s_2}{\sqrt{s_3}} \tag{2.102}$$

for the cross-covariances.

2.4.4 Third-order semiclassical truncation for single pair of degrees of freedom

Third-order moments are subject to linear Poisson brackets within a third-order truncation. In particular, the Poisson bracket of any pair of third-order moments is zero within this truncation, and we have linear brackets between second-order and third-order moments, such as

$$\{\Delta(q^2),\Delta(q^2\pi)\} = 2\Delta(q^3) \quad , \quad \{\Delta(q^2),\Delta(q\pi^2)\} = 4\Delta(q^2\pi) \quad , \quad \{\Delta(q^2),\Delta(\pi^3)\} = 6\Delta(q\pi^2) \tag{2.103}$$

and so on. Thanks to the truncation, the brackets still define a linear Lie algebra, but it is not semisimple because the third-order moments span an Abelian ideal. This seven-dimensional Lie algebra is the semidirect product $\mathrm{sp}(2,\mathbb{R}) \ltimes \mathbb{R}^4$ where $\mathrm{sp}(2,\mathbb{R})$, spanned by the second-order moments, acts on $\mathbb{R}^4$, spanned by the third-order moments, according to

$$A = -\frac{1}{2}\Delta(\pi^2) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \tag{2.104}$$

$$B = \frac{1}{2}\Delta(q^2) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{2.105}$$

$$C = \Delta(q\pi) = \begin{pmatrix} -3 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix} \tag{2.106}$$

using (2.51). Computing the Casimir

$$K = -\frac{1}{2}(AB + BA) - \frac{1}{4}C^2 = -\frac{15}{4}\mathbb{I} = -\frac{3}{2}\left(\frac{3}{2} + 1\right)\mathbb{I}\,, \tag{2.107}$$

this action is recognized as the spin-3/2 representation of $\mathrm{sp}(2, \mathbb{R})$.

Guided by our second-order examples, we make the choice

$$\Delta(q^2) = s_1^2 \tag{2.108}$$

$$\Delta(q\pi) = s_1\, p_1 \tag{2.109}$$

as the first step in the introduction of canonical coordinates. Suitable variables on the hypersurface Poisson orthogonal to (s_1, p_1) are

$$\begin{aligned}
f_1 &= \Delta(q^2)\Delta(\pi^2) - \Delta(q\pi)^2 \\
f_2 &= \Delta(q^2)\frac{\Delta(q^2\pi)}{\Delta(q^3)} - \Delta(q\pi) \\
f_3 &= \frac{\Delta(q^2)^2}{\Delta(q^3)^2}\left(\Delta(q^2\pi)^2 - \Delta(q\pi^2)\Delta(q^3)\right) \\
f_4 &= 2\Delta(q\pi) + \Delta(q^2)\frac{\Delta(q^3)\Delta(\pi^3) - \Delta(q\pi^2)\Delta(q^2\pi)}{\Delta(q^2\pi)^2 - \Delta(q\pi^2)\Delta(q^3)}\,.
\end{aligned}$$

The dimension of the Poisson manifold at third order is $D = 7$, while the rank of the Poisson tensor is six. We therefore expect three degrees of freedom and one Casimir function. One additional coordinate Poisson commuting with (s_1, p_1) is needed to have seven independent variables. Since the Poisson brackets of f_i are closed, the last variable Poisson commuting with (s_1, p_1) has to be the Casimir function, which by ansatz can be found to be

$$U_1 = 4\left(\Delta(q\pi^2)^2 - \Delta(q^2\pi)\Delta(\pi^3)\right)\left(\Delta(q^2\pi)^2 - \Delta(q^3)\Delta(q\pi^2)\right) \tag{2.110}$$

$$- \left(\Delta(q^2\pi)\Delta(q\pi^2) - \Delta(q^3)\Delta(\pi^3)\right)^2\,. \tag{2.111}$$

To initiate the next step, we choose

$$s_2 = f_3 \tag{2.112}$$

and integrate its flow equations. The resulting expressions tell us that

$$p_2 = \frac{6f_2 + f_4}{16s_2}\,, \tag{2.113}$$

while

$$g_1 = f_1 + \frac{(6f_2 + f_4)^2}{16} \quad , \quad g_2 = -\frac{1}{2}f_2 - \frac{1}{4}f_4 \tag{2.114}$$

Poisson commute with s_2 but not with p_2. After a further transformation of variables, we obtain the remaining canonical pair

$$s_3 = \frac{g_2}{\sqrt{s_2}} \tag{2.115}$$

$$p_3 = -\frac{2g_1 - 7s_2 + 10p_3^2 s_2}{6\sqrt{s_2}(-1 + 4p_3^2)}\,, \tag{2.116}$$

as can be checked directly.

The resulting faithful canonical realization is given by the second-order moments

$$\Delta(\pi^2) = p_1^2 + \frac{f_1(s_2, p_2, s_3, p_3)}{s_1^2} \tag{2.117}$$

$$\Delta(q\pi) = s_1 p_1 \tag{2.118}$$

$$\Delta(q^2) = s_1^2 \tag{2.119}$$

where

$$f_1(s_2, p_2, s_3, p_3) = -3\sqrt{s_2}\left(4s_3^2 - 1\right)p_3 + \frac{1}{2}\left(7 - 10s_3^2\right)s_2 - 16s_2^2 p_2^2\,, \tag{2.120}$$

and third-order moments

$$\Delta(\pi^3) = \frac{1}{\sqrt{s_2}s_1^3}\Phi(s_i, p_j)\left(\frac{U_1}{16s_2 s_3^2 - 4s_2}\right)^{1/4} \tag{2.121}$$

$$\Delta(q\pi^2) = \frac{1}{s_1\sqrt{s_2}}\left(p_1 s_1 + (s_3 - 1)\sqrt{s_2} + 4s_2 p_2\right) \times \left(p_1 s_1 + (s_3 + 1)\sqrt{s_2} + 4s_2 p_2\right)\left(\frac{U_1}{16s_2 s_3^2 - 4s_2}\right)^{1/4} \tag{2.122}$$

$$\Delta(q^2\pi) = \frac{1}{\sqrt{s_2}}\left(p_1 s_1^2 + s_1\left(p_3\sqrt{s_2} + 4s_2 p_2\right)\right)\left(\frac{U_1}{16s_2 s_3^2 - 4s_2}\right)^{1/4} \tag{2.123}$$

$$\Delta(q^3) = \frac{s_1^3}{\sqrt{s_2}}\left(\frac{U_1}{16s_2s_3^2-4s_2}\right)^{1/4} \tag{2.124}$$

with

$$\begin{aligned}\Phi(s_i,p_j) &= p_1^3s_1^3+3p_1^2s_1^2\sqrt{s_2}s_3+3p_1s_1s_2\left(s_3^2+4s_1p_1p_2-1\right)+64p_2^3s_2^3 \\ &\quad +s_2^{3/2}s_3\left(s_3^2+24s_1p_1p_2-7\right)+48p_2^2s_2^{5/2}s_3+12p_2s_2^2\left(s_3^2+4s_1p_1p_2-1\right).\end{aligned} \tag{2.125}$$

2.4.5 Momentum dependence

In [100], the moments are quadratic in the new momentum p_s. This property is useful because it implies an effective Hamiltonian (4.6) with standard kinetic term, quadratic in the classical momentum π (the expectation value) and the new momentum p_s related to $\Delta(\pi^2)$:

$$\begin{aligned}\langle\hat{H}\rangle &= \frac{\langle\hat{\pi}^2\rangle}{2m}+V(\hat{q})=\frac{\pi^2+\Delta(\pi^2)}{2m}+V(q)+\frac{1}{2}V''(q)\Delta(q^2)+\cdots \\ &= \frac{\pi^2}{2m}+\frac{p_s^2}{2m}+\frac{U}{2m}+V(q)+\frac{1}{2}V''(q)s^2+\cdots\end{aligned} \tag{2.126}$$

The corresponding property for a bosonic realization implies that generators of a Lie algebra have some terms bilinear in the boson variables. (However, bosonic realizations corresponding to canonical realizations of moment algebras cannot be completely bilinear, owing to Casimir terms such as U/s^2.) Our third-order realization for a single classical degree of freedom is similar in that $\Delta(\pi^2)$ is quadratic in the new momenta, altough with s-dependent coefficients.

Unlike the example of a single pair of degrees of freedom, the moments for two pairs of degrees of freedom, given so far, are not quadratic in the new momenta. In fact, we can prove by ansatz that, for a second-order semiclassical truncation for two classical degrees of freedom, there is no faithful representation quadratic in momenta with s-independent coefficients. The Poisson tensor has rank eight, so that we are looking for four canonical pairs (s_j,p_i) and two Casimir functions.

We write

$$\begin{aligned}
\Delta(\pi_1^2) &= p_1^2 + p_3^2 + F_1(s_i)p_1 + F_2(s_i)p_3 + F(s_i) \\
\Delta(\pi_2^2) &= p_2^2 + p_4^2 + G_1(s_i)p_2 + G_2(s_i)p_4 + G(s_i) \\
\Delta(\pi_1\pi_2) &= p_1p_2 + p_3p_4 + H_1(s_i)p_1 + H_2(s_i)p_2 + H_3(s_i)p_3 + H_4(s_i)p_4 + H_5(s_i)
\end{aligned} \tag{2.127}$$

and choose

$$\Delta(q_1^2) = s_1^2 + s_3^2 \quad , \quad \Delta(q_2^2) = s_2^2 + s_4^2 \quad , \quad \Delta(q_1q_2) = s_1s_2 + s_3s_4\,. \tag{2.128}$$

A realization of the entire algebra can be generated by taking Poisson brackets: We can compute

$$\Delta(\pi_1\pi_2) = \frac{1}{4}\left\{\left\{\Delta(q_1q_2), \Delta(\pi_2^2)\right\}, \Delta(\pi_1^2)\right\} \tag{2.129}$$

and, given this moment,

$$\Delta(q_1\pi_2) = \frac{1}{2}\{\Delta(q_1^2), \Delta(\pi_1\pi_2)\} \quad , \quad \Delta(q_2\pi_1) = \frac{1}{2}\{\Delta(q_2^2), \Delta(\pi_1\pi_2)\}\,. \tag{2.130}$$

Finally, once we know these three moments, we compute

$$\Delta(q_1\pi_1)+\Delta(q_2\pi_2) = \{\Delta(q_1q_2), \Delta(\pi_1\pi_2)\} \quad , \quad -\Delta(q_1\pi_1)+\Delta(q_2\pi_2) = \{\Delta(q_1\pi_2), \Delta(q_2\pi_1)\} \tag{2.131}$$

from which $\Delta(q_1\pi_1)$ and $\Delta(q_2\pi_2)$ follow from linear combinations. If $F_1 = F_2 = F_3 = 0$, $G_1 = G_2 = G_3 = 0$, and $H_1 = H_2 = H_3 = H_4 = H_5 = 0$, we have a non-faithful realization because there are no Casimir variables. We therefore have to find suitable functions depending on two additional variables, U_1 and U_2, such that the required Poisson brackets are realized.

Evaluating all Poisson brackets for consistency conditions, such as $\{\Delta(\pi_1^2), \Delta(\pi_2^2)\} = 0$, we find the following mapping:

$$\Delta(q_1^2) = s_1^2 + s_3^2 \tag{2.132}$$

$$\Delta(q_1\pi_1) = s_1p_1 + s_3p_3 + \frac{1}{2}s_1s_2U_1\left(\frac{1}{s_2^2} - \frac{1}{s_1^2}\right) + \frac{1}{2}s_3s_4U_2\left(\frac{1}{s_4^2} - \frac{1}{s_3^2}\right) \tag{2.133}$$

$$\Delta(\pi_1^2) = p_1^2 + p_3^2 + p_1s_2U_1\left(\frac{1}{s_2^2} - \frac{1}{s_1^2}\right) + p_3s_4U_2\left(\frac{1}{s_4^2} - \frac{1}{s_3^2}\right) \tag{2.134}$$

$$+\frac{1}{4}s_2^2U_1^2\left(\frac{1}{s_2^2}-\frac{1}{s_1^2}\right)^2+\frac{1}{4}s_4^2U_2^2\left(\frac{1}{s_4^2}-\frac{1}{s_3^2}\right)^2$$

for the first classical degree of freedom,

$$\begin{aligned}
\Delta(q_2^2) &= s_2^2+s_4^2 && (2.135)\\
\Delta(q_2\pi_2) &= s_2p_2+s_4p_4+\frac{1}{2}s_1s_2U_1\left(\frac{1}{s_1^2}-\frac{1}{s_2^2}\right)+\frac{1}{2}s_3s_4U_2\left(\frac{1}{s_3^2}-\frac{1}{s_4^2}\right) && (2.136)\\
\Delta(\pi_2^2) &= p_2^2+p_4^2+p_2s_1U_1\left(\frac{1}{s_1^2}-\frac{1}{s_2^2}\right)+p_4s_3U_2\left(\frac{1}{s_3^2}-\frac{1}{s_4^2}\right) && (2.137)\\
&\quad +\frac{1}{4}s_1^2U_1^2\left(\frac{1}{s_1^2}-\frac{1}{s_2^2}\right)^2+\frac{1}{4}s_3^2U_2^2\left(\frac{1}{s_3^2}-\frac{1}{s_4^2}\right)^2
\end{aligned}$$

for the second classical degree of freedom, and

$$\begin{aligned}
\Delta(q_1q_2) &= s_1s_2+s_3s_4 && (2.138)\\
\Delta(q_1\pi_2) &= s_1p_2+s_3p_4+\frac{1}{2}s_1^2U_1\left(\frac{1}{s_1^2}-\frac{1}{s_2^2}\right)+\frac{1}{2}s_3^2U_2\left(\frac{1}{s_3^2}-\frac{1}{s_4^2}\right) && (2.139)\\
\Delta(q_2\pi_1) &= s_2p_1+s_4p_3+\frac{1}{2}s_2^2U_1\left(\frac{1}{s_2^2}-\frac{1}{s_1^2}\right)+\frac{1}{2}s_4^2U_2\left(\frac{1}{s_4^2}-\frac{1}{s_3^2}\right) && (2.140)\\
\Delta(\pi_1\pi_2) &= p_1p_2+p_3p_4+\frac{1}{2}p_1s_1U_1\left(\frac{1}{s_1^2}-\frac{1}{s_2^2}\right)+\frac{1}{2}p_2s_2U_1\left(\frac{1}{s_2^2}-\frac{1}{s_1^2}\right) && (2.141)\\
&\quad +\frac{1}{2}p_3s_3U_2\left(\frac{1}{s_3^2}-\frac{1}{s_4^2}\right)+\frac{1}{2}p_4s_4U_2\left(\frac{1}{s_4^2}-\frac{1}{s_3^2}\right)\\
&\quad -\frac{1}{4}s_1s_2U_1^2\left(\frac{1}{s_2^2}-\frac{1}{s_1^2}\right)^2-\frac{1}{4}s_3s_4U_2^2\left(\frac{1}{s_4^2}-\frac{1}{s_3^2}\right)^2
\end{aligned}$$

for the cross-covariances.

If the two free parameters U_1 and U_2 were independent Casimir functions, we would have a faithful canonical realization. However, the rank of the Jacobian of the transformation from (s_i, p_j, U_I) to the moments can be seen to equal seven, and therefore the realization is not faithful. Moreover, the quadratic Casimir of the algebra,

$$C_2 = \mathrm{tr}\left((\tau\Delta)^2)\right), \qquad (2.142)$$

can be computed explicitly and does not equal a function of U_1 and U_2 — it depends

on the coordinates as well. If the map were faithful, we would have

$$\frac{\partial C_2}{\partial s_i} = \frac{\partial C_2}{\partial p_j} = 0\,. \tag{2.143}$$

Finally, we note that the canonical transformation

$$\begin{aligned} P_1 &= p_1 + \frac{1}{2} s_2 U_1 \left(\frac{1}{s_2^2} - \frac{1}{s_1^2} \right) \quad , \quad P_2 = p_2 + \frac{1}{2} s_1 U_1 \left(\frac{1}{s_1^2} - \frac{1}{s_2^2} \right) \\ P_3 &= p_3 + \frac{1}{2} s_4 U_2 \left(\frac{1}{s_4^2} - \frac{1}{s_3^2} \right) \quad , \quad P_4 = p_4 + \frac{1}{2} s_3 U_2 \left(\frac{1}{s_3^2} - \frac{1}{s_4^2} \right) \end{aligned}$$

and $S_i = s_i$ maps our realization to the non-faithful

$$\begin{aligned} &\Delta(q_1^2) = S_1^2 + S_3^2 \quad , \quad \Delta(q_1\pi_1) = S_1 P_1 + S_3 P_3 \quad , \quad \Delta(\pi_1^2) = P_1^2 + P_3^2 \\ &\Delta(q_2^2) = S_2^2 + S_4^2 \quad , \quad \Delta(q_2\pi_2) = S_2 P_2 + S_4 P_4 \quad , \quad \Delta(\pi_2^2) = P_2^2 + P_4^2 \\ &\Delta(q_1 q_2) = S_1 S_2 + S_3 S_4 \quad , \quad \Delta(q_1\pi_2) = S_1 P_2 + S_3 P_4 \\ &\Delta(q_2\pi_1) = S_2 P_1 + S_4 P_3 \quad , \quad \Delta(\pi_1\pi_2) = P_1 P_2 + P_3 P_4\,, \end{aligned}$$

in which there are no free parameters that could play the role of Casimir functions. The only possibilities are therefore realizations non-quadratic in momenta, or with non-standard, s-dependent kinetic terms. None of these options can lead to a bilinear bosonic realization.

2.4.6 Realizations of $\mathrm{sp}(2n, \mathbb{R})$

The isomorphism between second-order semiclassical truncations and $\mathrm{sp}(2n, \mathbb{R})$ implies that faithful bosonic realizations of $\mathrm{sp}(4, \mathbb{R})$ cannot be bilinear in the boson variables. This result underlines some of the difficulties in finding such realizations pointed out in [119, 120]. Given the generators A_{ij} $(i \leq j)$, B_{ij} $(i \leq j)$ and C_{ij}, $i, j = 1, \ldots, N$, of $\mathrm{sp}(2N, \mathbb{R})$ with relations (5.26), it is easy to see that an explicit isomorphism between $\mathrm{sp}(2N, \mathbb{R})$ and the second-order semiclassical truncation with N classical degrees of freedom is given by

$$A_{ij} = \Delta(\pi_i \pi_j) \quad , \quad B_{ij} = \Delta(q_i q_j) \quad , \quad C_{ij} = \Delta(q_i \pi_j)\,. \tag{2.144}$$

In particular, for $\mathrm{sp}(4, \mathbb{R})$ we obtain a realization from (2.93)–(2.102) with

four bosonic variables $b_1 = \frac{1}{\sqrt{2}}(s_1 + ip_1)$, $b_2 = \frac{1}{\sqrt{2}}(s_2 + ip_2)$, $b_3 = \frac{1}{\sqrt{2}}(s_3 + ip_3)$ and $b_4 = \frac{1}{\sqrt{2}}(s_4 + ip_4)$, in addition to two Casimir variables U_1 and U_2. We do not reproduce here all generators obtained by substituting bosonic variables in (2.93)–(2.102), but note that the resulting expressions are rather different from the non-faithful form (5.25). Even the moments that are bilinear in bosonic variables, such as $B_{11} = s_1^2 = \frac{1}{2}(b_1 + b_1^*)^2$ or $C_{11} = s_1 p_1 = \frac{1}{2} i\left((b_1^*)^2 - b_1^2\right)$, depend on different combinations of the b_i. These changes are required to maintain the reality conditions implied by a bosonic realization. Moreover, our realization brings in the two Casimir variables U_1 and U_2 in a way that requires a non-bilinear realization.

2.5 Parametric resonance of fluctuations in coupled oscillators

In order to illustrate the usefulness of canonical realizations for physical applications, we analyze the problem of parametric resonance in a quantum system of coupled oscillators, based on the classical Hamiltonian

$$H = \frac{1}{2}\left(\pi_1^2 + \pi_2^2\right) + \frac{1}{2}\left(q_1^2 + q_2^2\right) + \gamma(t) q_1 q_2 \,. \tag{2.145}$$

If $\gamma(t)$ is a small periodic function, one can apply time-dependent perturbation theory to the corresponding quantum problem. However, if $\gamma(t)$ has twice the natural frequency ($\omega = 1$) of the uncoupled system, as we will show, parametric resonance leads to large fluctuations that may violate the perturbation assumption. Our second-order canonical realization, on the other hand, presents exact results for the quadratic Hamiltonian (2.145), which we display here in analytic form. The canonical nature of our system allows us to adapt standard classical methods of parametric resonance to the quantum problem.

A time independent canonical rotation by $\frac{1}{4}\pi$ radians decouples the two oscillators:

$$H = \frac{1}{2}\bar{\pi}_1^2 + \frac{1}{2}\bar{\pi}_2^2 + \frac{1}{2}(1 + \gamma(t))\bar{q}_1^2 + \frac{1}{2}(1 - \gamma(t))\bar{q}_2^2 \tag{2.146}$$

in the rotated canonical variables $(\bar{q}_i, \bar{\pi}_j)$. The quantizations of (2.145) and (2.146) are unitarly equivalent, but the quantization of (2.146) is easier to analyze and will be used here.

In a canonical realization of the second-order semiclassical truncation, the quantum Hamiltonian takes the form

$$\begin{aligned} H_{\rm Q} &= \tfrac{1}{2}\bar{\pi}_1^2 + \tfrac{1}{2}\bar{\pi}_2^2 + \tfrac{1}{2}(1+\gamma)\bar{q}_1^2 + \tfrac{1}{2}(1-\gamma)\bar{q}_2^2 \\ &+ \tfrac{1}{2}p_1^2 + \tfrac{1}{2}p_2^2 + \tfrac{1}{2}\tfrac{U_1}{s_1^2} + \tfrac{1}{2}\tfrac{U_2}{s_2^2} + \tfrac{1}{2}(1+\gamma)s_1^2 + \tfrac{1}{2}(1-\gamma)s_2^2 \,. \end{aligned} \tag{2.147}$$

Since the oscillators are decoupled, we have used two individual realizations for a single degree of freedom, and can set $U_1 = U_2 = 1/4$ (using $\hbar = 1$) with zero cross-correlations for the ground state. Moreover, all cross-correlations should remain zero in this coordinate system, because their equations of motion form a four dimensional autonomous system that is non-degenerate. Once the analysis has been done in this coordinate system the results can be transformed into the original coordinate system by applying the inverse of the canonical rotation. The coupling in the original system then illustrates some features of our new canonical variables, such as the correlation angle θ introduced in Sec. **??**.

Unlike the classical Hamiltonian, the quantum Hamiltonian $H_{\rm Q}$ is not quadratic. As we will see, the nonlinear nature of the fluctuation dynamics implies new resonance properties for suitable choices of $\gamma(t)$. The Hamiltonian (2.147) is the sum of four uncoupled Hamiltonians, two classical ones and two for the fluctuations. In order to isolate the dynamics of fluctuations, we can focus on one of the fluctuation Hamiltonians,

$$H_{\rm fluc} = \frac{1}{2}p_s^2 + \frac{U}{2s^2} + \frac{1}{2}\,(1+\gamma)\,s^2 \,. \tag{2.148}$$

We recognize this as the radial part of the Hamiltonian of a two-dimensional harmonic oscillator, such that $\frac{1}{2}U/s^2$ is analogous to the centrifugal term. Introducing a spurious degree of freedom, ϕ, we make the identifications

$$U = \text{const} = L^2 = (s^2\dot{\phi})^2 \geq \frac{1}{4} \tag{2.149}$$

$$x = s\cos(\phi) \quad , \quad y = s\sin(\phi) \quad , \quad s^2 = x^2 + y^2 \,. \tag{2.150}$$

The fluctuation Hamiltonian

$$H_{\rm fluc}^{xy} = \frac{1}{2}p_x^2 + \frac{1}{2}p_y^2 + \frac{1}{2}\,(1+\gamma)\,x^2 + \frac{1}{2}\,(1+\gamma)\,y^2 \tag{2.151}$$

is now quadratic, but with additional degrees of freedom.

Equation (2.149) gives us constraints on the initial values. Starting in the harmonic-oscillator ground state, we have the initial values $s_0 = 1/\sqrt{2}$ and $p_{s,0} = 0$ as well as $U = 1/4$. Thus, $x_0^2 + y_0^2 = \frac{1}{2}$ and $x_0\dot{x}_0 + y_0\dot{y}_0 = 0$. Moreover, $s^2\dot{\phi} = \sqrt{U} = \frac{1}{2}$ implies $\dot{\phi}_0 = 1$. Finally, there is an arbitrary initial phase $\alpha = \phi_0$ which arises because of the spurious nature of the coordinate ϕ. We thus arrive at the initial conditions

$$x_0 = \frac{1}{\sqrt{2}}\cos(\alpha) \quad , \quad y_0 = \frac{1}{\sqrt{2}}\sin(\alpha) \tag{2.152}$$

$$p_{x0} = -\frac{1}{\sqrt{2}}\sin(\alpha) \quad , \quad p_{y0} = \frac{1}{\sqrt{2}}\cos(\alpha) \tag{2.153}$$

using $L = x_0 p_{y0} - y_0 p_{x0} = 1/2$. Each of the two oscillators starts with a non-zero fluctuation energy because of Heisenberg's uncertainty principle.

We now choose $\gamma = \gamma_0 \sin(2\Omega t)$, where Ω is a parameter we can tune. The choice of $\Omega \approx 1$ is of particular interest because it causes the fluctuations to grow parametrically. We proceed by analyzing the equations of motion of one of the auxiliary quantum degrees of freedom, x:

$$\ddot{x} + (1 + \gamma_0 \sin(2\Omega t))\, x = 0\,. \tag{2.154}$$

We make the ansatz

$$x(t) = A(t)\cos(\Omega t) + B(t)\sin(\Omega t) \tag{2.155}$$

where A and B are assumed to vary slowly compared with the trigonometric functions. Our initial conditions imply $A(0) = x_0$ and $B(0) = p_{x0}$.

We now apply standard methods of parametric resonance. Using (2.154) and neglecting second-order derivatives of A and B as well as higher-frequency terms, we find

$$\dot{A} = \frac{\gamma_0}{4\Omega}A - \frac{1}{2\Omega}\left(\Omega^2 - 1\right)B \tag{2.156}$$

$$\dot{B} = \frac{1}{2\Omega}\left(\Omega^2 - 1\right)A - \frac{\gamma_0}{4\Omega}B\,. \tag{2.157}$$

This system of linear equations has the eigenvalues

$$\lambda_{\pm} = \pm\sqrt{\left(\frac{\gamma_0}{4\Omega}\right)^2 - \left(\frac{\Omega^2-1}{2\Omega}\right)^2}. \tag{2.158}$$

Therefore, if $\Omega \in \left[\sqrt{1-\gamma_0/2}, \sqrt{1+\gamma_0/2}\right]$ there is one solution that grows exponentially, and one that decays exponentially. For generic initial conditions, this system has the solution

$$A = x_0 \cosh(\lambda t) + x_0 \frac{\gamma_0}{4\Omega}\frac{\sinh(\lambda t)}{\lambda} - p_{x0}\left(\frac{\Omega^2-1}{2\Omega}\right)\frac{\sinh(\lambda t)}{\lambda} \tag{2.159}$$

$$B = \left(\cosh(\lambda t) - \frac{\gamma_0}{4\Omega}\frac{\sinh(\lambda t)}{\lambda}\right) p_{x0} + x_0\left(\frac{\Omega^2-1}{2\Omega}\right)\frac{\sinh(\lambda t)}{\lambda}. \tag{2.160}$$

The case $\Omega = 1$ leads to more manageable solutions:

$$A = x_0 \exp\left(\frac{\gamma_0}{4}t\right) \quad , \quad B = p_{x0}\exp\left(-\frac{\gamma_0}{4}t\right) \tag{2.161}$$

and thus

$$x(t) = \frac{1}{\sqrt{2}}\cos(\alpha)\exp\left(\frac{\gamma_0}{4}t\right)\cos(t) - \frac{1}{\sqrt{2}}\sin(\alpha)\exp\left(-\frac{\gamma_0}{4}t\right)\sin(t) \tag{2.162}$$

for the required initial values. Similarly, the second auxiliary degree of freedom has the solution

$$y(t) = \frac{1}{\sqrt{2}}\sin(\alpha)\exp\left(\frac{\gamma_0}{4}t\right)\cos(t) + \frac{1}{\sqrt{2}}\cos(\alpha)\exp\left(-\frac{\gamma_0}{4}t\right)\sin(t). \tag{2.163}$$

For the fluctuations, we obtain

$$s_1^2 = x^2 + y^2 = \frac{1}{2}\exp\left(\frac{\gamma_0 t}{2}\right)\cos(t)^2 + \frac{1}{2}\exp\left(-\frac{\gamma_0 t}{2}\right)\sin(t)^2 \tag{2.164}$$

and, making the replacement $\gamma_0 \to -\gamma_0$,

$$s_2^2 = \frac{1}{2}\exp\left(-\frac{\gamma_0 t}{2}\right)\cos(t)^2 + \frac{1}{2}\exp\left(\frac{\gamma_0 t}{2}\right)\sin(t)^2. \tag{2.165}$$

The system has now been approximately solved in this coordinate system using an adiabatic approximation at (2.156). We still need to rotate back to the original

coordinate system. For global linear transformations the moments of the states transform like tensors

$$\Delta = \mathcal{O}^\dagger \bar{\Delta} \mathcal{O} \tag{2.166}$$

because the Poisson structure is conserved by this transformation. Using (2.166) we find,

$$\Delta(q_1 q_2) = \frac{1}{2}(s_1^2 - s_2^2) \tag{2.167}$$

$$\Delta(q_1^2) = \Delta(q_2^2) = \frac{1}{2}\left(s_1^2 + s_2^2\right) . \tag{2.168}$$

We can isolate the canonical angle of the correlation function

$$\theta = \arccos\left(\frac{\Delta(q_1 q_2)}{\sqrt{\Delta(q_1^2)\Delta(q_2^2)}}\right) \tag{2.169}$$

which, in the late-time limit, reduces to linear growth,

$$\theta_\infty \sim 2t\,. \tag{2.170}$$

The canonical angle therefore phase locks with the pumping signal. The moment $\Delta(q_1\pi_1)$ can be found as well, with the result

$$\Delta(q_1\pi_1) = \frac{1}{2}(s_1 p_1 + s_2 p_2) = \frac{\gamma}{8}\sinh\left(\frac{1}{2}\gamma t\right). \tag{2.171}$$

The momentum dispersion is more complicated and we omit it here, but it can be derived analytically. We can however write down the Heisenberg uncertainty for each oscillator,

$$U_{1/2} = \frac{1}{16}\frac{14 + \gamma^2 + (2+\gamma^2)\cos(4t) + 16\cosh(\gamma t) + 4\cosh(2\gamma t)\sin(2t)^2 - 4\gamma\sin 4t\sinh t\gamma}{6 + 2\cos(4t) - 2\cos 4t\cosh t\gamma + 2\cosh t\gamma}$$

with exponential asymptotic behavior

$$U_\infty \sim \frac{1}{16}\exp(\gamma t)\,. \tag{2.172}$$

The quadratic Casimir, by contrast, is an exact constant of motion for this system, which can be confirmed explicitly despite the complexity of some of the correlation

functions, and even after using an adiabatic approximation:

$$C_2(t) \equiv \frac{1}{2} \tag{2.173}$$

This analysis would have been harder using other methods. The canonical structure of our realization helped us to map the non-linear fluctuation dynamics to a two-dimensional linear system. It therefore allowed us to make direct contact with the literature on parametric resonance, without having to reinvent this analysis for the corresponding ten-dimensional autonomous system of quantum moments. Furthermore, the usage of canonical variables is fairly general as it only relies on the Poisson bracket of the moments and not on the specific Hamiltonian. The effort put into finding this canonical mapping can therefore be spent in other problems as well.

Chapter 3
Canonical tunneling time in ionization experiments

3.1 Introduction

Our goal in this chapter is to apply the methods developed in chapter 2 to the problem of tunneling times. That is, we want to address the question "How much time does a particle take to tunnel through a barrier?". Detailed observations of atom ionization have recently become possible with attoclock experiments [44,69,70], suggesting comparisons with various predictions of tunneling times. The theoretical side of the question, however, remains largely open: Different proposals of how to define tunneling times have been made through almost nine decades, yielding widely diverging predictions and physical interpretations [71, 72]. Even the extraction of tunneling times from experiments has been performed in different ways [47–52], and the original conclusion of a non-zero result has been challenged [53–55]. The situation therefore remains far from being clarified, and a continuing analysis of fundamental aspects of tunneling is important.

A recent approach to understand the tunneling dynamics in this context is the application of Bohmian quantum mechanics [56, 57], in which the prominent role played by trajectories provides a more direct handle on tunneling times [79]. However, through initial conditions, the ensemble of trajectories remains subject to statistical fluctuations. An alternative trajectory approach, which we will develop in this paper, is to consider, in an extension of Ehrenfest's theorem, the evolution of expectation values and fluctuations, possibly together with higher-order moments

of a state. By including moments of a probability distribution, such an approach remains statistical in order to capture quantum properties, but it provides a unique trajectory starting with the expectation values and fluctuations of a given initial state. The ensemble of trajectories used in Bohmian quantum mechanics is replaced by a single trajectory in an extended phase space, enlarged by fluctuations and higher moments as non-classical dimensions.

In the context of tunneling, a semiclassical version of this proposal has been used occasionally in quantum chemistry [99, 100], which we extend here to higher orders and apply to models of atom ionization. Unlike Bohmian quantum mechanics, these methods present an approximation to standard quantum mechanics, rather than a new formulation. Nevertheless, since they lead to a single trajectory rather than a statistical ensemble of trajectories, they provide a crucial advantage which, we hope, can help to clarify the question of tunneling times in atom ionization.

In [79], it has been shown that a trajectory approach based on Bohmian quantum mechanics reliably shows non-zero tunneling times in atomic models of ionization. There is therefore a tension with recent evaluations of ionization experiments which give the impression of zero tunneling delays [54]. The latter results are based on a definition of the tunneling exit time through classical back-propagation [53]: Since the energy of a tunneling electron in a time-dependent electric field is not conserved and usually unkonwn in experiments, it is difficult to apply the intuitive definition of the tunneling exit as the time when the electron's energy equals the classical potential. As an alternative, classical back-propagation evolves the final state of a measured electron back toward the atom using classical equations of motion, and defines the tunneling exit as the time when the momentum in the direction of the electric field is zero, taking the point closest to the atom in the event that this condition may be realized multiple times. As already noted in [79], this condition is conceptually problematic because it uses classical physics near a turning point, where the equations governing a classically back-propagated trajectory are usually expected to break down. We will use our single-trajectory approach to compare a quantum trajectory with a classical back-propagated one.

In addition, our analysis will allow us to derive further properties of the tunneling process. In order to obtain a single trajectory describing an evolving quantum state, we write evolution of a quantum state in terms of a classical-type system with quantum corrections, in which the expectation values of position and momen-

tum are coupled to fluctuations. The coupling terms, quite generally, lower the classical barrier such that the classical-type system can move "around" it in an extended phase space with a real-valued velocity. This detour has a certain duration, depending on initial conditions, and provides a natural definition of tunneling time.

It turns out that several new ingredients are necessary compared with existing treatments in quantum chemistry. For instance, semiclassical states are not always sufficient for a full description of tunneling. This fact is not surprising because, intuitively, a tunneling wave splits up into two wave packets separated by the barrier width. Deep tunneling then implies states with large fluctuations, even if each wave packet remains sharp and perhaps nearly Gaussian. Moreover, fluctuation terms do not always lower the barrier enough to make tunneling possible at all energies for which quantum tunneling occurs. In [100], the classical-type system used for tunneling has been extended to moments of up to fourth order, with a clear improvement of predicted tunneling times closer to what follows from wave-function evolution. However, the extension was done mainly at a numerical level, which does not provide much intuition about the tunneling process in a given potential. To second order, by contrast, an effective potential was used in [99, 100] which shows how the classical barrier can be lowered by quantum fluctuations. One of our main new ingredients is an extension of such effective potentials to higher orders.

In Sec. 3.2 we describe quantum dynamics using canonical semiclassical methods and present a new effective potential that includes effects from higher-order moments. In Sec. 3.3, we introduce various models of atom ionization in which our methods can be applied, and discuss specific results focusing on tests of tunneling conditions and the definition of tunneling times.

3.2 Quantum dynamics by canonical effective methods

Using canonical effective methods [92, 93], we describe the dynamics of a quantum state by coupled ordinary differential equations for the expectation values $x = \langle\hat{x}\rangle$ and $p = \langle\hat{p}\rangle$ coupled to central, Weyl-ordered moments

$$\Delta(x^a p^b) = \langle(\hat{x} - x)^a (\hat{p} - p)^b\rangle_{\rm Weyl}\,. \tag{3.1}$$

(In this notation, the usual fluctuations are written as $\Delta(x^2) = (\Delta x)^2$ and $\Delta(p^2) = (\Delta p)^2$, while $\Delta(xp)$ is the covariance.)

The Hamiltonian operator $H(\hat{x}, \hat{p})$ implies the quantum Hamiltonian

$$\begin{aligned} H_{\rm Q} &= \langle H(\hat{x} + (\hat{x} - x), \hat{p} + (\hat{p} - p))\rangle \\ &= H(x,p) + \sum_{n=2}^{\infty} \sum_{a=0}^{n} \left(\begin{array}{c} n \\ a \end{array} \right) \frac{\partial^n H(x,p)}{\partial x^a \partial p^{n-a}} \Delta(x^a p^{n-a}) \end{aligned} \tag{3.2}$$

with the classical Hamiltonian $H(x,p)$. Hamiltonian equations for moments are generated using the Poisson bracket

$$\{\langle \hat{A}\rangle, \langle \hat{B}\rangle\} = \frac{\langle [\hat{A}, \hat{B}]\rangle}{i\hbar}\,, \tag{3.3}$$

derived from the commutator and extended to moments by using linearity and the Leibniz rule.

Unfortunately, the Poisson brackets between moments are rather complicated at higher orders, and they are not canonical. For instance,

$$\{\Delta(x^2), \Delta(xp)\} = 2\Delta(x^2) \quad , \quad \{\Delta(x^2), \Delta(p^2)\} = 4\Delta(xp) \quad , \quad \{\Delta(xp), \Delta(p^2)\} = 2\Delta(p^2)\,, \tag{3.4}$$

corresponding to the Lie algebra $\mathrm{sp}(2, \mathbb{R})$, but those of higher moments are in general non-linear. For these second-order moments, canonical variables were introduced in [99, 100]:

$$s = \sqrt{\Delta(x^2)} \quad , \quad p_s = \frac{\Delta(xp)}{\sqrt{\Delta(x^2)}} \tag{3.5}$$

together with a third variable, $U = \Delta(x^2)\Delta(p^2) - \Delta(xp)^2$, which has zero Poisson brackets with s and p_s. Inverting these relationships, we write the second-order moments

$$\Delta(x^2) = s^2 \quad , \quad \Delta(xp) = sp_s \quad , \quad \Delta(p^2) = p_s^2 + \frac{U}{s^2} \tag{3.6}$$

in terms of canonical variables (s, p_s) and a conserved quantity U. To second order, the quantum Hamiltonian can then be expressed as

$$\langle \hat{H}\rangle = \frac{\langle \hat{p}^2\rangle}{2m} + \langle V(\hat{x})\rangle$$

$$\approx \frac{\langle\hat{p}\rangle^2}{2m} + \frac{(\Delta p)^2}{2m} + V(\langle\hat{x}\rangle) + \frac{1}{2}V''(\langle\hat{x}\rangle)(\Delta x)^2 = \frac{p^2+p_s^2}{2m} + V_{\rm eff}(x,s) \quad (3.7)$$

with the effective potential

$$V_{\rm eff}(x,s) = V(x) + \frac{U}{2ms^2} + \frac{1}{2}V''(x)s^2\,. \quad (3.8)$$

An extension to higher orders turns out to be more involved, but it can be accomplished with the new methods developed in [115]. The canonical form of higher-order moments then gives useful higher-order effective potentials, and it suggests closure conditions, in the sense of [101], that can be used to turn the infinite set of moments into finite approximations.

We introduce closure conditions based on the following properties of higher moments which we have confirmed for up to fourth order [65]: the second-order variable s also contributes to an n-th order moment, in the form $\langle(\hat{x}-\langle\hat{x}\rangle)^n\rangle \approx s^n$, in addition to terms that depend on new degrees of freedom. Moments of odd and even order, respectively, often behave rather differently from each other. For instance, a Gaussian has zero odd-order moments, a property which extends to generic states that evolve adiabatically in symmetric potentials [92]. This difference is reflected in mathematical properties of the canonical variables. At third order, for instance, there are three canonical coordinates, s_1, s_2 and s_3, such that $\langle(\hat{x}-\langle\hat{x}\rangle)^3\rangle \propto s_1^3+s_2^3+s_3^3$. The constant of proportionality has zero Poisson brackets with the canonical variables but is state dependent. As an approximation, we set this constant equal to zero, reducing the number of degrees of freedom. If we assume this behavior also for orders greater than four, we can complete the Taylor expansion in (3.2) and derive the all-orders effective potential

$$\begin{aligned} V_{\rm eff}(x,s) &= \frac{U}{2ms^2} + V(x) + \sum_{n=1}^{\infty}\frac{1}{2n!}\frac{{\rm d}^{2n}(V(x))}{{\rm d}x^{2n}}s^{2n} \\ &= \frac{U}{2ms^2} + \frac{1}{2}\left(V(x+s)+V(x-s)\right)\,. \end{aligned} \quad (3.9)$$

Heuristically, therefore, the particle does not follow a potential local in x, but rather is feeling around itself at a distance s. This distance increases as the wave function spreads out.

We have moved beyond the semi-classical approximation by replacing a strict

truncation with a specific behavior of the moments. This extension is crucial for our purposes because tunneling states or the ground states of an electron in most atoms are not semi-classical. A semi-classical approximation should then not be expected to give accurate results in situations where the tunneling times are very long, or the electron spends a fair amount of time in states close to the ground state.

3.3 Effective theory of tunneling ionization

In order to test various aspects that have been found to be relevant for tunneling times in ionization experiments, we discuss properties and results of different models. An application to tunneling ionization requires an extension of (3.9) to three dimensions. The main question is then how to deal with cross-correlations between different coordinates, which significantly enlarge the phase space. Motivated by the intuition that a tunneling wave packet should split up predominantly in the direction of the force that lowers the confining potential of a bound state, we assume that the main moments to be considered are the two fluctuations (position and momentum) in the direction of the force. These moments then play the role of reaction coordinates [66], which reduce a large parameter space to a few significant variables.

The relationship to the direction of the force implies a crucial difference between the treatment of a constant force and time-dependent, rotating forces as used in attoclock experiments. We first deal with examples subject to a constant force in order to illustrate the tunneling process with our new methods, and then show how time-dependent forces alter the conclusions.

3.3.1 Coulomb potential in a static electromagnetic field

As usual, we can treat tunneling ionization as a a single electron moving in an effective potential with two contributions: a spherically symmetric term for interactions with the nucleus and the remaining electrons, and a linear potential in the direction of the electric field. Assuming that correlations between the independent coordinates can be ignored, an approximation that can be expected to be valid during most of the tunneling process which affects mainly one of the

coordinates, the all-orders effective potential (3.9) for the 3-dimensional Coulomb interaction and the electric field strength F is then

$$V_{\text{eff}}(x_i, s_j) = \sum_{i=1}^{3} \frac{U}{2s_i^2} + \frac{1}{8} \sum_{\{n_i=0,1\}} V\left(x_i + (-1)^{n_i} s_i\right) , \tag{3.10}$$

where

$$V(\vec{x}) = -\frac{1}{|\vec{x}|} - \vec{x} \cdot \vec{F} - \frac{\alpha_I \vec{F} \cdot \vec{x}}{|\vec{x}|^3} \tag{3.11}$$

is the classical potential and α_I is the static polarizability of the ion. (We set $\vec{x} = (x, y, z)$ and use atomic units $\hbar = e = m_e = k_e = 1$ throughout the paper.)

Evolution in the effective potential requires initial values of x_i, s_i, p_i and p_{s_i}. Since these describe expectation values and fluctuations, they could in principle be determined from an initial atomic state. However, it is more useful to minimize the energy in the field-free ($\vec{F} = 0$) effective potential (3.10), in order to fix these initial values within our approximation. That is, to get initial values for the canonical variables we minimize $\frac{1}{2}\sum(p_i^2 + p_{s_i}^2) + V_{\text{eff}}(\vec{x}, \vec{s})$ in the absence of the electric field. We find

$$s_i^0 = \frac{3\sqrt{3}}{4} \quad \text{and} \quad p_i^0 = p_{s_i}^0 = x_i^0 = 0 \tag{3.12}$$

for $i = 1, 2, 3$. These values, taken as initial conditions for tunneling with a non-zero field, result in a ionization potential of $I_p = -2/9$ which in our model corresponds the ground-state energy E_{ground} in the absence of the electric field.

We choose our coordinate system such that the x_3-axis points in the direction of the force. Figure 3.1 shows the ground-state equipotential line of (3.10) in the $x_3 - s_3$ plane for both Argon ($\alpha_I = 7$) and Krypton ($\alpha_I = 11$), as well as the behavior of the fluctuation parameter s_3 with respect to the direction along x_3. When the field strength is small enough, the equipotential line of the ground state literally forms a tunnel that the electron has to follow in order to escape. The tunneling time is related to the amount of time spent in this tunnel. At this point, we can see the importance of our extension beyond semiclassical effective potentials. The quadratic s-term in (3.8) reduces the classical barrier monotonically in the s-direction, giving us a steep slope instead of a tunnel. Numerical solutions in such a potential show that the resulting tunneling times would be too large because

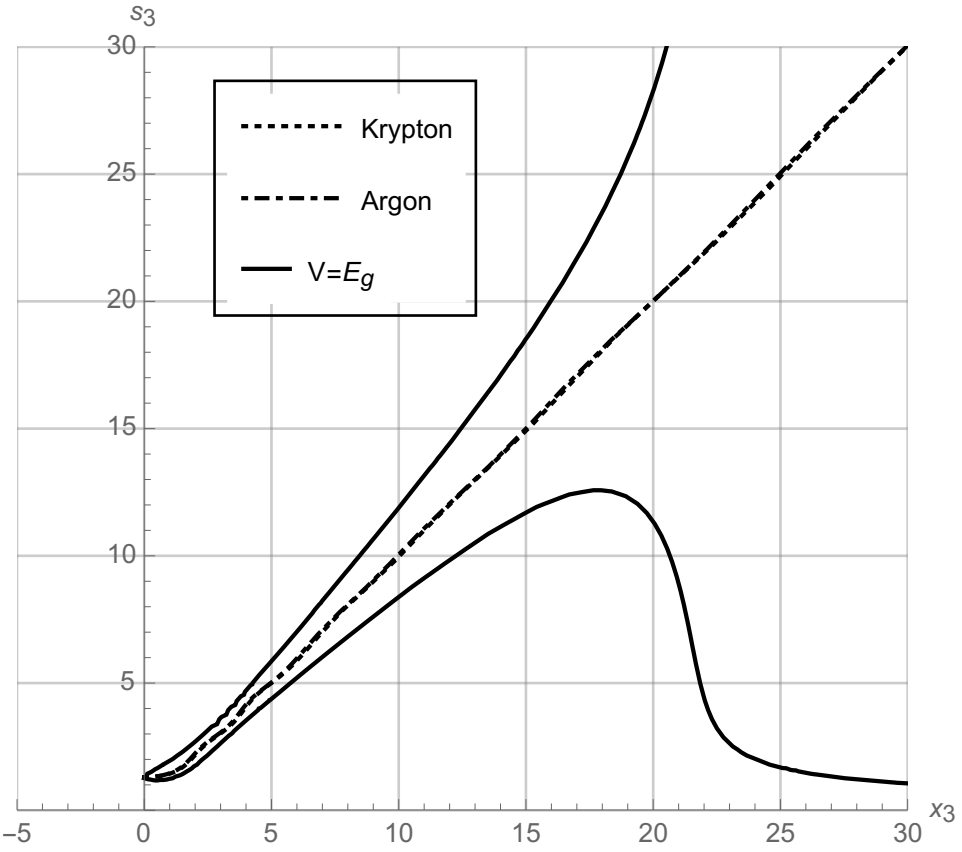

Figure 3.1. A contour plot of the effective potential for both Argon ($\alpha_I = 7$) and Krypton ($\alpha_I = 11$). The solid curve is the equipotential line, $V_{\text{eff}} = E_{\text{ground}} = -2/9$ for the approximate ground-state energy corresponding to (3.12). It shows the location of the classical barrier in the presence of a field $F = 0.015$ (a laser intensity of $I \sim 0.8 \cdot 10^{14}\text{W/cm}^2$). The path of the electron is shown here by the (almost overlapping) dashed lines for Argon and Krypton. The electron escaping from either atom has to travel along an actual tunnel, formed by the equi-potential line in phase space.

trajectories get dragged into the s-direction with little movement in the x-direction. The tunnel in our all-orders potential, by contrast, guides the trajectories such that they still move substantially in the x_3-direction. Corresponding tunneling times are significantly shorter.

Our dynamical system contains not only expectation values but also the fluctuation variables s_i and p_{s_i}, related to Δx_i and Δp_i as in (3.6). As shown in Fig. 3.2, our effective evolution is self-consistent in the sense that it is indeed only the fluctuation s_3 in the direction of the force (our reaction coordinate) that increases

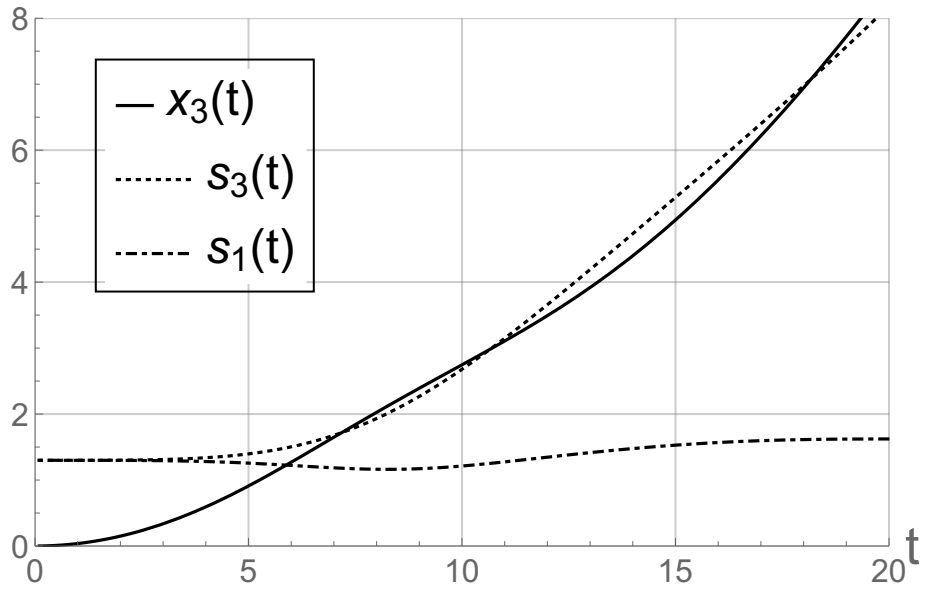

Figure 3.2. Trajectories of the tunneling coordinate x_3, its fluctuation s_3 and the fluctuation s_1 for Argon. The behavior for Krypton is qualitatively similar.

significantly, while s_1 and s_2 remain nearly constant. Nevertheless, the behavior of the transversal position fluctations, shown in Fig. 3.3 for the example of s_1 at the tunneling exit, is also of interest: There is a local minimum with a value less than the ground-state fluctuation (3.12). At higher intensities, the fluctuations level off because in a strong field they do not have much time to change. Moreover, these fluctuations depend more strongly on the element used compared to the trajectories in Fig. 3.1 for variables in the direction of the force, or the tunneling time to which we turn now.

Using the all-orders potential in a static field, we estimate the tunneling time in Argon and Krypton as a function of the laser intensity. The tunneling time is determined by how long the particle travels from one turning point to another in a state parameterized by x_i and s_i. The tunneling times for both Argon and Krypton in the range of laser intensities used in [70], are shown in Fig. 3.4. We see tunneling at all relevant scales, and qualitative agreement with the calculations from Wigner formalism used in [70].

Traditionally, proposed tunneling times have often been expressed as integral formulas, motivated by the WKB approximation. Our effective potential can be used to derive a new version if we eliminate some of the basic variables in further

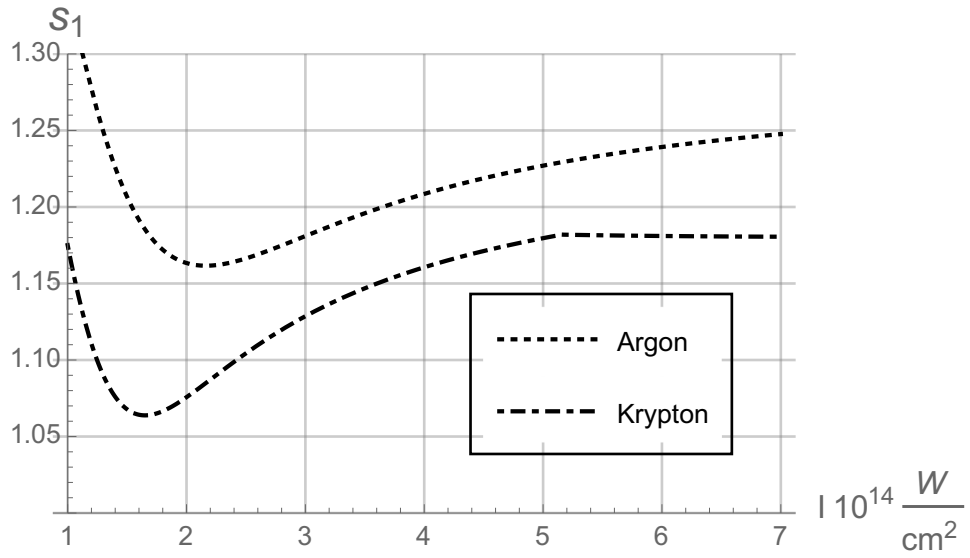

Figure 3.3. The transverse exit fluctuation s_1 over the observable range of laser intensities for Argon and Krypton.

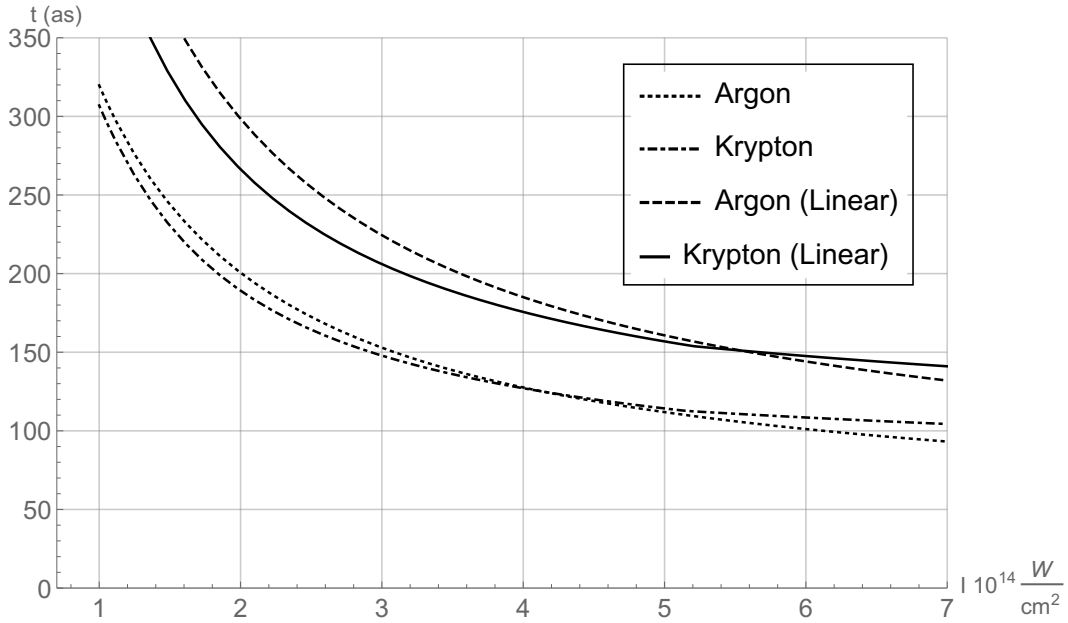

Figure 3.4. Tunneling times for Argon and Krypton. The dashed (Argon) and solid (Krypton) lines correspond to the approximation (3.13) with $s_3 \approx x_3$. The range of the laser intensity is obtained by scaling the electric field $I = \frac{1}{2}c\epsilon_0 F^2$. Time variables are scaled to atto-seconds from atomic units.

approximations. As suggested by Figs. 3.1 and 3.2, we may assume that $s_3 \approx x_3$ inside the barrier. The tunneling time can then be written as

$$\tau \approx \int_0^{x_3^*} \frac{\mathrm{d}x_3}{p_3} \approx \int_0^{x_3^*} \frac{\mathrm{d}x_3}{\sqrt{-E_{\mathrm{ground}} - V_{\mathrm{eff}}(x_i, \tilde{s}_i)}}\,, \tag{3.13}$$

where $\tilde{s}_3 = x_3$ and x_3^* is the tunneling exit position. The values of x_1 and x_2 are assumed zero, while $\tilde{s}_1$ and $\tilde{s}_2$ retain their ground-state values. The qualitative behavior of the tunneling time in Fig. 3.4 under this approximation is not too far from the results of our full computation.

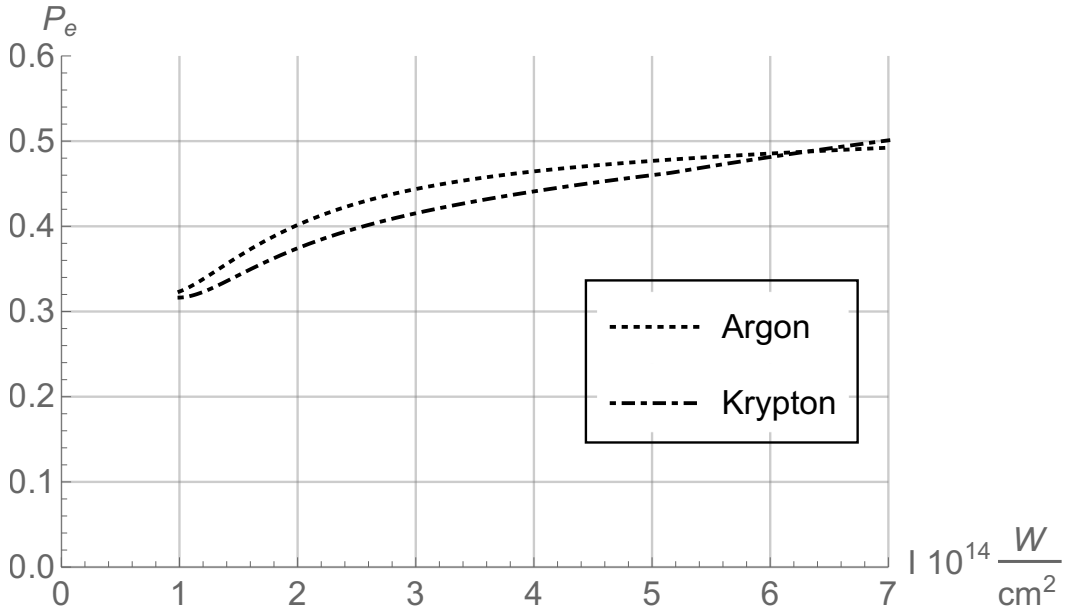

Figure 3.5. Exit momenta for the electron as a function of the laser intensity. They have the same qualitative behavior as in [70] with an agreement of order of magnitude.

Our method also yields the momentum p_3 at the tunnel exit, shown in Fig. 3.5. The longitudinal momentum is non-zero because the electron exits the tunnel with momentum in the direction of the force: As shown in Fig. 3.1, in the effective potential, the classical turning point is replaced by an actual tunnel exit. Our effective potential therefore presents a self-contained model in which several observational features are qualitatively reproduced, without any free parameters beyond the coefficients used to define the classical potential. However, it requires an extension to time-dependent forces modelling laser fields.

3.3.2 Time-dependent, circularly polarized electric fields

If the direction of the force is not constant, tunneling should affect the moments of more than one degree of freedom. If the force is rotating at constant angular velocity ω, we can nevertheless find suitable reaction coordinates by transforming to a frame co-rotating with the force. It is sufficient to start with a two-dimensional system in the plane in which the force is rotating. For instance, the example used in [54] is a two-dimensional, time-dependent vector potential

$$\vec{A}(t) = \frac{A_0}{\sqrt{1+\epsilon^2}} \cos^4(\omega t/2N) \begin{pmatrix} \cos(\omega t) \\ \epsilon \sin(\omega t) \end{pmatrix} \tag{3.14}$$

for N cycles of frequency ω, with ellipticity ϵ. The corresponding electric field is

$$\vec{E} = -\frac{\mathrm{d}\vec{A}}{\mathrm{d}t} = \frac{A_0\omega}{\sqrt{1+\epsilon^2}} \cos^4(\omega t/2N) \begin{pmatrix} \sin(\omega t) + \frac{2}{N}\tan(\omega t/2N)\cos(\omega t) \\ \epsilon\left(-\cos(\omega t) + \frac{2}{N}\tan(\omega t/2N)\sin(\omega t)\right) \end{pmatrix}. \tag{3.15}$$

Specialized to two cycles, $N = 2$, and circular polarization, $\epsilon = 1$, also as in [54], we have

$$\vec{E} = \frac{A_0\omega}{\sqrt{2}} \cos^3(\omega t/4) \begin{pmatrix} \sin(5\omega t/4) \\ \cos(5\omega t/4) \end{pmatrix} = \frac{A_0\omega}{\sqrt{2}} \cos^3(\omega t/4) S \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{3.16}$$

with the orthogonal matrix

$$S = \begin{pmatrix} \sin(5\omega t/4) & -\cos(5\omega t/4) \\ \cos(5\omega t/4) & \sin(5\omega t/4) \end{pmatrix}. \tag{3.17}$$

In terms of the electric field, we can write the Hamiltonian for a negatively charged particle as

$$H = \frac{1}{2}\vec{p}^2 + \vec{r}\cdot\vec{E} + V(r)\,. \tag{3.18}$$

In co-rotating coordinates

$$\vec{R} = S^{-1}\vec{r} \quad , \quad \vec{P} = S^{-1}\vec{p} \tag{3.19}$$

we have

$$H = \frac{1}{2}\vec{P}^2 + \vec{R}\cdot\vec{E}_0 + V(R) + \frac{5\omega}{4}\left(P_1R_2 - P_2R_1\right) \tag{3.20}$$

with an electric field

$$\vec{E}_0 = S^{-1}\vec{F} = \frac{A_0\omega}{\sqrt{2}}\cos^3(\omega t/4)\begin{pmatrix}1\\0\end{pmatrix}, \tag{3.21}$$

which is not constant but points in a fixed direction. The fluctuations in this direction are our reaction coordinates.

The transformation to a co-rotating frame shows that the two-dimensional nature of tunneling in circularly polarized electric fields is not essential, but it turns out that the non-static behavior of the field amplitude is important. This behavior can be studied by Bohmian quantum mechanics in one-dimensional models [79], or by our effective potentials as we will do in the rest of this paper.

For our methods, in the one dimensional case, it is of advantage to have a smooth potential which is finite everywhere. Instead of the Coulomb potential or the truncated version of [79], we therefore consider a one-dimensional model for a Gaussian potential well in a time-dependent electric field:

$$V(x,t) = -\frac{e^{-x^2}}{2} + x\,F(t)\,. \tag{3.22}$$

The potential depth is chosen so that the ground state energy agrees with E_{ground}. As the time-dependent electric field, we choose, as in [79],

$$F(t) = \begin{cases} -F_0\sin(\omega t)^2\sin(\omega t) & \text{if } 0 < t < \frac{\pi}{\omega} \\ 0 & \text{otherwise,} \end{cases} \tag{3.23}$$

which has an amplitude of F_0, frequency $\omega = 0.05811$, and starts at time $t = 0$. Compared with [54], this field belongs to a half-cycle pulse, $N = 1/2$. The corresponding intensities are considered in the observed regime. We will use the form (3.23) in our examples, and later on comment on some of the differences compared with (3.21).

We use this model in order to probe different definitions of the time when the electron exits the tunnel. The standard definition of tunneling exit points equates the energy of the particle with the potential, at which time a classical turning point

would be reached in the absence of quantum corrections. As shown in [53–55], this condition cannot always be imposed in non-static situations, in which the energy of the electron is not constant and may not be known in an experiment. As an alternative, these papers proposed classical back-propagation as a new method, combined with a definition of the tunneling exit as the time when the momentum of the particle in the direction of the force, evaluated on a classically back-propagated trajectory, is zero. However, while this condition is of advantage in evaluations of experimental results [54,55], it is questionable, as also pointed out in [79], because it makes use of a classical property (zero longitudinal momentum at a classical turning point) in a region where classical physics is known to be inadequate. Our methods describe tunneling by a single quantum trajectory, which we will compare directly with the back-propagated classical trajectory in order to see possible deviations.

3.3.3 Definition of tunneling time for dynamic fields

The main quantity of conceptual interest is called "tunneling traversal time" in [79], which is the time the electron spends in a classically forbidden region between two turning points. In a constant field, the positions of turning points depend only on the initial energy of the electron and can be easily determined, but the definition is more difficult to implement when the dynamical behavior of the force is crucial [54].

As a solution, [54] proposed the method of classical back-propagation in order to determine the "tunneling exit time" defined as the point in time when the electron reenters a classically allowed region. By definition, the tunneling exit time is therefore a point in time, while the tunneling traversal time is a duration. The examples considered in [54] suggested near-zero tunneling exit times, which has to be interpreted in the context of the pulse (3.21) with maximum intensity at time zero. In the terminology of [79], the tunneling exit time of [54] is therefore equal to the "tunneling ionization time" defined as the duration between the maximum of the external force and the time when the electron reenters a classically allowed region.

The tunneling ionization time can be accessed in observations more directly than the tunneling traversal time. But it does not give us a full picture of the tunneling process because the electron may well start tunneling before the external force has reached its maximum. The near-zero tunneling exit times or tunneling

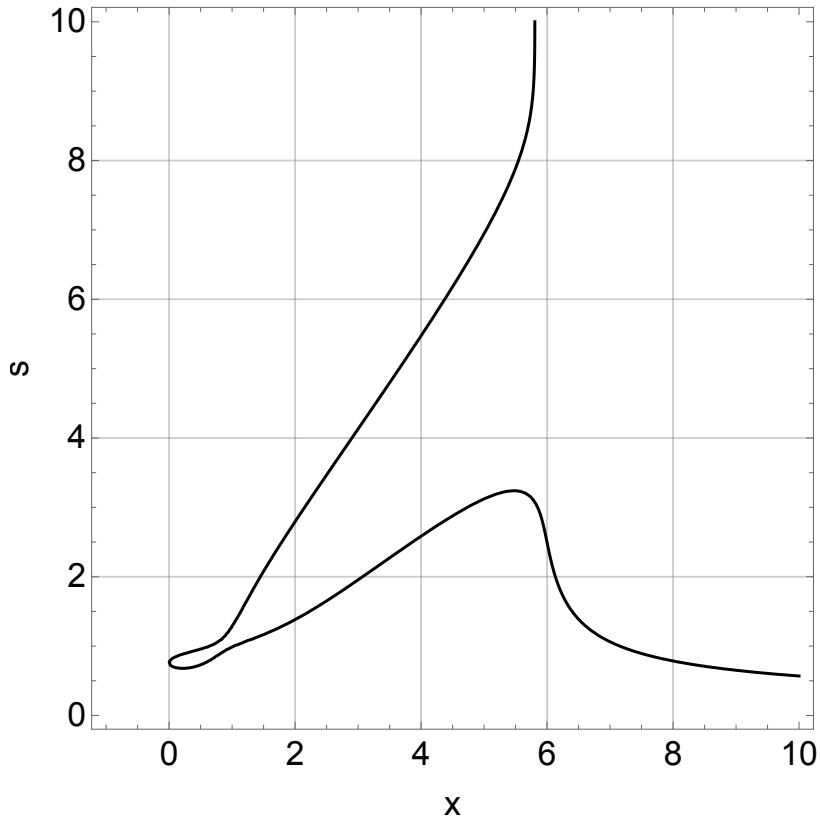

Figure 3.6. Equipotential plot of the all orders at potental at $t = 16$, about half-way to the wave peak.

ionization times of [54] therefore do not imply that the electron tunnels without any delay. The example of tunneling times given in [79] illustrates this difference, which we can show explicitly using our effective potential: As shown in Figs. 3.6 and 3.7, the tunnel has already opened as early as halfway through the build-up of the external force.

In the next subsection, we will analyze tunneling exit criteria, and then return to the question of tunneling traversal.

3.3.4 Tunneling exit criteria for dynamic fields

For the time-dependent potential (3.22) we should use a definition of tunneling exit time which can account for non-adiabatic effects. For instance, the energy

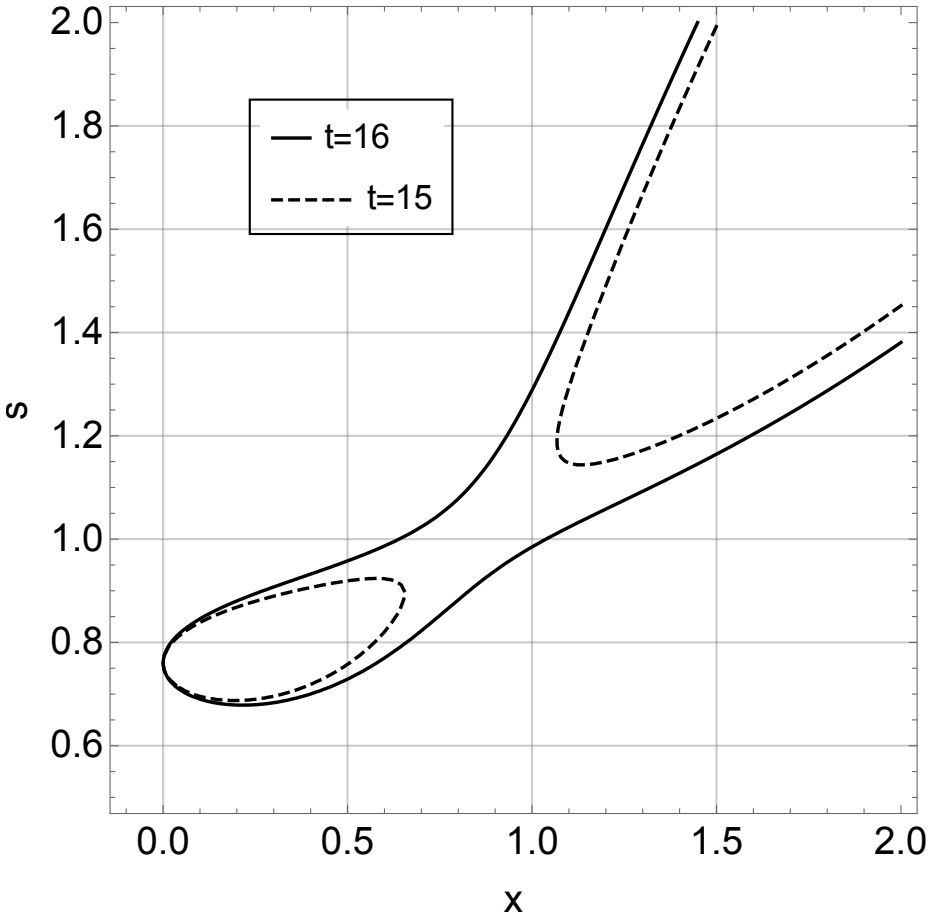

Figure 3.7. Zoom-in of Fig. 3.6 on the area of interest. The dashed contour is from $t = 15$ at which time the tunneling channel has not completely opened. A little while later, at $t = 16$, the tunneling channel is open and the particle can leave.

condition

$$H_{\mathrm{Q}}(p(t), p_s(t), x(t), s(t); t) - x(t)\, F(t) = 0 \tag{3.24}$$

gives us a finite time because we always have $V_{\mathrm{eff}} < 0$ when the term $U/2ms^2$ can be ignored. This definition focuses on the energy gain in an external force: By the time the electron reaches zero energy, it is in an allowed region for any negative potential. In this condition, quantum effects can be significant, for instance when the kinetic energy $p_s^2/2m$ of fluctuations raises the energy to positive values; see Fig. 3.9 below. The condition is adapted to non-adiabatic situations, in the sense that the dynamically changing energy is kept track of. While this criterion includes non-adiabatic effects, the quantum dynamics is approximated by an all orders

Hamiltonian. The canonical tunneling exit time is taken to be the instant when (3.24) is satisfied.

We present results from numerical simulations with the quantum Hamiltonian (3.7) for an effective potential (3.10) and the initial conditions (3.12). We mainly show the tunneling exit time $\tau_{\rm ex}$ by extracting the instant when the interaction-free part of the quantum Hamiltonian (3.24) crosses the time axis. From this value, we are able to determine the tunneling ionization time $\tau_{\rm ion} = \tau_{\rm ex} - \tau_{\rm max}$, which is defined with respect to the instant of maximum field, $t = \pi/2\omega$ in (3.23); see Fig. 3.8. In particular, the tunneling ionization time $\tau_{\rm ion}$ is several atomic units for a field amplitude $F_0 = 0.14$ and becomes smaller for higher intensity pulses. Figure 3.9 shows that the "quantum" kinetic energy $T_Q = p_s^2/2m$ is important for an evaluation of this condition. The tunneling exit time of the electron in Fig. 3.8 explicitly indicates non-zero tunneling ionization time for a dynamic barrier, similarly to what has been obtained in [47, 48, 70] but on a smaller scale.

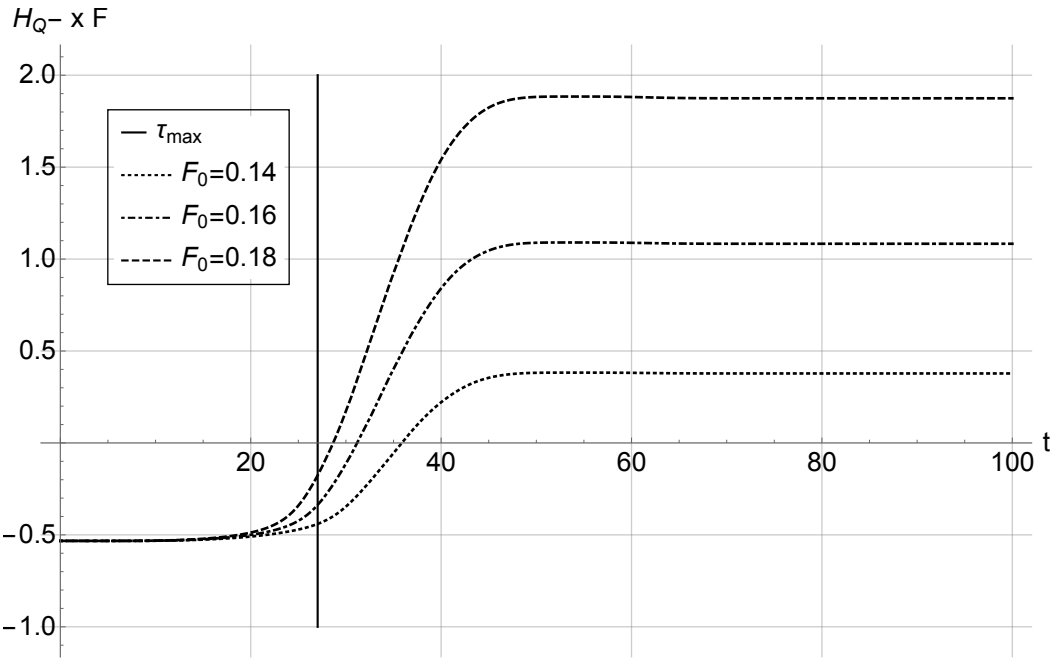

Figure 3.8. The tunneling exit time as an energy condition: $H_{\rm Q} - x\,F = 0$. The intermittent lines represent this condition with respect to time parameter t for three different electric field amplitudes (corresponding to an intensity range of $F_0^2 \sim [6 \times 10^{14}, 12 \times 10^{14}]\,{\rm W/cm^2}$). The vertical solid line indicates the instant of maximum field strength at $\tau_{\rm max} \sim 27$ atomic units.

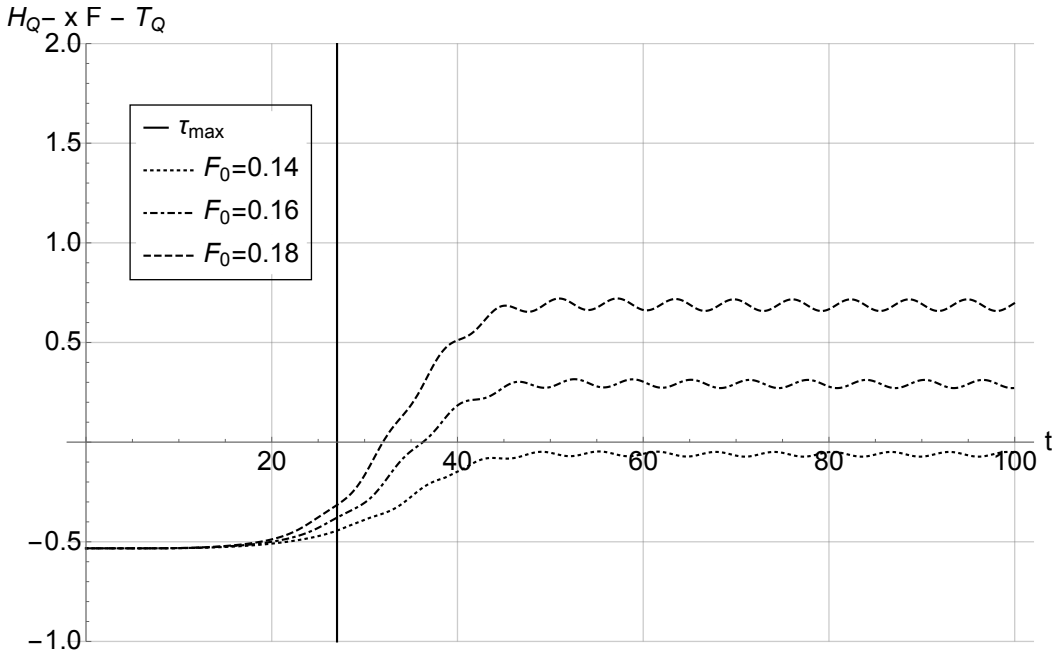

Figure 3.9. The energy as a function of time, with the kinetic term of the quantum degrees of freedom removed.

In addition, laser pulses of sufficiently high frequency do not lead to tunneling if we keep the same maximal field amplitude for varying frequencies; see Fig. 3.10. This implication is easy to understand because less energy then falls on the atom. However, if we use pulses with various frequencies and intensities such that there is always the same energy hitting the atom, we find that, as the frequency rises, the tunneling exit criterion gives ionization times that tend to zero. In this limit, most of the energy reaches the atom close to the wave peak. The result is conceptually similar to the traditional distinction between tunneling ionization and multiphoton ionization based on the Keldysh parameter $\gamma_{\mathrm{K}} = \omega\tau_{\mathrm{K}}$ with $\tau_{\mathrm{K}} = \sqrt{2|I_p|}/F$ [67, 68]. If $\gamma_{\mathrm{K}} \gg 1$, the pulse frequency ω is too large to allow a process of duration τ_{K} to be completed during a laser cycle, which suggests that tunneling does not take place at high frequency. However, the Keldysh time τ_{K} refers to the ionization potential I_p and is therefore adapted to a static electric field during tunneling.

Our method of approximating quantum dynamics allows us to compare different possible tunneling criteria, in particular criteria based on momentum and energy conditions for the tunnel exit. The recent study [54], analyzing a model for a

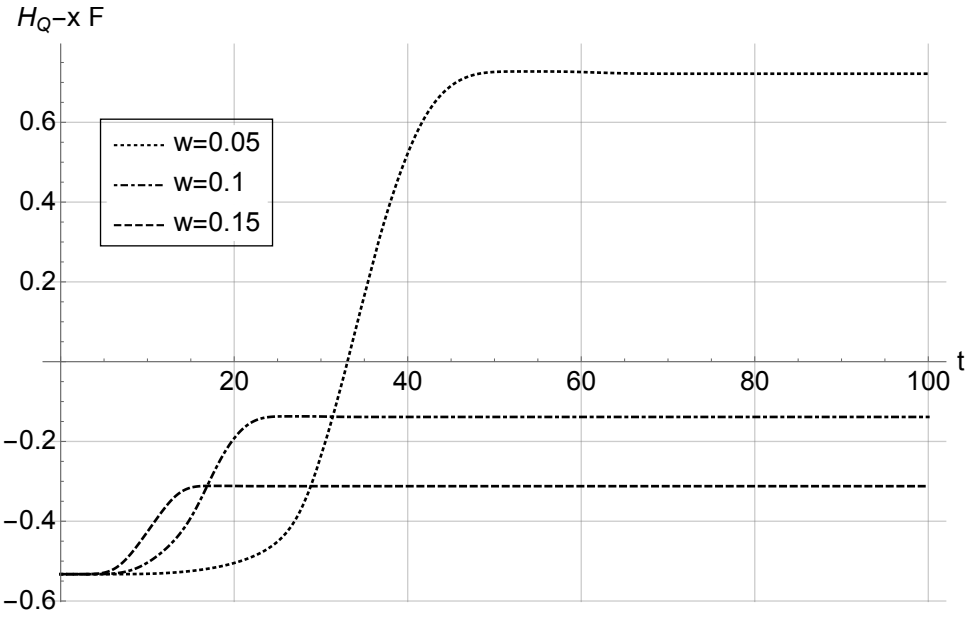

Figure 3.10. Above a certain critical frequency we no longer obtain tunneling according to the condition (3.24).

single active electron in a helium atom, obtains a near-zero ionization time using classical backpropagation and zero longitudinal momentum to define the tunneling exit time. The basic idea of classical backpropagation is to evolve the initial state quantum-mechanically forward to some time after the laser pulse has ended. Then, the classically transmitted ionized part of the wave packet is backpropagated and tunneling exit properties are extracted corresponding to the specific tunneling criterion applied.

We can compare the momentum condition with the energy condition that we introduced in (3.24). First, we evolve the system by the quantum Hamiltonian in (3.7) forward to some late time, $t \sim 150$. Then, using the final values of $\{\langle\hat{x}\rangle, \langle\hat{p}\rangle\}$ at the late time as initial conditions of position and momentum $\{x_{\rm bp}, p_{\rm bp}\}$, we use the classical Hamiltonian $H_{\rm cl} \equiv p^2/2 + V(x)$ to backpropagate classically to an early time. Figure 3.11 shows that the backpropagation trajectory of the particle stays rather close to the quantum evolved trajectory. However, the backpropagated trajectory deviates from the effective trajectory around the instant ($t \approx 27$) when the electric field amplitude is maximum, close to the tunneling exit, where it bounces off the potential well. In Fig. 3.12 we show how the tunneling exit time is

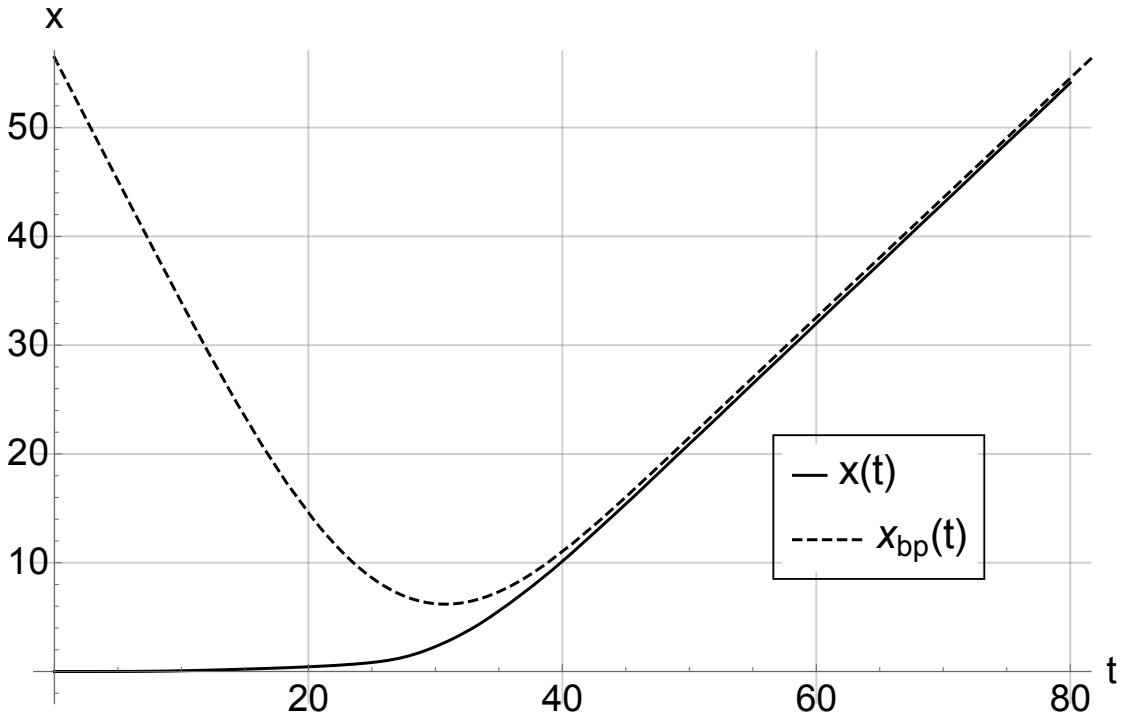

Figure 3.11. Quantum trajectory (solid line) going forwards and the classical trajectory (dashed line) being back propagated in time. The quantum Hamiltonian is responsible for the evolution of the quantum trajectory. The back propagated trajectory is obtained by first evolving the classical trajectory backward in time with the initial condition of the quantum trajectory at some later time.

realized with respect to the momentum condition based on classical backpropagation. There is a non-zero tunneling ionization time $\tau_{\text{ion}} \sim 3$ (atomic units) in qualitative agreement with but smaller than what we obtained from the energy condition.

So far, our results have been shown for a half-cycle pulse (3.23), while [54] used a two-cycle pulse. We repeated our calculations for one- and two-cycle pulses while keeping the same frequency used in the half-cycle pulse, see Fig. 3.13. Figures 3.14 and 3.15 confirm our general findings, and they show that tunneling is possible for significantly larger field amplitudes than for a half-cycle pulse (for which less energy falls on the atom). The frequency dependence of tunneling times can also be confirmed. More cycles in a pulse of the same frequency produce a longer tunneling ionization time according to both criteria evaluated here because the field intensity rises more slowly for bigger N.

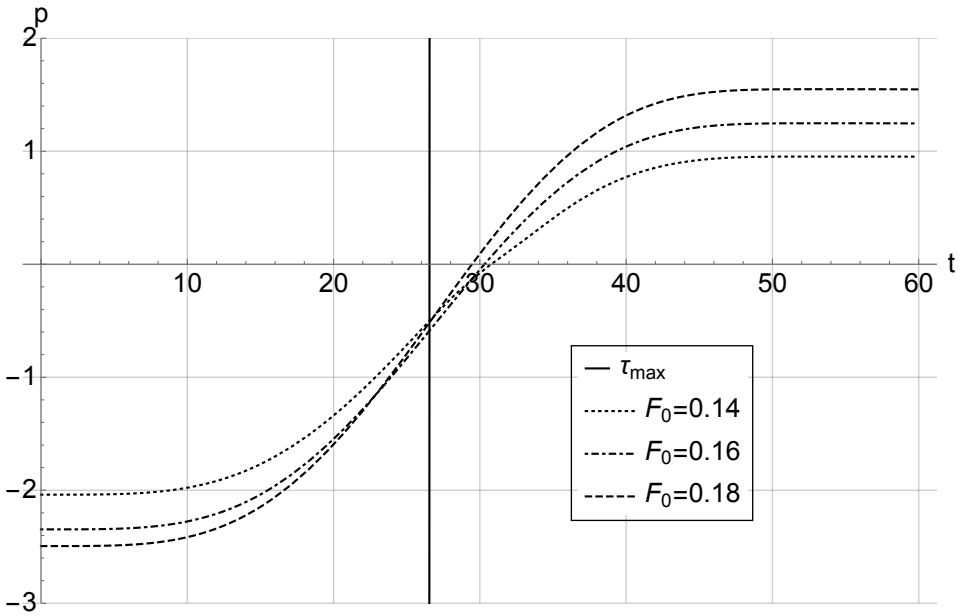

Figure 3.12. Momentum, as a function of time, being back propagated in time. The intermittent lines represent the momentum condition with respect to time parameter t for the same three different electric field amplitudes used for the energy condition. The vertical line indicates the instant of maximum field strength $\tau_{\max} \sim 27$ atomic units.

3.3.5 Tunneling dynamics of Hydrogen in three dimensions

As the most realistic one of our models, we now consider the three dimensional case of a Hydrogen atom in a time dependent electric field

$$H = \frac{1}{2}|\vec{p}|^2 - \frac{1}{|\vec{r}|} + \vec{r}\cdot\vec{E}(t)\,, \tag{3.25}$$

where we use a half cycle pulse

$$\vec{E}(t) = -E_0 \sin^2(\omega t)\theta(t)\theta(\pi/\omega - t) \begin{pmatrix} \sin(\omega t) \\ \cos(\omega t) \\ 0 \end{pmatrix}. \tag{3.26}$$

The classical Hamiltonian at (3.25) has the all-orders quantization given in (3.10).

We use the definition of the tunnel exit time as the moment when the quantum Hamiltonian with the electric field term removed is zero: $H_Q - \vec{r}\cdot\vec{E}(t) = 0$. The ionization time is then defined as the difference between the time of the maximum

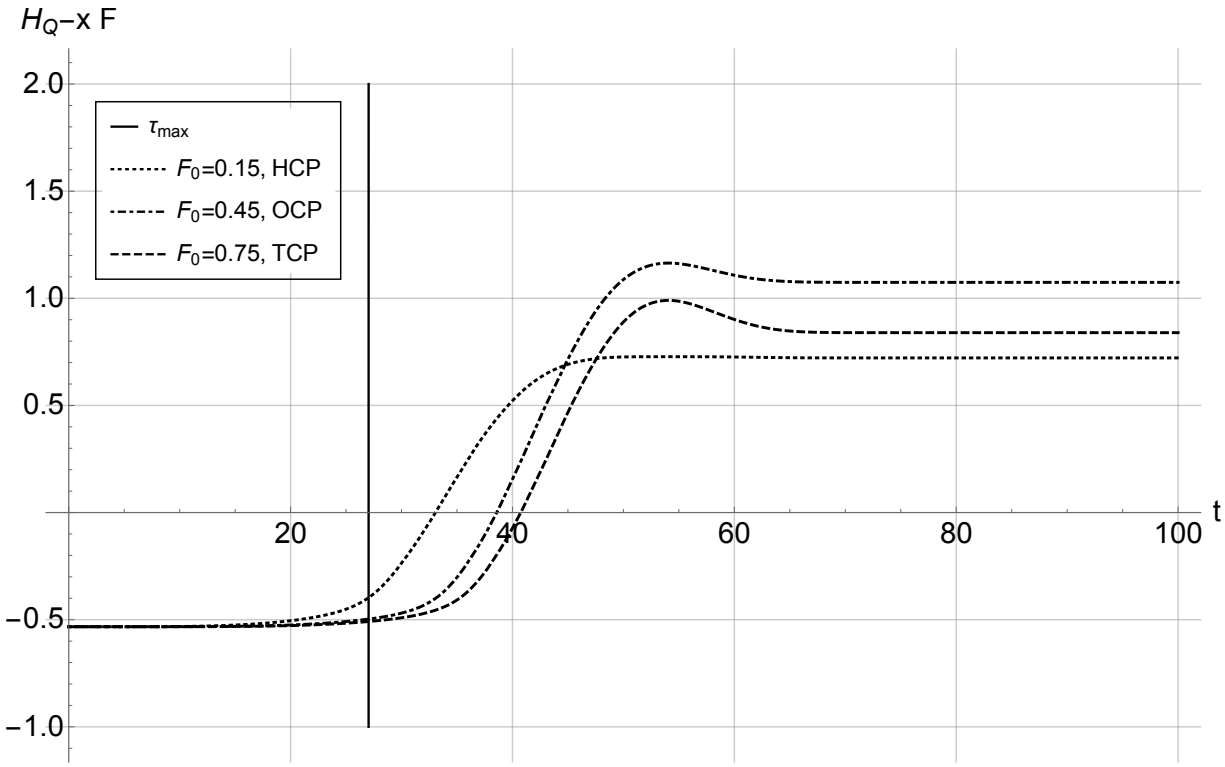

Figure 3.13. The tunneling energy condition as a function of time for various pulses with different field amplitudes: HCP (half-cylce pulse, $F_0 = 0.15$), OCP (one-cycle pulse, $F_0 = 0.45$), TCP (two-cycle pulse, $F_0 = 0.75$).

electric field strength and the exit time, $\tau_{\text{ion}} = \tau_{\text{ex}} - \tau_{\text{max}}$, and shown in Fig. 3.16. Depending on the peak laser intensity, we find an ionization time that is either positive or negative. We can easily understand this result as showing that the electron can tunnel well before the peak reaches the atom, provided the intensity of the pulse is large enough. However, a negative ionization time does not imply that there is no tunneling delay.

Other observables are also accessible as well as correlations between them. Figures 3.17 and 3.18 show that the spot size of the electron jet, defined as the geometric mean of the transversal fluctuations, depends monotonically on the exit time. This result indicates that there is indeed a tunneling delay, or at least non-trivial tunneling dynamics, even if the ionization time is negative: The larger the exit time, the more time there is for the wave packet to spread out. Additionally, the tunneling time depends monotonically on the offset angle, see Figures 3.19 and

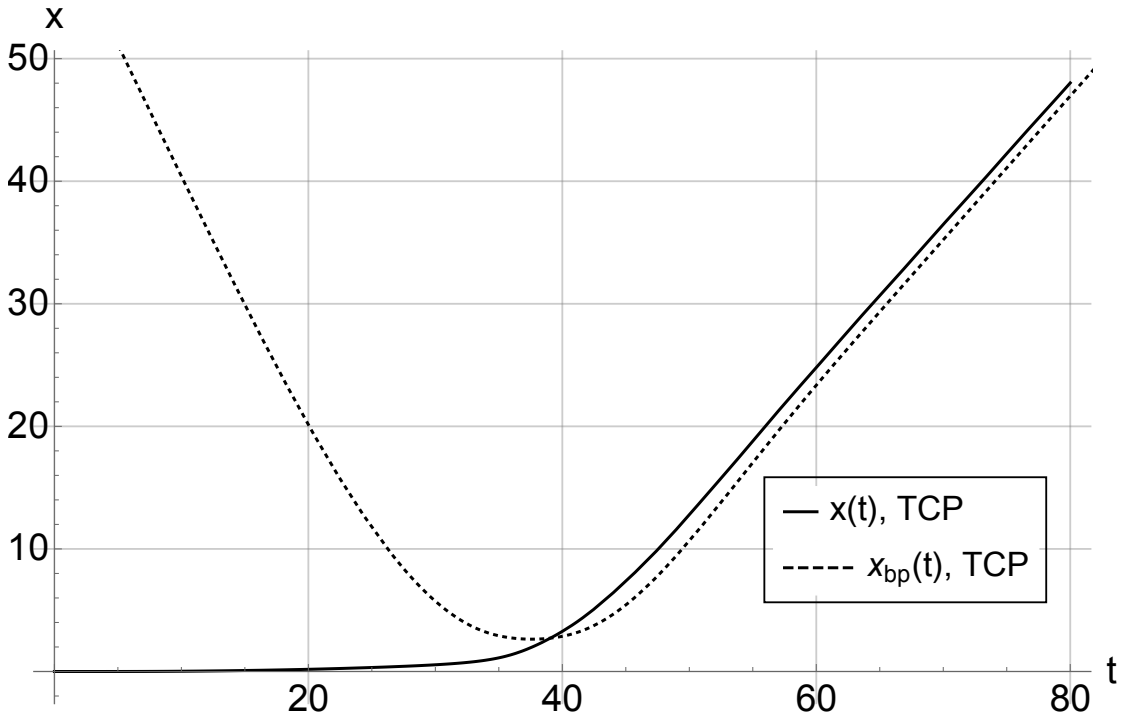

Figure 3.14. Quantum trajectory (solid line) going forwards and the classical trajectory (dashed line) being back propagated in time for a two-cycle pulse. The quantum Hamiltonian is responsible for the evolution of the quantum trajectory.

3.20.

3.3.6 Alternate Definition of tunneling time

The transverse fluctuations used to define the spot size have an interesting dynamics which can be used to define the tunneling exit time in an inherently quantum way, rather than using classical dynamics as in backpropagation. As indicated by Fig. 3.2, and confirmed below for the 3-dimensional non-static model, the transversal fluctuations have three phases. Initially, the particle is confined for some time and the fluctuations stay constant near their ground-state values. During tuneling in the second phase, the state and its fluctuations undergo a more complicated dynamics. After tunneling and when the pulse has ended, during the third phase transversal fluctuations grow linearly as is well-known for a free particle. These phases are clearly demarcated in a plot of the fluctuations, which are readily accessible from simulations in our effective potential.

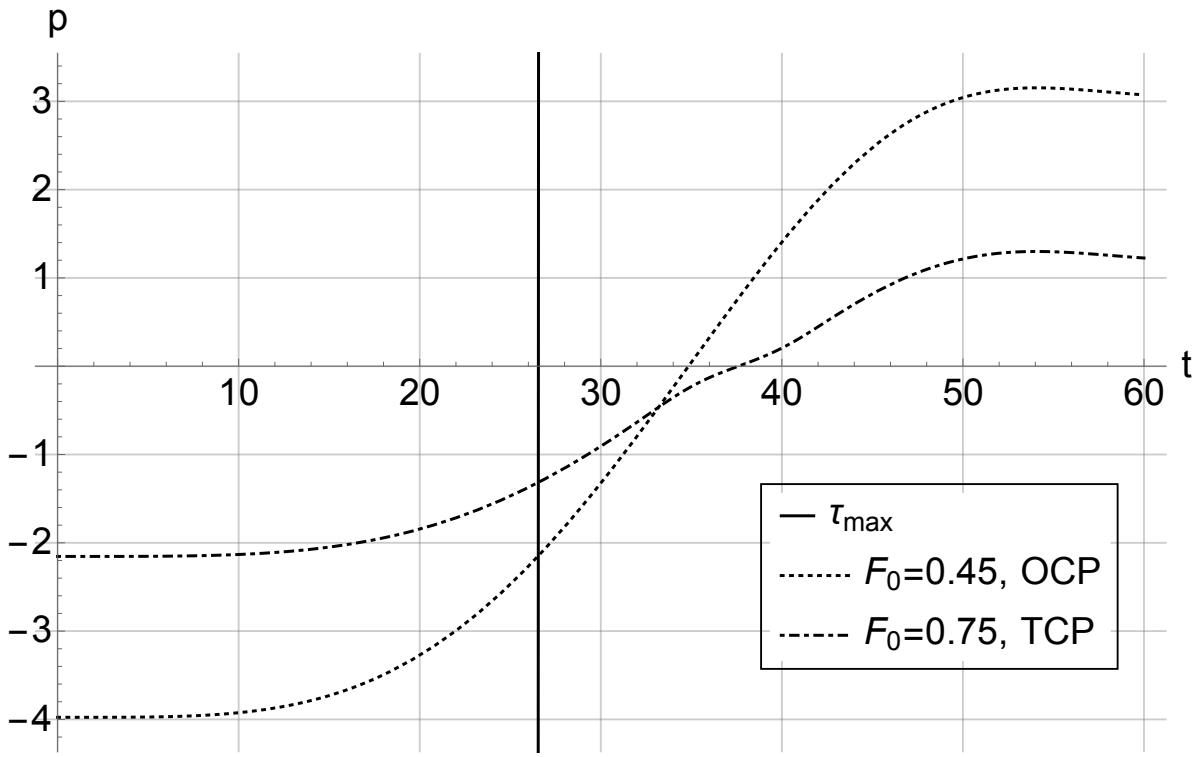

Figure 3.15. Momentum, as a function of time, being back propagated in time for both one- and two-cycle pulses. The intermittent lines represent the momentum condition with respect to time parameter t for the same three electric field amplitudes used for the energy condition.

Nevertheless, extracting the transverse fluctuations is not entirely trivial. To do so, we transform to the co-rotating frame in which some fluctuation parameters s_i are transverse to the external force at all times. Under global rotations, the second-order position moments of a state, defined in general as

$$\Delta_{ij} = \langle (\hat{r}_i - \langle \hat{r}_i \rangle)(\hat{r}_j - \langle \hat{r}_j \rangle) \rangle \,, \tag{3.27}$$

transform in the following way

$$\bar{\Delta}_{ij} = \mathcal{O}_{ki} \Delta_{kl} \mathcal{O}_{lj} \,, \tag{3.28}$$

where $\mathcal{O}_{ij}$ is the rotation matrix that acts on position coordinates. This transfor-

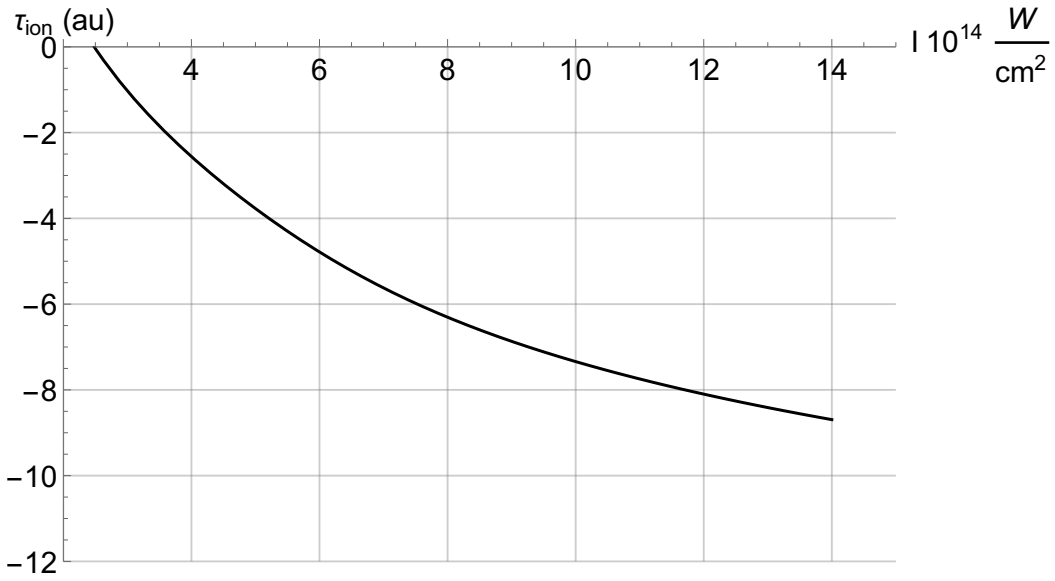

Figure 3.16. Ionization time as a function of the laser intensity in the 3-dimensional model (3.25).

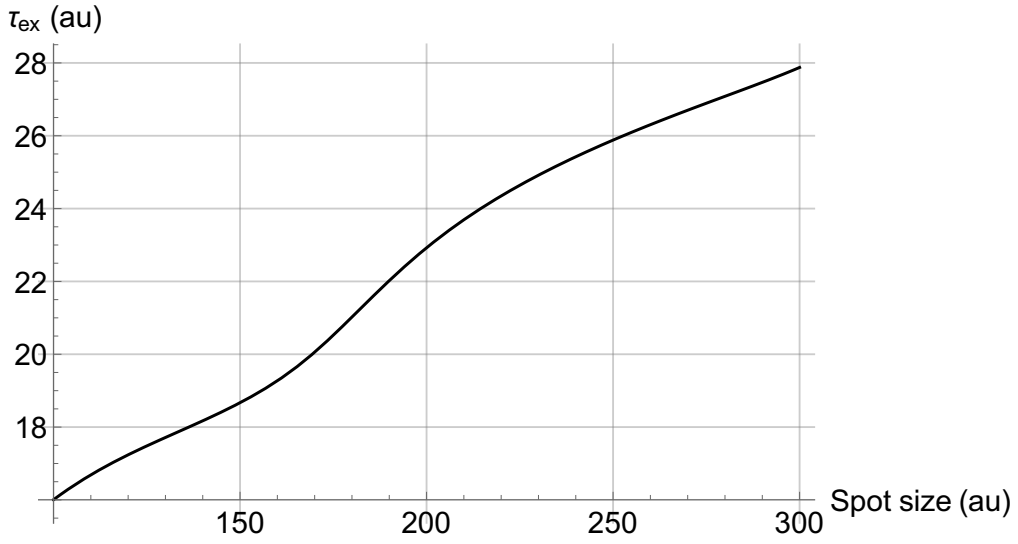

Figure 3.17. The exit time as a function of the spot size at a distance of 1000 atomic units.

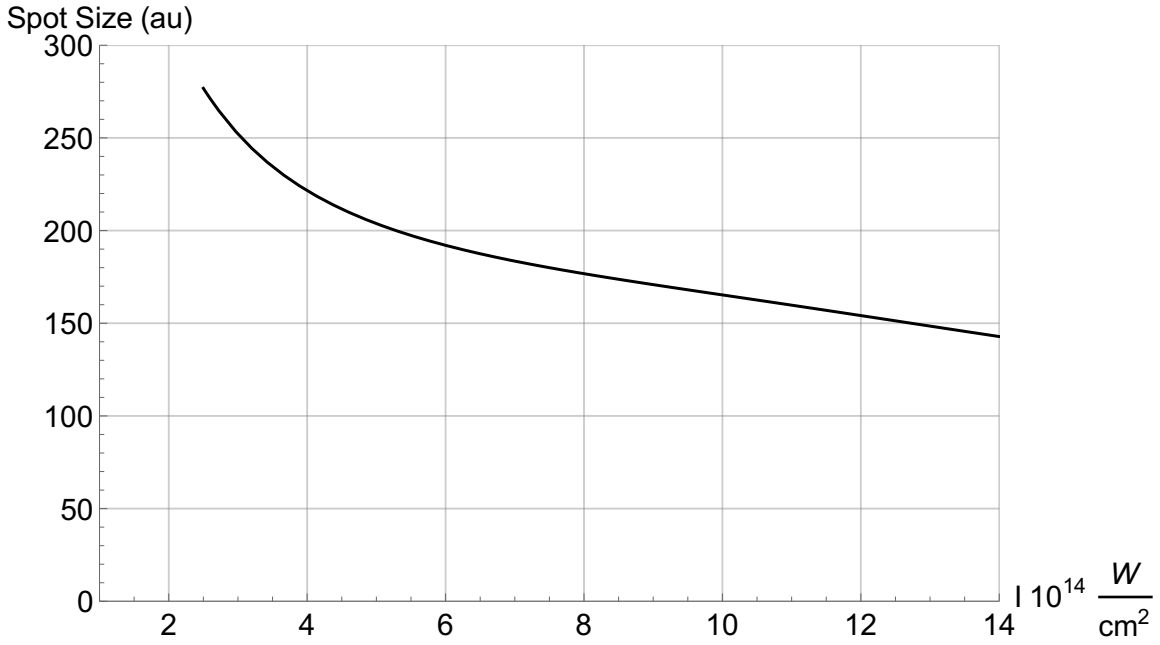

Figure 3.18. Spot size of the wave packet a distance of 1000 atomic units from the atom.

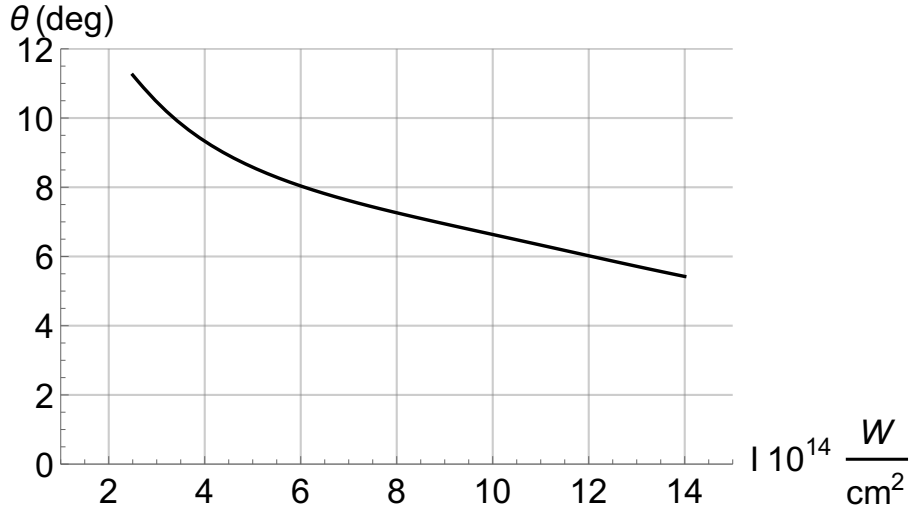

Figure 3.19. Off-set angle of the ionized part of the wave packet.

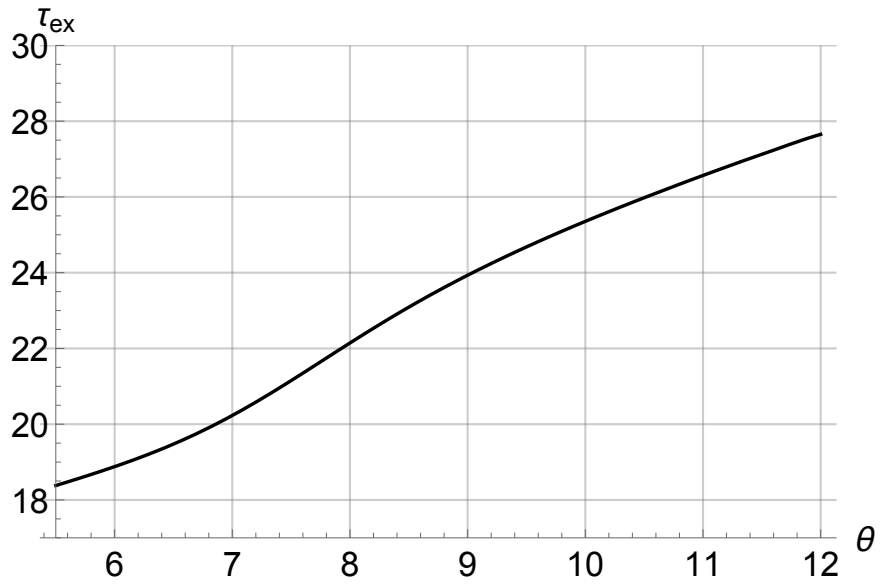

Figure 3.20. Tunneling exit time in terms of the offset angle.

mation results in the transverse fluctuation

$$s_{\mathrm{T}} = \sqrt{\cos^2\left(\theta(t)\right)s_x^2 + \sin^2\left(\theta(t)\right)s_y^2} \tag{3.29}$$

where θ is the offset angle as a function of time.

The transversal fluctuation during the tunneling process is shown in Fig. 3.21, together with two linear fits of the first and final stages. The resulting tunneling exit times in Fig. 3.22 are less than the time of the peak at $t \approx 27$, so that we obtain negative tunneling ionization times based on this criterion, similar to Fig. 3.16. However, the extrapolated time in Fig. 3.21 lies somewhere in the middle of the second stage, and therefore does not mark the end of the tunneling process.

We have to look at the tunneling dynamics in more detail in order to identify the end of tunneling. In Fig. 3.23 we show the second time derivative of the transversal fluctuation as a function of time, which can be interpreted as an effective force that causes the spreading. The three phases are clearly visible, with significant time dependence and a rich dynamics only in the important second phase during which tunneling happens. The time where there is a negative force is interesting, because it could be interpreted as a squeezing the particle state as it passes through the tunnel. The last local maximum and the last inflection point, indicated in the

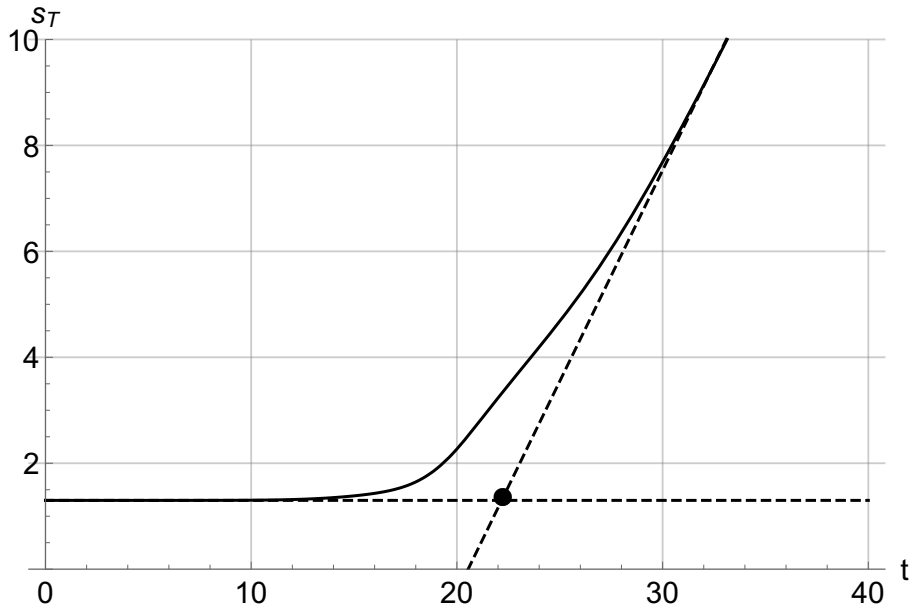

Figure 3.21. The transverse fluctuations as a function of time. The tangent lines of the linear regions are plotted in the dotted lines, and their intersection is marked with a dot.

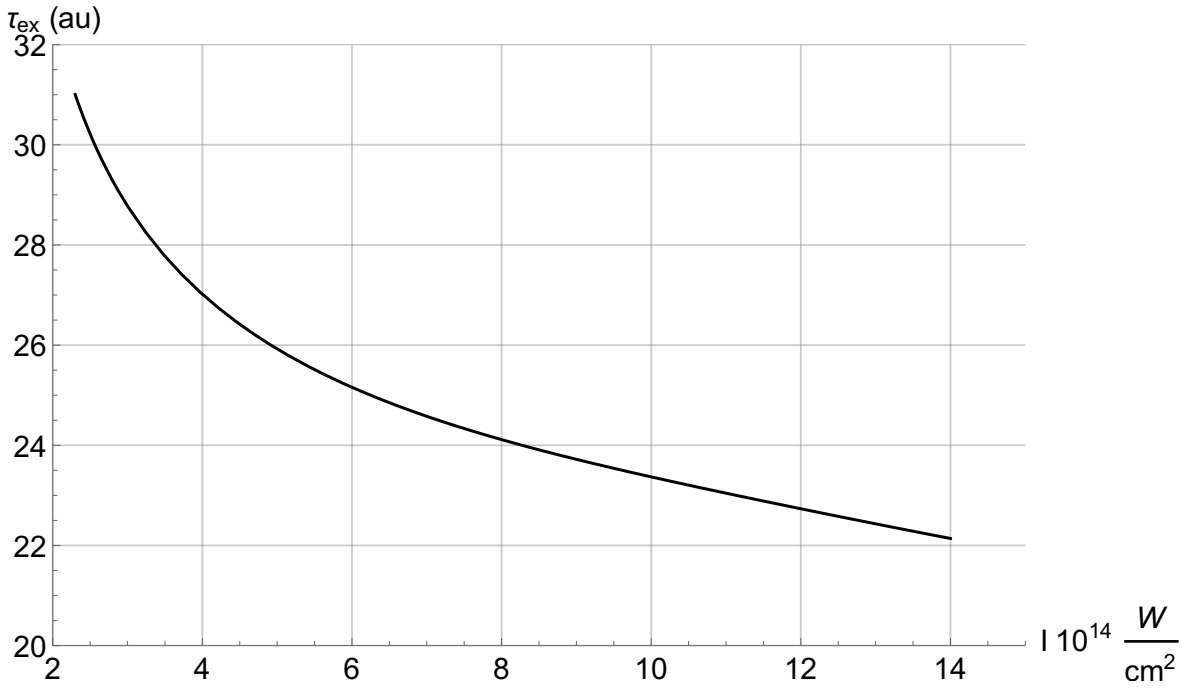

Figure 3.22. Alternative tunnel exit time, based on the fitting process shown in Fig. 3.21, as a function of the intensity.

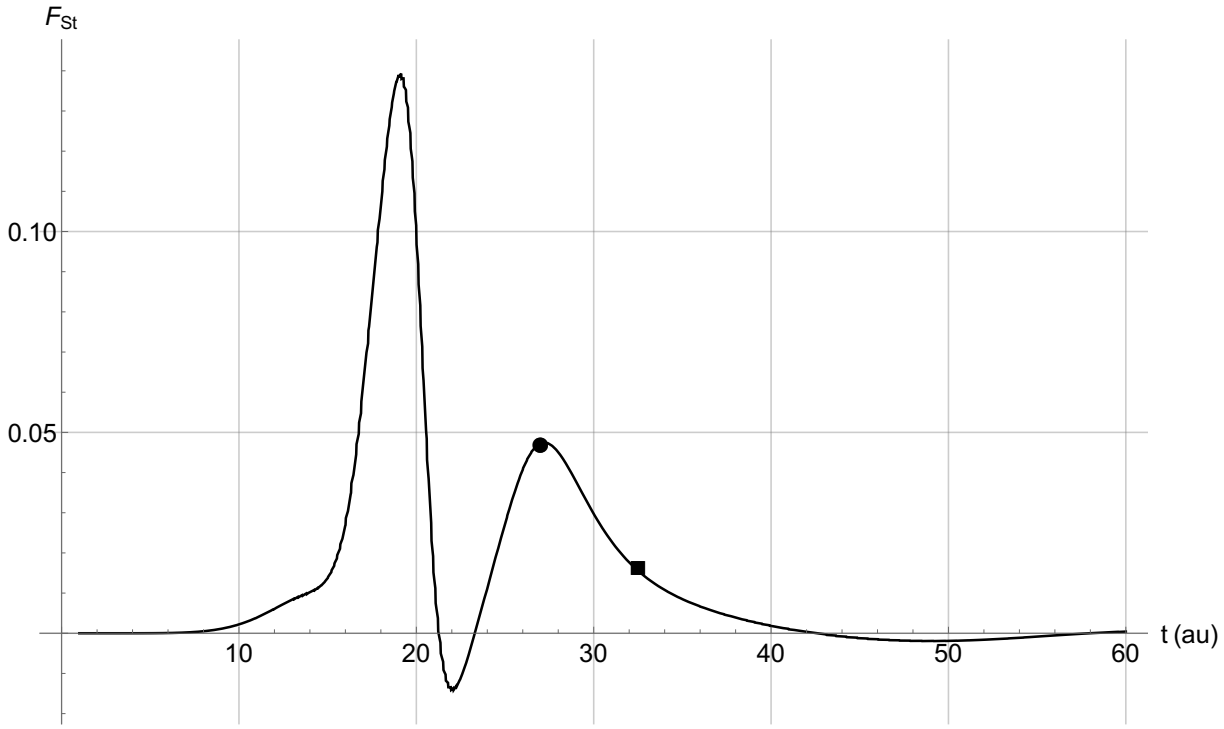

Figure 3.23. The effective force acting on the transverse fluctuations. We see a rich structure in the force as the particle goes through the tunneling region. The filled circle and square represent the last local maximum and the inflection point, respectively.

plot, are very close to the wave peak and gives the time of the maximum force on the transverse fluctuations. In particular, the last inflection point can be used as an indicator for the tunneling exit. For a range of laser intensities, the resulting tunneling exit times are shown in Fig. 3.24. In the entire range shown in this diagram, the exit time is greater than the time of maximum intensity at $t \approx 27$, and a positive tunneling ionization time of a few atomic units is obtained.

3.4 Summary

In summary, our main result — an all-orders effective potential — makes possible a detailed analysis of the tunneling dynamics in various situations. It agrees well with observed features and is able to make new predictions. Numerical solutions give us an efficient way of generating data about the state of the electron which can be compared with observations. Our method, perhaps in combination with

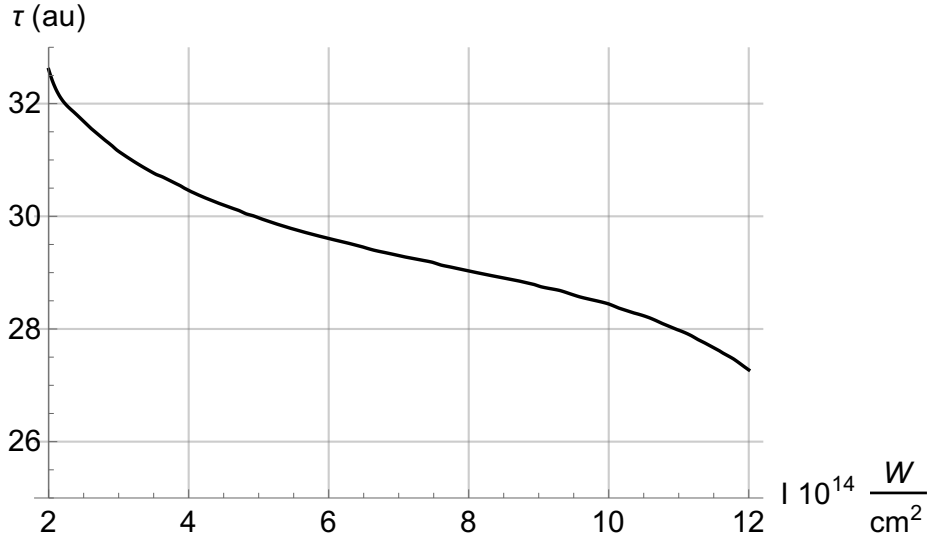

Figure 3.24. Tunneling time based on the last inflection point of the tunneling phase force.

numerical simulations of multi-electron wave functions, can therefore be used to turn ionization experiments into indirect microscopes focused on the atomic state.

We have found qualitative agreement between our approximation and the exact Bohmian treatment. In particular, there is always a tunneling delay. One advantage of our new methods is that we have a single effective trajectory describing the quantum state through its expectation values and moments. This trajectory can directly be compared with the classical back-propagated trajectory, showing crucial deviations near the tunneling exit. In specific examples, classical back-propagation tends to underestimate the tunneling exit time. Our results therefore indicate non-zero tunneling times, but by about an order of magnitude less than what had initially been extracted from experiments. In particular, the tunneling time in a half-cycle pulse is significantly less than the tunneling time in a static field at a level of the maximum field of the pulse, which is not surprising once the importance of non-adiabatic effects has been realized [53, 79].

We also found that the definition of tunneling ionization time in non-constant fields, given by the difference of the tunneling exit time and the time of maximal field strength, does not give a full picture of the tunneling dynamics. In particular, it is possible for the electron to start tunneling well before the maximum field is reached. The entire tunneling process then takes longer than indicated by the

tunneling ionization time, considered mainly in [54]. The tunneling traversal time, used in [79], gives a more complete picture of time-dependent tunneling. In our examples, we see that a tunnel opens up already at weak fields: The intensity assumed in the static example of Fig. 3.1 is about one tenth of the intensity used in our non-static examples, such as Fig. 3.8; see also Fig. 3.7.

Unfortunately, it is difficult to extract the full traversal time from experiments, but we have given examples of indirect signatures, such as the spot size based on fluctuations, which could be useful in this context. Moreover, if the spot size and a corresponding longitudinal fluctuation can be measured, one could use it, along with the final expectation values of position and momentum, as initial conditions for *semiclassical backpropagation* defined as in [53] but using our effective dynamics instead of the classical dynamics. This process would eliminate potential problems of classical backpropagation near turning points.

Chapter 4
Effective potentials from semi-classical truncations

4.1 Introduction

In this chapter we extend the methods laid out in chapter 2 to more general effective potentials and to higher semi-classical orders. Our methods are tested by taking the adiabatic limit and comparing with known results. In particular we are able to reproduce some basic results from quantum field theory. Beyond reproducing some known results, we are able to add something new by getting analytic formulas for the moments in an adiabatic state. Given the canonical structure of our variables, we are able to examine the thermodynamics of our effective potentials, allowing us to compute the moments in some thermal equilibrium with an external reservoir. We also discuss how the purity of a quantum states can correspond to its moments. We argue that some parameters in out mapping should correspond to parameters that parametrize the purity of the state.

Semiclassical physics can often be described by classical equations of motion amended by correction terms and possible new degrees of freedom. For instance, Ehrenfest's theorem shows that the expectation values of position and momentum in an evolving quantum state obey equations of motion which are identical with the classical equations to zeroth order in $\hbar$ but, in general, have a modified quantum force given by $-\langle \nabla V(\hat{x}) \rangle$ not equal to the classical force $-\nabla V(\langle \hat{x} \rangle)$ evaluated at $\langle \hat{x} \rangle$. The difference depends on $\langle \hat{x} \rangle$, but also on the variance $(\Delta x)^2$ and higher moments, which constitute new, non-classical degrees of freedom.

A moment expansion can be used to derive quantum corrections systematically. In this way, one can formulate quantum dynamics as classical-type dynamics on an extended phase space, given by expectation values and moments equipped with a Poisson bracket that follows from the commutator of operators [92, 93]. Moments, however, do not directly form canonical variables on this Poisson manifold, which complicates some of the usual procedures of canonical mechanics. Darboux' theorem guarantees the existence of local canonical coordinates, but it is not always easy to find them. Using a procedure we developed in [115], as well as other new methods, we present here detailed derivations of canonical variables for moments of up to fourth order for a single degree of freedom, as well as to second order for a pair of degrees of freedom. The resulting expressions can be used to make interesting observations about the behavior of states, and they are crucial for the derivation of effective potentials. We present several applications, including tunneling which is also discussed in more detail in [95].

4.2 Canonical Effective Methods

We use a quantum system of N degrees of freedom with basic operators $\hat{q}_j$ and $\hat{\pi}_k$, $1 \leq j, k \leq N$ that are canonically conjugate,

$$[\hat{q}_j, \hat{\pi}_k] = i\hbar\delta_{jk}\,. \tag{4.1}$$

In a semiclassical truncation [92, 93], the state space is described by a finite-dimensional phase space with coordinates given by the basic expectation values $q_j = \langle\hat{q}_j\rangle$ and $\pi_k = \langle\hat{\pi}_k\rangle$ and, for positive integers k_i and l_i such that $\sum_{i=1}^{N}(k_i+l_i) \geq 2$, the moments

$$\Delta\left(q_1^{k_1}\cdots q_N^{k_N}\pi_1^{l_1}\cdots\pi_N^{l_N}\right) = \langle(\hat{q}_1-q_1)^{k_1}\cdots(\hat{q}_N-q_N)^{k_N}(\hat{\pi}_1-\pi_1)^{l_1}\cdots(\hat{\pi}_N-\pi_N)^{l_N}\rangle_{\rm Weyl}\,, \tag{4.2}$$

where the product of operators is Weyl (totally symmetrically) ordered. The phase-space structure is defined by the Poisson bracket

$$\{\langle\hat{A}\rangle, \langle\hat{B}\rangle\} = \frac{1}{i\hbar}\langle[\hat{A}, \hat{B}]\rangle\,, \tag{4.3}$$

extended to all moments by using linearity and the Leibniz rule. The phase space has boundaries according to Heisenberg's uncertainty relation

$$\Delta(q_j^2)\Delta(\pi_k^2) - \Delta(q_j\pi_k)^2 \geq \frac{\hbar^2}{4}\delta_{jk} \tag{4.4}$$

and higher-order analogs.

Any given state (which may be pure or mixed) is therefore represented by a point in phase space defined by the corresponding basic expectation values and moments. A state is considered semiclassical if its moments obey the hierarchy

$$\Delta\left(q_1^{k_1}\cdots q_N^{k_N}\pi_1^{l_1}\cdots\pi_N^{l_N}\right) = O\left(\hbar^{\frac{1}{2}\sum_n(l_n+k_n)}\right) \tag{4.5}$$

which is satisfied, for instance, by a Gaussian, but includes also a more general class of states. A semiclassical truncation of order s of the quantum system is defined as the submanifold spanned by the basic expectation values and moments such that $\sum_n(l_n+k_n)\leq s$, which implies variables up to order $\frac{1}{2}s$ in $\hbar$ according to the semiclassical hierarchy. The Poisson bracket that results from (4.3) can consistently be restricted to any semiclassical truncation by ignoring in $\{\Delta_1,\Delta_2\}$ all terms of order higher than s in moments. In this restriction, the product of a moment of order s_1 and a moment of order s_2 is considered of semiclassical order s_1+s_2, while the product of a moment of order s_1 with $\hbar^{s_2}$ is of order s_1+2s_2 [96]. For given s, the Poisson tensor on the semiclassical truncation of order s is, in general, not invertible. Therefore, semiclassical truncations and the resulting effective potentials cannot be formulated within symplectic geometry.

The Hamilton operator $\hat{H}$ determines a Hamilton function $\langle\hat{H}\rangle$ on state space, which can be restricted to any semiclassical truncation of order s to define an effective Hamilton function of semiclassical order s. We assume that each contribution to the Hamilton operator is Weyl-ordered in basic operators. Any Hamilton operator that does not obey this condition can be brought to Weyl-ordered form by using the canonical commutation relations, which results in terms that explicitly depend on $\hbar$. In order to compute an effective Hamiltonian of order s for a given Hamilton operator $H(\hat{q}_j,\hat{\pi}_k)$, we use

$$H_{\mathrm{eff},s} \;=\; \langle H(\hat{q}_j+(\hat{q}_j-q_j),\hat{\pi}_k+(\hat{\pi}_k-\pi_k))\rangle \tag{4.6}$$

$$= H(q_j,\pi_k) + \sum_{\sum_n (j_n+k_n)=2}^{s} \frac{\partial^n H(q,\pi)}{\partial q_1^{j_1}\cdots\partial q_N^{j_N}\,\partial \pi_1^{k_1}\cdots\partial\pi_N^{k_N}} \frac{\Delta\left(q_1^{j_1}\cdots q_N^{j_N}\pi_1^{k_1}\cdots\pi^{k_N}\right)}{j_1!\cdots j_N!k_1!\cdots k_N!}\,.$$

This expansion is reduced to a finite sum if $\hat{H}$ is polynomial in basic operators, in which case the expansion serves the purpose of expressing the expectation value of products of basic operators in terms of central moments. For a non-polynomial Hamilton operator, the expansion is a formal power series in $\hbar$. The definition of our Poisson bracket ensures that Hamilton's equations

$$\dot{f}(\langle\cdot\rangle,\Delta) = \{f(\langle\cdot\rangle,\Delta), H_{\text{eff,s}}\} \tag{4.7}$$

on any semiclassical truncation are consistent with Heisenberg's equations of motion evaluated in a state.

4.2.1 Examples

For a single pair of classical degrees of freedom, $N = 1$, the phase space of the semiclassical truncation of order two is five-dimensional (and therefore cannot be symplectic). In addition to the basic expectation values q and π, there are two fluctuation variables, $\Delta(q^2)$ and $\Delta(\pi^2)$, and the covariance $\Delta(q\pi)$. The non-zero Poisson brackets of these variables are given by

$$\{q,\pi\} = 1 \tag{4.8}$$
$$\{\Delta(q^2),\Delta(q\pi)\} = 2\Delta(q^2) \tag{4.9}$$
$$\{\Delta(q\pi),\Delta(\pi^2)\} = 2\Delta(\pi^2) \tag{4.10}$$
$$\{\Delta(q^2),\Delta(\pi^2)\} = 4\Delta(q\pi) \tag{4.11}$$

which are linear and equivalent to the Lie algebra $\mathrm{sp}(2,\mathbb{R})$.

More generally, the second-order semiclassical truncation for N pairs of classical degrees of freedom is equivalent to $\mathrm{sp}(2N,\mathbb{R})$ [115]. Third-order semiclassical truncations also have linear Poisson brackets which are no longer semisimple: Within a higher-order semiclassical truncation, the Poisson bracket of two third-order moments is a sum of fourth-order moments and products of second-order moments, all of which are of order four and set to zero in a third-order truncation. Moreover, the Poisson bracket of a second-order moment and a third-order moment

is proportional to a third-order moment, for instance

$$\{\Delta(q^2),\Delta(q^2\pi)\}=2\Delta(q^3) \quad , \quad \{\Delta(q^2),\Delta(q\pi^2)\}=4\Delta(q^2\pi) \quad , \quad \{\Delta(q^2),\Delta(\pi^3)\}=6\Delta(q\pi^2) \tag{4.12}$$

for $N=1$. The third-order moments in a semiclassical truncation of order three therefore form an Abelian ideal, and the corresponding Lie algebra is not semisimple. (For $N=1$, the Lie algebra is the semidirect product $\mathrm{sp}(2,\mathbb{R})\ltimes\mathbb{R}^4$ where $\mathrm{sp}(2,\mathbb{R})$ acts according to its spin-3/2 representation [115].)

For orders higher than three, the Poisson brackets are non-linear and therefore do not define Lie algebras. A general expression is given by [92, 97]

$$\begin{aligned}\{\Delta(q^bp^a),\Delta(q^dp^c)\} &= a\,d\,\Delta(q^bp^{a-1})\Delta(q^{d-1}p^c)-bc\Delta(q^{b-1}p^a)\Delta(q^dp^{c-1})\\ &\quad+\sum_{\text{odd }n=1}^{M}\left(\frac{i\hbar}{2}\right)^{n-1}K^n_{abcd}\,\Delta(q^{b+d-n}p^{a+c-n})\end{aligned} \tag{4.13}$$

where $M=\min(a+c,b+d,a+b,c+d)$ and

$$K^n_{abcd}=\sum_{m=0}^{n}(-1)^m m!(n-m)!\binom{a}{m}\binom{b}{n-m}\binom{c}{n-m}\binom{d}{m}\,. \tag{4.14}$$

The inclusion of only odd n in the sum ensures that all coefficients are real. Terms containing $\Delta(q)$ or $\Delta(p)$ are considered zero: They correspond to expectation values of the form $\langle\hat{a}-a\rangle=0$ which are identically zero.

4.2.2 Purity

The collection of all moments determines a state, provided it obeys conditions that follow from uncertainty relations. Since moments are defined using expectation values, which can be computed from a pure or mixed state, they may describe a pure or mixed state. In general, it is not easy to determine the purity of a state described by moments without first reconstructing a density matrix from them. As we will see, however, canonical variables for moments can provide indications as to possible impurity parameters. In preparation of this application, we discuss here ingredients for possible reconstructions of states from a given set of moments.

If the state is pure, it is sufficient to consider only the moments $\Delta(q^n)$ and $\Delta(q^{n-1}\pi)$ to reconstruct a wave function [92]. For instance, we can use Hermite

polynomials $H_n(q)$ and their coefficients $h_{n,l}$ defined such that $H_n(q) = \sum_l h_{n,l} q^l$. The expectation values $a_n = \langle \hat{q}^n \rangle$ can then be used to compute

$$c_n = \sum_l h_{n,l} a_l = \int \mathrm{d}q |\psi(q)|^2 H_n(q)\,, \tag{4.15}$$

from which we obtain the probability density

$$|\psi(q)|^2 = e^{-q^2} \sum_n \frac{c_n}{2^n \pi n!} H_n(q) \tag{4.16}$$

using the orthonormality relation of Hermite polynomials.

Using $b_n = \langle \hat{q}^n \hat{\pi} \rangle$, the phase $\alpha(q)$ of the wave function $\psi(q) = \exp(i\alpha(q))|\psi(q)|$ then follows from

$$\begin{aligned}
\mathrm{Re} b_n &= \mathrm{Re} \int \mathrm{d}q \psi^* q^n \frac{\hbar}{i} \frac{\mathrm{d}\psi}{\mathrm{d}q} && (4.17)\\
&= \mathrm{Re} \int \mathrm{d}q e^{-i\alpha} |\psi| q^n \frac{\hbar}{i} \left(i \frac{\mathrm{d}\alpha}{\mathrm{d}q} e^{i\alpha} |\psi| + e^{i\alpha} \frac{\mathrm{d}|\psi|}{\mathrm{d}q} \right) && (4.18)\\
&= \hbar \int \mathrm{d}q |\psi|^2 q^n \frac{\mathrm{d}\alpha}{\mathrm{d}q}\,. && (4.19)
\end{aligned}$$

If we define

$$d_n = \sum_l h_{n,l} \mathrm{Re} b_n = \hbar \int \mathrm{d}q |\psi|^2 \frac{\mathrm{d}\alpha}{\mathrm{d}q} H_n(q)\,, \tag{4.20}$$

we reconstruct

$$\frac{\mathrm{d}\alpha}{\mathrm{d}q} = \frac{e^{-q^2}}{\hbar |\psi|^2} \sum_n \frac{d_n}{2^n \pi n!} H_n(q)\,. \tag{4.21}$$

Integration gives $\alpha(q)$ up to an arbitrary constant phase.

In order to reconstruct a density matrix, we need all moments. First, position moments are given by

$$\Delta(q^a) = \mathrm{tr}((\hat{q} - \langle \hat{q} \rangle)^a \hat{\rho}) = \int (q - \langle \hat{q} \rangle)^a \rho(q,q) \mathrm{d}q \tag{4.22}$$

from which we can reconstruct the diagonal part $\rho(q,q)$ using orthogonal polynomials. Using momentum-dependent moments, we can compute the values of

$$\mathrm{tr}((\hat{q} - \langle \hat{q} \rangle)^a \hat{\pi}^b \hat{\rho}) = \left(\frac{\hbar}{i} \right)^b \int (q - \langle \hat{q} \rangle)^a \left. \frac{\partial^b \rho(y,q)}{\partial y^b} \right|_{y=q} \mathrm{d}q \tag{4.23}$$

and use them in

$$\begin{aligned}\sum_b \frac{1}{b!}\left(\frac{id}{\hbar}\right)^b \mathrm{tr}((\hat{q}-\langle\hat{q}\rangle)^a\hat{\pi}^b\hat{\rho}) &= \int (q-\langle\hat{q}\rangle)^a \sum_b \frac{d^b}{b!}\left.\frac{\partial^b\rho(y,q)}{\partial y^b}\right|_{y=q} \mathrm{d}q \\ &= \int (q-\langle\hat{q}\rangle)^a \rho(q+d,q)\mathrm{d}q \end{aligned} \tag{4.24}$$

to reconstruct $\rho(q+d,q)$ for arbitrary q and d.

In a semiclassical truncation we have incomplete information about the moments and it may be impossible to tell with certainty whether truncated moments correspond to a pure or mixed state. However, if there are parameters that appear only in moments of the form $\Delta(q^a\pi^b)$ with $b>1$, they may be considered candidates for impurity parameters. We will see several examples in our derivation of canonical variables for moments.

4.2.3 Casimir–Darboux coordinates

Since the brackets (4.13) are non-canonical, it is not possible to interpret the moments directly in terms of configuration variables and momenta. However, the Darboux theorem and its generalization to Poisson manifolds guarantees that one can always choose coordinates that are canonical, together with a set of Casimir coordinates that have vanishing Poisson brackets with all other variables. The required transformation from moments to Casimir–Darboux variables of this form is, in general, non-linear. In [115], we have developed a systematic method to derive such transformations, based on a proof of Darboux' theorem given in [98]. We have applied this method to semiclassical truncations in [115], which we review here with further details in the relevant integrations.

4.2.3.1 Single pair of degrees of freedom at second order

We illustrate the method for the case of a semiclassical truncation of order two for a single canonical pair of degrees of freedom. In this case, Casimir–Darboux variables had already been found independently in [99, 100].

The relevant Poisson brackets of second-order moments are given in (4.8). The procedure starts by choosing a function that plays the role of the first canonical coordinate. It is convenient to have a quantum fluctuation as one of the configuration

variables, and therefore we choose $s = \sqrt{\Delta(q^2)}$. This function, viewed formally as a Hamiltonian, is the generator of a Hamiltonian flow on phase space defined by

$$\frac{\mathrm{d}f(\Delta(q^2), \Delta(q\pi), \Delta(\pi^2)}{\mathrm{d}\epsilon} = \{f(\Delta(q^2), \Delta(q\pi), \Delta(\pi^2), s\}\,. \tag{4.25}$$

If we already knew canonical coordinates, it would be obvious that the Poisson bracket on the right-hand side of this equation changes only the variable p_s canonically conjugate to s, and therefore the derivative should be equal to the (negative) partial derivative of f by p_s. Since we do not know p_s yet, we revert this argument and implicitly define p_s such that the derivatives in (4.25) equal the negative partial deirvative by p_s for any function f. In particular, for the three second-order moments we obtain

$$\frac{\partial\Delta(q^2)}{\partial p_s} = -\{\Delta(q^2), \sqrt{\Delta(q^2)}\} = 0 \tag{4.26}$$

$$\frac{\partial\Delta(q\pi)}{\partial p_s} = -\{\Delta(q\pi), \sqrt{\Delta(q^2)}\} = \sqrt{\Delta(q^2)} = s \tag{4.27}$$

$$\frac{\partial\Delta(\pi^2)}{\partial p_s} = -\{\Delta(\pi^2), \sqrt{\Delta(q^2)}\} = 2\frac{\Delta(q\pi)}{\sqrt{\Delta(q^2)}} = 2\frac{\Delta(q\pi)}{s}\,. \tag{4.28}$$

By construction, these are partial differential equations in which s is held constant. We can easily solve (4.27) by

$$\Delta(q\pi) = sp_s + f_1(s) \tag{4.29}$$

with a free function f_1 depending only on s. Inserting this solution in (4.28), we have

$$\Delta(\pi^2) = p_s^2 + 2\frac{f_1(s)}{s}p_s + f_2(s) \tag{4.30}$$

with another free function f_2 depending only on s.

Computing $\{\Delta(q\pi), \Delta(\pi^2)\}$ using the canonical nature of the variables s and p_s, and requiring that it equal $2\Delta(\pi^2)$ implies two equations:

$$\frac{\mathrm{d}f_1}{\mathrm{d}s} = \frac{f_1}{s} \quad , \quad \frac{\mathrm{d}f_2}{\mathrm{d}s} = 2\frac{f_1}{s^2}\frac{\mathrm{d}f_1}{\mathrm{d}s} - 2\frac{f_2}{s}\,. \tag{4.31}$$

They are solved by

$$f_1(s) = U_2 s \quad , \quad f_2(s) = \frac{U_1}{s^2} + U_2^2 \tag{4.32}$$

with constants U_1 and U_2. We can eliminate U_2 by a canonical transformation replacing p_s with $p_s + U_2$. The constant U_1 is the Casimir coordinate. The resulting moments in terms of Casimir–Darboux variables are

$$\Delta(q^2) = s^2 \quad , \quad \Delta(q\pi) = sp_s \quad , \quad \Delta(\pi^2) = p_s^2 + \frac{U_1}{s^2} \tag{4.33}$$

as in [99, 100].

In general, it may be difficult to recognize a variable such as U_1 as a Casimir coordinate. In such a case, the flow generated by s or $s^2 = \Delta(q^2)$ is again useful:

$$\frac{\mathrm{d}\Delta(q\pi)}{\mathrm{d}\epsilon} = -2\Delta(q^2) \quad , \quad \frac{\mathrm{d}\Delta(\pi^2)}{\mathrm{d}\epsilon} = -4\Delta(q\pi)\,. \tag{4.34}$$

The solutions are similar to what we already used, $\Delta(q\pi)[\epsilon] = -2\Delta(q^2)\epsilon + d$ for the first equation and $\Delta(\pi^2)[\epsilon] = 4\Delta(q^2)\epsilon^2 - 4d\epsilon + e$ for the second equation, with constants d and e. But now we use these equations to eliminate ϵ instead of solving for p_s. Inserting $\epsilon = \frac{1}{2}(d - \Delta(q\pi)[\epsilon])/s^2$ in $\Delta(\pi^2)[\epsilon]$ implies

$$\Delta(\pi^2)[\epsilon] = \frac{\Delta(q\pi)[\epsilon]^2}{\Delta(q^2)} - 3\frac{d^2}{\Delta(q^2)} + e\,. \tag{4.35}$$

The combination $U_1 = \Delta(q^2)\Delta(\pi^2)[\epsilon] - \Delta(q\pi)[\epsilon]^2 = -3d^2 + es^2$ is therefore independent of ϵ. Since $\mathrm{d}U_1/\mathrm{d}\epsilon = \{U_1, \Delta(q^2)\} = 0$, U_1 is a coordinate Poisson orthogonal to s. It is also Poisson orthogonal to p_s by construction, and therefore represents the Casimir variable of this system.

4.2.3.2 Single pair of degrees of freedom at third order

We now try to find an extension of our Casimir–Darboux coordinates to third order. There are now seven moments, and the rank of the Poisson tensor shows that there is a single Casimir variable. We must therefore derive two additional pairs of canonical degrees of freedom. Since Darboux coordinates are defined only up to canonical transformations, the form in which they appear in the moments is not unique and subject to choices. For now, we make a choice motivated by the canonical form we just derived at second order: We assume that $\Delta(q^2)$ depends

only on one of the new canonical pairs,

$$\Delta(q^2) = s_1^2 \tag{4.36}$$

from which it quickly follows, by a calculation similar to our second-order example, that

$$\Delta(q\pi) = s_1\, p_1 \tag{4.37}$$

is a consistent (but not unique) choice of introducing the first momentum.

The remaining canonical pairs must be such that they have zero Poisson brackets with s_1 and p_1, or with $\Delta(q^2)$ and $\Delta(q\pi)$ according to our first choices. The same procedure that we used to derive U_1 as a coordinate Poisson orthogonal to both s and p_s at second order can also be used here, but now we have five additional moments which should be expressed in terms of functions Poisson orthogonal to s and p_s. By systematically computing the flows of all the remaining moments generated by s_1 and p_1 and eliminating flow parameters, it follows that the following functions of moments are Poisson orthogonal to s_1 and p_1:

$$\begin{aligned}
f_1 &= \Delta(q^2)\Delta(\pi^2) - \Delta(q\pi)^2 \\
f_2 &= \Delta(q^2)\frac{\Delta(q^2\pi)}{\Delta(q^3)} - \Delta(q\pi) \\
f_3 &= \frac{\Delta(q^2)^2}{\Delta(q^3)^2}\left(\Delta(q^2\pi)^2 - \Delta(q\pi^2)\Delta(q^3)\right) \\
f_4 &= 2\Delta(q\pi) + \Delta(q^2)\frac{\Delta(q^3)\Delta(\pi^3) - \Delta(q\pi^2)\Delta(q^2\pi)}{\Delta(q^2\pi)^2 - \Delta(q\pi^2)\Delta(q^3)}\,.
\end{aligned}$$

One additional variable can be derived independently from the Casimir function of the Lie algebra that corresponds to third-order moments,

$$\begin{aligned}
f_5 := U_1^4 &= \left(\Delta(q^2\pi)\Delta(q\pi^2) - \Delta(q^3)\Delta(\pi^3)\right)^2 && (4.38)\\
&\quad -4\left(\Delta(q\pi^2)^2 - \Delta(q^2\pi)\Delta(\pi^3)\right)\left(\Delta(q^2\pi)^2 - \Delta(q^3)\Delta(q\pi^2)\right) && (4.39)
\end{aligned}$$

(The fourth power of U_1 is chosen such that U_1 is of third order just like the moment order considered here.) While f_5 Poisson commutes with all other f_i, (f_1, f_2, f_3, f_4)

have non-linear brackets

$$\begin{aligned}
\{f_1, f_2\} &= 2f_1 + 2f_2^2 + 4f_3 && (4.40)\\
\{f_1, f_3\} &= 12f_2f_3 + 2f_3f_4 && (4.41)\\
\{f_1, f_4\} &= -4f_1 - f_4^2 + 4f_3 - (2f_2 + f_4)^2 && (4.42)\\
\{f_2, f_3\} &= -4f_3 && (4.43)\\
\{f_2, f_4\} &= -4f_2 - 2f_4 && (4.44)\\
\{f_3, f_4\} &= -8f_3 && (4.45)
\end{aligned}$$

with one another.

We are now ready to choose our second configuration variable. We define

$$s_2 = f_3\,, \tag{4.46}$$

such that

$$\frac{\partial f_1}{\partial p_2} = -12s_2f_2 - 2s_2f_4 \quad , \quad \frac{\partial f_2}{\partial p_2} = 4s_2 \quad , \quad \frac{\partial f_4}{\partial p_2} = -8s_2 \tag{4.47}$$

can be used to determine the second momentum variable. Integrating the last two equations and inserting the results in the first one gives

$$\begin{aligned}
f_1 &= -16s_2^2p_2^2 - s_2\,(12g_2 + 2g_4)\,p_2 + g_1 && (4.48)\\
f_2 &= 4s_2p_2 + g_2 && (4.49)\\
f_4 &= -8s_2p_2 + g_4 && (4.50)
\end{aligned}$$

with three functions g_1, g_2 and g_4 independent of p_2. (They can therefore depend on s_2 and the remaining canonical pair, s_3 and p_3, as well as the Casimir variable U_1.) Since we are interested in deriving p_2, we can choose the free functions such that it is easy to invert (4.48), (4.49) or (4.50) for p_2. A wrong choice at this point could result in a degenerate system that does not allow us to derive all canonical pairs. Since we know how many canonical pairs we obtain, a little bit of trial and error quickly shows when a choice is suitable. If we choose $g_4 = -6g_2$, we obtain

$$p_2 = \frac{6f_2 + f_4}{16s_2} \tag{4.51}$$

from a combination of (4.49) and (4.50), as well as

$$g_1 = f_1 + \frac{(6f_2 + f_4)^2}{16} \quad , \quad g_2 = -\frac{1}{2}f_2 - \frac{1}{4}f_4\,. \tag{4.52}$$

By construction, g_1 and g_2 do not depend on p_2, but we have not made sure yet that they do not depend on s_2 either. Since s_2 is defined as s_3, the Poisson brackets (4.40)–(4.45) can be used to show that g_1 and g_2 do, in fact, depend on s_2. The same Poisson brackets determine the canonical flow generated by p_2 in (4.51) on g_1 and g_2. By eliminating the flow parameter as in some of the previous steps, we find that the combinations

$$p_3 = \frac{g_2}{\sqrt{s_2}} \tag{4.53}$$

$$s_3 = \frac{2g_1 - 7s_2 + 10p_3^2 s_2}{6\sqrt{s_2}(4p_3^2 - 1)} \tag{4.54}$$

are independent of s_2 and are therefore Poisson orthogonal to all previously constructed canonical pairs. They determine our final pair (s_3, p_3).

In order to express moments in terms of canonical pairs and the Casimir variable, we insert the functions

$$f_1 = 3\sqrt{s_2}\left(-1 + 4p_3^2\right) s_3 + \frac{1}{2}\left(7s_2 - 10s_2 p_3^2\right) - 16 s_2^2 p_2^2 \tag{4.55}$$

$$f_2 = \sqrt{s_2}p_3 + 4s_2 p_2 \tag{4.56}$$

$$f_3 = s_2 \tag{4.57}$$

$$f_4 = -4\sqrt{s_2}p_3 - 8s_2 p_2 \tag{4.58}$$

$$f_5 = U_1^4 \tag{4.59}$$

in (4.38) and (4.38) and invert the resulting relations for

$$\Delta(q^2) = s_1^2 \quad , \quad \Delta(q\pi) = s_1 p_1 \tag{4.60}$$

$$\Delta(\pi^2) = p_1^2 + \frac{f_1}{s_1^2} = p_1^2 + \frac{3\sqrt{s_2}\,(4p_3^2 - 1)\,s_3 + \frac{1}{2}s_2\,(7 - 10p_3^2) - 16 s_2^2 p_2^2}{s_1^2} \tag{4.61}$$

$$\Delta(\pi^3) = \frac{U_1}{s_1^3\sqrt{2s_2^{3/2}\sqrt{1 - 4p_3^2}}}\Phi(s_i, p_i) \tag{4.62}$$

$$\Delta(q\pi^2) = \frac{U_1}{s_1\sqrt{2s_2^{3/2}\sqrt{1-4p_3^2}}}\left(p_1 s_1 + (p_3-1)\sqrt{s_2} + 4s_2p_2\right) \tag{4.63}$$

$$\times\left(p_1 s_1 + (1+p_3)\sqrt{s_2} + 4s_2p_2\right) \tag{4.64}$$

$$\Delta(q^2\pi) = \frac{U_1}{\sqrt{2s_2^{3/2}\sqrt{1-4p_3^2}}}\left(p_1 s_1^2 + s_1\left(p_3\sqrt{s_2} + 4s_2p_2\right)\right) \tag{4.65}$$

$$\Delta(q^3) = \frac{U_1 s_1^3}{\sqrt{2s_2^{3/2}\sqrt{1-4p_3^2}}}, \tag{4.66}$$

where

$$\Phi(s_i,p_i) = p_1^3s_1^3 + 3p_1^2p_3s_1^2\sqrt{s_2} + 3p_1s_1s_2\left(-1+p_3^2+4p_1s_1p_2\right) + 64p_2^3s_2^3 \tag{4.67}$$
$$+p_3s_2^{3/2}\left(-7+p_3^2+24p_1p_2s_1\right) + 48p_3p_2^2s_2^{5/2} + 12p_2s_2^2\left(-1+p_3^2+4p_1s_1p_2\right).$$

More compactly, some of the momentum-dependent moments can be written as

$$\Delta(\pi^3) = \frac{U_1\left(P^3-3P-4p_3s_2^{3/2}\right)}{s_1^3\sqrt{2s_2^{3/2}\sqrt{1-4p_3^2}}} \tag{4.68}$$

$$\Delta(q\pi^2) = \frac{U_1\left(P^2-s_2\right)}{s_1\sqrt{2s_2^{3/2}\sqrt{1-4p_3^2}}} \tag{4.69}$$

$$\Delta(q^2\pi) = \frac{U_1 s_1 P}{\sqrt{2s_2^{3/2}\sqrt{1-4p_3^2}}} \tag{4.70}$$

if we introduce $P = p_1s_1 + p_3\sqrt{s_2} + 4s_2p_2$. Note that s_3 does not appear in any $\Delta(q^a\pi^b)$ with $b \leq 1$, and may therefore be a candidate for the impurity of a state.

4.2.3.3 Third order by ansatz

As we have seen, several choices have to be made in the process of deriving Casimir–Darboux coordinates. Some choices may lead to degenerate systems in which a smaller number of canonical pairs results, and which should therefore be discarded. However, even within the class of non-degenerate systems, there cannot be a unique set of Casimir–Darboux coordinates because one can always apply canonical transformations of Darboux variables. Depending on the application, some choices

may lead to more useful realizations of canonical variables than others. Staying with the third-order system for a single pair of canonical degrees of freedom, we now apply an alternative method which works by ansatz and therefore is somewhat less systematic than the previous procedure. However, it makes it easier to implement certain properties such as a simplified version of $\Delta(\pi^2)$ in (4.61) with s_i-independent coefficients. As we will see, such a version greatly simplifies the effective dynamics, but it does not always exist, in particular if we have more than one pair of classical degrees of freedom.

We make the ansatz

$$\Delta(\pi^2) = \sum_{i=1}^{3} p_i^2 + F(s_1, s_2, s_3) \quad , \quad \Delta(q\pi) = \sum_{i=1}^{3} s_i p_i \tag{4.71}$$

$$\Delta(q^2) = \sum_{i=1}^{3} s_i^2 \quad , \quad \Delta(q^3) = \sum_{i=1}^{3} s_i^3 \tag{4.72}$$

introducing three canonical pairs, as required. The function $F(s_1, s_2, s_3)$, which is assumed to be independent of the momenta, is subject to consistency conditions that follow from the required Poisson brackets of moments. Once we have a consistent F, we can generate all the remaining moments by taking successive Poisson brackets with $\Delta(\pi^2)$:

$$\Delta(q^{m-1}\pi^{n+1}) = -\frac{1}{2m}\left\{\Delta(\pi^2), \Delta(q^m\pi^n)\right\} , \tag{4.73}$$

starting with $m = 3$, $n = 0$ in which case we have defined $\Delta(q^3)$ in (4.72) and can derive

$$\Delta(q^2\pi) = \sum_i p_i s_i^2 \tag{4.74}$$

$$\Delta(q\pi^2) = \sum_i p_i^2 s_i - \frac{1}{4}\sum_i s_i^2 \frac{\partial F}{\partial s_i} \tag{4.75}$$

$$\Delta(\pi^3) = \sum_i p_i^3 - \frac{1}{4}\sum_i p_i \left(4s_i \frac{\partial F}{\partial s_i} + \sum_j s_j^2 \frac{\partial^2 F}{\partial s_i \partial s_j}\right) . \tag{4.76}$$

Since we have explicitly used all three canonical pairs expected for a third-order truncation, F depends on one further parameter, U, which will be the Casimir coordinate. Since F and therefore U appear only in moments which have at least two momentum factors, U is a candidate for an impurity parameter in this mapping.

Equation (4.73) also applies to second-order moments, $m+n=2$. Since we have defined all three second-order moments in (4.71), we obtain consistency conditions on F. We first compute

$$\{\Delta(\pi^2), \Delta(q^2)\} = -4\sum_i s_i p_i \tag{4.77}$$

and from this

$$\{\Delta\pi^2, \{\Delta(\pi^2), \Delta(q^2)\}\} = 8\sum_i p_i^2 - 4\sum_i s_i \frac{\partial F}{\partial s_i}\,. \tag{4.78}$$

The condition

$$\{\Delta\pi^2, \{\Delta(\pi^2), \Delta(q^2)\}\} = 8\Delta(\pi^2) \tag{4.79}$$

then implies

$$\sum_i s_i \frac{\partial F}{\partial s_i} = -2F \tag{4.80}$$

and therefore F is homogeneous of degree -2 if all s_i are rescaled by the same constant.

Applying further Poisson brackets with $\Delta(\pi^2)$ does not give new conditions. For instance,

$$0 = \Big\{\Delta(\pi^2), \Big\{\Delta(\pi^2), \Big\{\Delta(\pi^2), \Delta(q^2)\Big\}\Big\}\Big\} \tag{4.81}$$

is equivalent to

$$0 = 8\left(3\sum_i p_i \frac{\partial F}{\partial s_i} + \sum_{i,j} p_i s_j \frac{\partial^2 F}{\partial s_i \partial s_j}\right)\,. \tag{4.82}$$

Since the s_i and p_i can be varied independently, the condition implies that all three $\partial F/\partial s_i$ are homogeneous of degree -3 if all s_i are rescaled by the same constant, which follows from F being of degree -2.

Another consistency condition can be derived by looking at the third order moments:

$$0 = \Big\{\Delta(\pi^2), \Big\{\Delta(\pi^2), \Big\{\Delta(\pi^2), \Big\{\Delta(\pi^2), \Delta(q^3)\Big\}\Big\}\Big\}\Big\} \tag{4.83}$$

is equivalent to

$$0 \;=\; 6\sum_i p_i^2 \frac{\partial F}{\partial s_i} + 4\sum_{ij} p_i s_i p_j \frac{\partial^2 F}{\partial s_i \partial s_j} + \frac{1}{2}\sum_{ijk} s_i^2 p_j p_k \frac{\partial^3 F}{\partial s_i \partial s_j \partial s_k} \tag{4.84}$$

$$-\frac{3}{2}\sum_i s_i\left(\frac{\partial F}{\partial s_i}\right)^2-\frac{1}{4}\sum_{ij}s_i^2\frac{\partial F}{\partial s_j}\frac{\partial^2 F}{\partial s_i\partial s_j}\,. \tag{4.85}$$

This condition is generally independent from (4.80). For example, the solution $F=\sum_i U/s_i^2$ of (4.80) is not a solution of (4.84).

One further condition has to be imposed, which is the invertibility of the mapping from moments to (s_i,p_{s_j}). (Otherwise one could choose the trivial solution $F=0$.) For any given F, this condition can be checked by computing the Jacobian of the transformation, and it is fulfilled, for instance, by the solutions

$$F(s_1,s_2,s_3)=\sum_{i<j}\frac{U}{(s_i-s_j)^2} \tag{4.86}$$

of (4.80) and (4.84), where U is the Casimir variable. Therefore, there is a faithful mapping from moments to canonical coordinates at the third order, such that moments are quadratic in the new momenta with s-independent coefficients. The ansatz used here provides a simplified procedure to compute Casimir–Darboux coordinates, but only if moments quadratic in momenta exist. The choice (4.86) is not unique, but it is interesting because for $U>0$ it implies repulsive potentials between the s_i in an effective potential.

At this point, we have obtained two different canonical systems for the third-order semiclassical truncation of a single classical degree of freedom, with Casimir variables U_1 and U, respectively. However, a direct comparison of these two versions of the Casimir variable is difficult because the two Poisson algebras we have canonically realized, in fact, differ from each other in a subtle way: For the mapping derived with the ansatz we have Poisson brackets of third order moments of the form $\left\{\Delta_i^3,\Delta_j^3\right\}=\mathcal{O}(\hbar^2)$. The right-hand side is considered zero in a third-order semiclassical truncation, which corresponds to an $\hbar$-order of 3/2. For the mapping derived systematically, however, we were able to exactly impose $\left\{\Delta_i^3,\Delta_j^3\right\}=0$. Therefore, the two Casimir variables are likely to differ from each other by terms of the order $\hbar^2$.

Nevertheless, it is instructive to compute the Poisson bracket of the moments derived with the ansatz with the Casimir U_1 that was derived systematically. Assuming that s and p are of the order $\mathcal{O}(\sqrt{\hbar})$ in a semiclassical state, computer algebra shows that the Taylor expansion of the Poisson brackets $\{\Delta_{\text{ansatz}},U_1(\Delta_{\text{ansatz}})\}=\mathcal{O}(\hbar^{5/2})$

in $\sqrt{\hbar}$ is zero within the third-order truncation. Therefore, the Casimir variable derived systematically is a Casimir variable also for the realization derived using an ansatz, up to a truncation error.

4.2.3.4 Fourth order

The solution at the third order can be extended in a rather direct manner to the fourth order. Inspection of the rank of the Poisson tensor at this order shows that we expect five canonical pairs of quantum degrees of freedom and two Casimir variables. We then try the ansatz

$$\Delta(\pi^2) = \sum_{i=1}^{5} p_i^2 + \sum_{i>j} \frac{U}{(s_i - s_j)^2} \tag{4.87}$$

$$\Delta(q^2) = \sum_i s_i^2 \tag{4.88}$$

$$\Delta(q^3) = C \sum_i s_i^3 \,. \tag{4.89}$$

In addition to an extension of the third-order ansatz to five pairs of canonical degrees of freedom, we have inserted a new parameter C which will play the role of the second Casimir variable.

The moment $\Delta(q^4)$ can be generated from the Poisson bracket $\{\Delta(\pi q^2), \Delta(q^3)\} = 3\Delta(q^2)^2 - 3\Delta(q^4)$:

$$\Delta(q^4) = C^2 \sum_i s_i^4 + \sum_{i,j} s_i^2 s_j^2 \tag{4.90}$$

We also need to check that the Poisson bracket is consistent at this order. For instance, while an expansion of the right-hand side of

$$0 = \Big\{\Delta(\pi^2), \Big\{\Delta(\pi^2), \Big\{\Delta(\pi^2), \Big\{\Delta(\pi^2), \Big\{\Delta(\pi^2), \Delta(q^4)\Big\}\Big\}\Big\}\Big\}\Big\} \,, \tag{4.91}$$

would be too complex to be shown here, computer algebra confirms that (4.91) is indeed satisfied for our ansatz. This result supports the physical principle that (when $U > 0$) the quantum coordinates feel a repulsive potential between one another that goes as one over the square of the distance between them.

4.2.3.5 Second-order truncation for two pairs of classical degrees of freedom

For two pairs of classical degrees of freedom, we have a ten-dimensional submanifold of second-order moments. The Poisson tensor has rank eight, so that we have to construct four canonical pairs and two Casimir variables.

4.2.3.5.1 First step: The system contains two subalgebras that correspond to a single degree of freedom, given by $\langle\Delta(q_1^2), \Delta(q_1\pi_1), \Delta(\pi_1^2)\rangle$ and $\langle\Delta(q_2^2), \Delta(q_2\pi_2), \Delta(\pi_2^2)\rangle$. We can therefore make use of some of our previous derivations if we choose the first two configuration variables as $s_1 = \sqrt{\Delta(q_1^2)}$ and $s_2 = \sqrt{\Delta(q_2^2)}$. We obtain solutions similar to (4.29) and (4.30) with (4.32), but now the free functions $f_{q_1\pi_1}$, $f_{\pi_1^2}$, $f_{q_2\pi_2}$ and $f_{\pi_2^2}$ in

$$\Delta(q_1\pi_1) = s_1p_1 + f_{q_1\pi_1} \quad , \quad \Delta(\pi_1^2) = p_1^2 + 2\frac{p_1}{s_1}f_{q_1\pi_1} + f_{q_1\pi_1}^2 + \frac{f_{\pi_1^2}}{s_1^2} \tag{4.92}$$

and

$$\Delta(q_2\pi_2) = s_2p_2 + f_{q_2\pi_2} \quad , \quad \Delta(\pi_2^2) = p_2^2 + 2\frac{p_2}{s_2}f_{q_2\pi_2} + f_{q_2\pi_2}^2 + \frac{f_{\pi_2^2}}{s_2^2} \tag{4.93}$$

may still depend on the remaining two canonical pairs, as well as the two Casimirs.

Since $f_{q_1\pi_1}$, $f_{\pi_1^2}$, $f_{q_2\pi_2}$ and $f_{\pi_2^2}$ do not depend on s_1, p_1, s_2 and p_2 by construction, they parameterize coordinate Poisson orthogonal to the first two canonical pairs. However, it is convenient to choose $f_{q_1\pi_1} = 0 = f_{q_2\pi_2}$ because the condition of being Poisson orthogonal to s_1, p_1, s_2 and p_2 is then equivalent to having vanishing Poisson brackets with the basic moments $\Delta(q_1^2) = s_1^2$, $\Delta(q_1\pi_1) = s_1p_1$, $\Delta(q_2^2) = s_2^2$ and $\Delta(q_2\pi_2) = s_2p_2$. This leaves two functions,

$$f_{\pi_1^2} = s_1^2\Delta(\pi_1^2) - s_1^2p_1^2 = \Delta(q_1^2)\Delta(\pi_1^2) - \Delta(q_1\pi_1)^2 =: f_1 \tag{4.94}$$

and

$$f_{\pi_2^2} = s_2^2\Delta(\pi_2^2) - s_2^2p_2^2 = \Delta(q_2^2)\Delta(\pi_2^2) - \Delta(q_2\pi_2)^2 =: f_2\,, \tag{4.95}$$

out of the original free functions in (4.92) and (4.93), which we can easily write in terms of moments.

In addition to f_1 and f_2, we need four further functions that Poisson commute

with the first two canonical pairs, or with $\Delta(q_1^2)$, $\Delta(q_1\pi_1)$, $\Delta(q_2^2)$ and $\Delta(q_2\pi_2)$. As before, we find such variables by considering the flows generated by $\Delta(q_1^2)$, $\Delta(q_1\pi_1)$, $\Delta(q_2^2)$ and $\Delta(q_2\pi_2)$. For instance, for $\Delta(q_1\pi_1)$, the flows $\mathrm{d}/\mathrm{d}\epsilon = \{\cdot, \Delta(q_1\pi_1)\}$ on the remaining moments are

$$\begin{aligned} \frac{\mathrm{d}\Delta(q_1q_2)}{\mathrm{d}\epsilon} &= \Delta(q_1q_2) \quad , \quad \frac{\mathrm{d}\Delta(q_1\pi_2)}{\mathrm{d}\epsilon} = \Delta(q_1\pi_2) \quad , \quad \frac{\mathrm{d}\Delta(q_2\pi_1)}{\mathrm{d}\epsilon} = -\Delta(q_2\pi_1) \quad , \\ \frac{\mathrm{d}\Delta(\pi_1\pi_2)}{\mathrm{d}\epsilon} &= -\Delta(\pi_1\pi_2) \quad , \quad \frac{\mathrm{d}\Delta(q_1^2)}{\mathrm{d}\epsilon} = 2\Delta(q_1^2)\,. \end{aligned} \tag{4.96}$$

These linear differential equations can easily be solved by

$$\begin{aligned} \Delta(q_1q_2) &= c_1e^{\epsilon} \quad , \quad \Delta(q_1\pi_2) = c_2e^{\epsilon} \quad , \quad \Delta(q_2\pi_1) = c_3e^{-\epsilon} \quad , \\ \Delta(\pi_1\pi_2) &= c_4e^{-\epsilon} \quad , \quad \Delta(q_1^2) = c_5e^{2\epsilon}\,. \end{aligned} \tag{4.97}$$

By eliminating ϵ, we find that $\Delta(q_1q_2)\Delta(q_2\pi_1)$, $\Delta(q_1q_2)\Delta(\pi_1\pi_2)$, $\Delta(q_1\pi_2)\Delta(q_2\pi_1)$, $\Delta(q_1\pi_2)\Delta(\pi_1\pi_2)$ and $\Delta(q_1^2)\Delta(\pi_1\pi_2)\Delta(q_2\pi_1)$ Poisson commute with $\Delta(q_1\pi_1)$. However, these combinations are not necessarily invariant under the flows generated by $\Delta(q_1^2)$, $\Delta(q_2^2)$ and $\Delta(q_2\pi_2)$. After computing variables invariant with respect to any one of these four flows, we find that the combinations

$$f_3 = \Delta(q_1\pi_2)\Delta(q_2\pi_1) - \Delta(q_1q_2)\Delta(\pi_1\pi_2) \tag{4.98}$$

$$f_4 = \Delta(q_1^2)\frac{\Delta(q_2\pi_1)}{\Delta(q_1q_2)} - \Delta(q_1\pi_1) \tag{4.99}$$

$$f_5 = \Delta(q_2^2)\frac{\Delta(q_1\pi_2)}{\Delta(q_1q_2)} - \Delta(q_2\pi_2) \tag{4.100}$$

$$f_6 = \frac{\Delta(q_1^2)\Delta(q_2^2)}{\Delta(q_1q_2)^2}\,, \tag{4.101}$$

in addition to f_1 and f_2, are Poisson orthogonal to s_1, p_1, s_2 and p_2. Moreover, their mutual Poisson brackets are closed,

$$\{f_1, f_2\} = 0 = \{f_1, f_3\} = \{f_2, f_3\} \tag{4.102}$$

$$\{f_1, f_4\} = 2(f_1 + f_4^2) \quad , \quad \{f_1, f_5\} = 2f_3f_6 \quad , \quad \{f_1, f_6\} = 4f_4f_6 \tag{4.103}$$

$$\{f_2, f_4\} = 2f_3f_6 \quad , \quad \{f_2, f_5\} = 2(f_2 + f_5^2) \quad , \quad \{f_2, f_6\} = 4f_5f_6 \tag{4.104}$$

$$\{f_3, f_4\} = f_1 + f_3f_6 + f_4^2 \quad , \quad \{f_3, f_5\} = f_2 + f_3f_6 + f_5^2 \quad , \quad \{f_3, f_6\} = 2(f_4 + f_5)f_6 \tag{4.105}$$

$$\{f_4, f_5\} \;=\; (f_5 - f_4)f_6 \quad , \quad \{f_4, f_6\} = -2f_6(1 - f_6) = \{f_5, f_6\} \tag{4.106}$$

and therefore form a Poisson manifold on which we can iterate our procedure, expressing the f_1 in terms of further Casimir–Darboux variables.

4.2.3.5.2 Second step: We now define $s_3 = f_6$, equal to the inverse of the correlation between the two positions. It generates a flow to be identified with the negative partial derivative with respect tp p_3,

$$\frac{\partial f_1}{\partial p_3} \;=\; -\{f_1, f_6\} = -4s_3 f_4 \tag{4.107}$$

$$\frac{\partial f_2}{\partial p_3} \;=\; -4s_3 f_5 \quad , \quad \frac{\partial f_3}{\partial p_3} = -2s_3(f_4 + f_5) \tag{4.108}$$

$$\frac{\partial f_4}{\partial p_3} \;=\; 2s_3(1 - s_3) \quad , \quad \frac{\partial f_5}{\partial p_3} = 2s_3(1 - s_3)\,. \tag{4.109}$$

The last two equations are solved by

$$f_4 = 2s_3p_3(1 - s_3) + g_4 \quad \text{and} \quad f_5 = 2s_3p_3(1 - s_3) + g_5\,, \tag{4.110}$$

after which the remaining equations can be solved by

$$f_1 \;=\; -4s_3^2(1 - s_3)p_3^2 - 4s_3p_3g_4 + g_1 \tag{4.111}$$

$$f_2 \;=\; -4s_3^2(1 - s_3)p_3^2 - 4s_3p_3g_5 + g_2 \tag{4.112}$$

$$f_3 \;=\; -4s_3^2(1 - s_3)p_3^2 - 2s_3p_3(g_4 + g_5) + g_3\,. \tag{4.113}$$

The functions g_i are independent of p_3.

As before, a choice is required to proceed because we have five free functions g_i but only one more canonical pair and two Casimir variables. The choice $g_5 = -g_4$ simplifies f_3 and eliminates these functions from $f_4 + f_5$ according to (4.110) and we obtain our third momentum

$$p_3 = \frac{f_4 + f_5}{4s_3(1 - s_3)}\,. \tag{4.114}$$

We are left with four functions $g_1, \ldots, g_4$ which, by construction, are independent of p_3. But they may depend on s_3 and are therefore not Poisson orthogonal to the third canonical pair. In order to find combinations which Poisson commute with

p_3, we consider the flow generated by $f_4 + f_5 = 4s_3(1-s_3)p_3$. From

$$\begin{aligned} g_1 &= f_1 + \frac{(f_4+f_5)^2}{4(1-f_6)} + \frac{1}{2}\frac{(f_4+f_5)(f_4-f_5)}{1-f_6} && (4.115)\\ g_2 &= f_2 + \frac{(f_4+f_5)^2}{4(1-f_6)} - \frac{1}{2}\frac{(f_4+f_5)(f_4-f_5)}{1-f_6} && (4.116)\\ g_3 &= f_3 + \frac{(f_4+f_5)^2}{4(1-f_6)} && (4.117)\\ g_4 &= \frac{1}{2}(f_4-f_5)\,, && (4.118) \end{aligned}$$

We obtain the brackets

$$\begin{aligned} \{g_1, f_4+f_5\} &= 2(g_1 + s_3 g_3 + g_4^2) && (4.119)\\ \{g_2, f_4+f_5\} &= 2(g_2 + s_3 g_3 + g_4^2) && (4.120)\\ \{g_3, f_4+f_5\} &= g_1 + g_2 + 2s_3 g_3 + 2g_4^2 && (4.121)\\ \{g_4, f_4+f_5\} &= -2s_3 g_4\,. && (4.122) \end{aligned}$$

We see that $\{g_1 + g_2 - 2g_3, f_4 + f_5\} = 0$, and if we trace back all the dependencies on moments, we find that

$$g_1 + g_2 - 2g_3 = U_1 \tag{4.123}$$

is, in fact, the quadratic Casimir. The remaining independent variables can conveniently be chosen as $g_1 + g_2$, $g_1 - g_2$ and g_4, with mutual Poisson brackets

$$\begin{aligned} \{g_1+g_2, g_4\} &= g_1 - g_2 && (4.124)\\ \{g_1-g_2, g_4\} &= g_1 + g_2 - 2s_3 g_3 + 2\frac{1+s_3}{1-s_3} g_4^2 && (4.125)\\ \{g_1+g_2, g_1-g_2\} &= 4\frac{g_4}{1-s_3}(g_1 + g_2 + 2s_3 g_3 + 2g_4^2)\,. && (4.126) \end{aligned}$$

4.2.3.5.3 Final step: We now consider the flow $\partial/\partial s_3 = \{\cdot, p_3\}$, using (4.114):

$$\begin{aligned} \frac{\partial g_4}{\partial s_3} &= \frac{g_4}{2(s_3-1)} \quad , \quad \frac{\partial(g_1-g_2)}{\partial s_3} = \frac{g_1-g_2}{2s_3(1-s_3)} \quad ,\\ \frac{\partial(g_1+g_2)}{\partial s_3} &= \frac{g_1+g_2+2s_3g_3+2g_4^2}{2s_3(1-s_3)} = \frac{(g_1+g_2)(1+s_3) - s_3U_1 + 2g_4^2}{2s_3(1-s_3)} \end{aligned} \tag{4.127}$$

Solving these equations, we find that

$$h_1 = \frac{g_4}{\sqrt{s_3 - 1}} \tag{4.128}$$

$$h_2 = (g_1 - g_2)\sqrt{\frac{s_3 - 1}{s_3}} \tag{4.129}$$

$$h_3 = \frac{(1 - s_3)(g_1 + g_2) + s_3 U_1 + 2(1 + s_3)(1 - s_3)^{-1} g_4^2}{\sqrt{s_3}}\,, \tag{4.130}$$

in addition to U_1, are Poisson orthogonal to s_3 as well as p_3. They have closed brackets

$$\{h_1, h_2\} = h_3 \quad , \quad \{h_1, h_3\} = -h_2 \quad , \quad \{h_2, h_3\} = 8h_1 U_1 - 32h_1^3\,. \tag{4.131}$$

As our final canonical momentum, we choose $p_4 = h_1$. Its flow equations

$$\frac{\partial h_2}{\partial s_4} = -h_3 \quad , \quad \frac{\partial h_3}{\partial s_4} = h_2 \tag{4.132}$$

have trigonometric solutions with a phase that can be set to zero by shifting s_4. Therefore,

$$h_2 = A(p_4)\cos(s_4) \quad , \quad h_3 = A(p_4)\sin(s_4)\,. \tag{4.133}$$

The required Poisson brackets provide a condition on the function $A(p_4)$,

$$A(p_4)\frac{\mathrm{d}A(p_4)}{\mathrm{d}p_4} = -8p_4 U_1 + 32p_4^3\,, \tag{4.134}$$

solved by

$$A(p_4) = \sqrt{U_2 - 8p_4^2 U_1 + 16p_4^4}\,. \tag{4.135}$$

The new free parameter U_2 is a constant and is our second Casimir variable.

4.2.3.5.4 Casimir–Darboux variables: Inverting all intermediate relations, we obtain the moments in terms of Casimir–Darboux variables,

$$\Delta(q_1^2) = s_1^2 \quad , \quad \Delta(q_1\pi_1) = s_1 p_1 \tag{4.136}$$

$$\Delta(\pi_1^2) = p_1^2 + \frac{\Phi(s_3, p_3, s_4, p_4)}{s_1^2} \tag{4.137}$$

with

$$\begin{aligned}\Phi(s_3,p_3,s_4,p_4) &= -\frac{s_3+1}{s_3-1}p_4^2 - 4s_3\sqrt{s_3-1}p_3p_4 + 4s_3^2\left(s_3-1\right)p_3^2 \\ &+\frac{1}{2}\frac{s_3}{s_3-1}U_1 \\ &-\frac{1}{2}\frac{\sqrt{s_3}}{s_3-1}\sqrt{U_2-8p_4^2U_1+16p_4^4}\left(\sqrt{s_3-1}\cos\left(s_4\right)+\sin\left(s_4\right)\right),\end{aligned} \tag{4.138}$$

for moments of the second classical pair of degrees of freedom,

$$\Delta(q_2^2) = s_2^2 \quad , \quad \Delta(q_2\pi_2) = s_2p_2 \tag{4.139}$$

$$\Delta(\pi_2^2) = p_2^2 + \frac{\Gamma(s_3,p_3,s_4,p_4)}{s_2^2} \tag{4.140}$$

with

$$\begin{aligned}\Gamma(s_3,p_3,s_4,p_4) &= -\frac{s_3+1}{s_3-1}p_4^2 + 4s_3\sqrt{s_3-1}p_3p_4 + 4s_3^2\left(s_3-1\right)p_3^2 \\ &+\frac{1}{2}\frac{s_3}{s_3-1}U_1 \\ &-\frac{1}{2}\frac{\sqrt{s_3}}{s_3-1}\sqrt{U_2-8p_4^2U_1+16p_4^4}\left(-\sqrt{s_3-1}\cos\left(s_4\right)+\sin\left(s_4\right)\right),\end{aligned} \tag{4.141}$$

and

$$\begin{aligned}\Delta(\pi_1\pi_2) &= \frac{p_1p_2}{\sqrt{s_3}} + \sqrt{\frac{s_3-1}{s_3}}\left(\frac{p_2}{s_1}-\frac{p_1}{s_2}\right)p_4 \\ &-2\sqrt{s_3}\left(s_3-1\right)\left(\frac{p_1}{s_2}+\frac{p_2}{s_1}\right)p_3 + \frac{\left(3s_3-1\right)}{s_1s_2\sqrt{s_3}\left(s_3-1\right)}p_4^2 \\ &-4\frac{\left(s_3-1\right)s_3^{3/2}}{s_1s_2}p_3^2 - \frac{\sqrt{s_3}}{2s_1s_2\left(s_3-1\right)}U_1 \\ &+\frac{s_3}{2s_1s_2\left(s_3-1\right)}\sin\left(s_4\right)\sqrt{U_2-8p_4^2U_1+16p_4^4}\end{aligned} \tag{4.142}$$

$$\Delta(\pi_1q_2) = \frac{p_1s_2}{\sqrt{s_3}} + \sqrt{\frac{s_3-1}{s_3}}\frac{s_2}{s_1}p_4 - 2\left(s_3-1\right)\sqrt{s_3}\frac{s_2}{s_1}p_3 \tag{4.143}$$

$$\Delta(\pi_2q_1) = \frac{p_2s_1}{\sqrt{s_3}} - \sqrt{\frac{s_3-1}{s_3}}\frac{s_1}{s_2}p_4 - 2\left(s_3-1\right)\sqrt{s_3}\frac{s_1}{s_2}p_3 \tag{4.144}$$

$$\Delta(q_1q_2) = \frac{s_1s_2}{\sqrt{s_3}} \tag{4.145}$$

for the cross-covariances.

4.2.3.5.5 Canonical transformation: We can change our Darboux coordinates by canonical transformations. An intersting example is suggested by the trigonometric form in which s_4 appears in the equations derived so far, which can be extended to s_3 by using the canonical pair

$$\beta = \arctan\sqrt{s_3 - 1} \quad , \quad p_\beta = 2s_3\sqrt{s_3 - 1}p_3 \, . \tag{4.146}$$

Computing $s_3 = 1 + \tan^2\beta = 1/\cos^2\beta$, we see that the new variable β interprets the cross-correlation

$$\frac{\Delta(q_1q_2)}{\sqrt{\Delta(q_1^2)\Delta(q_2^2)}} = \frac{1}{\sqrt{s_3}} = \cos\beta \tag{4.147}$$

as an angle. Uncorrelated canonical pairs are therefore orthogonal to each other in the sense that $\cos\beta = 0$.

Because s_4 already appears in trigonometric functions in our realization, we rename it by defining

$$\alpha = s_4 \quad , \quad p_\alpha = p_4 \, . \tag{4.148}$$

The canonical mapping then takes the form

$$\Delta(q_1^2) = s_1^2 \quad , \quad \Delta(q_1\pi_1) = s_1p_1 \quad , \quad \Delta(\pi_1^2) = p_1^2 + \frac{\Phi}{s_1^2} \tag{4.149}$$

$$\Delta(q_2^2) = s_2^2 \quad , \quad \Delta(q_2\pi_2) = s_2p_2 \quad , \quad \Delta(\pi_2^2) = p_2^2 + \frac{\Gamma}{s_2^2} \tag{4.150}$$

where

$$\begin{aligned} \Phi(\beta, p_\beta, \alpha, p_\alpha) &= (p_\alpha - p_\beta)^2 \\ &\quad + \frac{1}{2\sin(\beta)^2}\left(U_1 - 4p_\alpha^2 - \sqrt{U_2 - U_1^2 + (U_1 - 4p_\alpha^2)^2}\sin(\alpha + \beta)\right) \end{aligned} \tag{4.151}$$

$$\begin{aligned} \Gamma(\beta, p_\beta, \alpha, p_\alpha) &= (p_\alpha + p_\beta)^2 \\ &\quad + \frac{1}{2\sin(\beta)^2}\left(U_1 - 4p_\alpha^2 - \sqrt{U_2 - U_1^2 + (U_1 - 4p_\alpha^2)^2}\sin(\alpha - \beta)\right) , \end{aligned} \tag{4.152}$$

as well as

$$\Delta(\pi_1\pi_2) = p_2p_2\cos(\beta) - \frac{\cos(\beta)}{s_1s_2}p_\beta^2 + \frac{\cos(\beta) + 2\cot(\beta)\csc(\beta)}{s_1s_2}p_\alpha^2 \tag{4.153}$$

$$
\begin{aligned}
&- \sin(\beta) p_\beta \left(\frac{p_2}{s_1} + \frac{p_1}{s_1}\right) + p_\alpha \sin(\beta) \left(\frac{p_2}{s_1} - \frac{p_1}{s_2}\right) \\
&- \frac{\cot(\beta)\csc(\beta)}{s_1 s_2} U_1 + \frac{\csc(\beta)^2 \sin(\alpha)}{2 s_1 s_2} \sqrt{16 p_\alpha^2 - 8 p_\alpha^2 U_1 + U_2}
\end{aligned}
$$

$$
\Delta(\pi_1 q_2) = p_1 s_2 \cos(\beta) + \sin(\beta) \frac{s_2}{s_1} (p_\alpha - p_\beta) \tag{4.154}
$$

$$
\Delta(\pi_2 q_1) = p_2 s_1 \cos(\beta) + \sin(\beta) \frac{s_1}{s_2} (p_\beta + p_\alpha) \tag{4.155}
$$

$$
\Delta(q_1 q_2) = s_1 s_2 \cos(\beta) \,. \tag{4.156}
$$

4.3 Applications

As shown in the preceding section, the inclusion of moments in semiclassical truncations leads to several new degrees of freedom. In this section, we highlight some of the physical effects implied by them. At the same time, we show that the form in which canonical variables appear in various realizations of the moment algebras suggests truncations to smaller canonical subsystems which are easier to analyze by analytic means and often show physical effects more intuitively.

4.3.1 Partition and two-point function of a free massive scalar field

Our first example is an application of the second-order mapping (4.33), rederived here from [99, 100], to a free field theory. We start with the Hamiltonian,

$$
H = \int \mathrm{d}x \left(\frac{1}{2}\pi^2 + \frac{1}{2} (\partial_x \phi)^2 + \frac{1}{2} m^2 \phi^2\right) \tag{4.157}
$$

of a 1-dimensional real scalar field with mass m. We transform to momentum space by writing

$$
\phi_k = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}x \, \phi(x) e^{-ikx} \quad , \quad \pi_k = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}x \, \pi(x) e^{-ikx} \tag{4.158}
$$

with a real wave number k. Reality of $\phi(x)$ and $\pi(x)$ implies that $\phi_k^* = \phi_{-k}$ and $\pi_k^* = \pi_{-k}$.

If we assume that the spatial manifold with coordinate x is compact and of length 2π, thus describing a scalar field on a unit circle, k takes integer values and

we have finite Poisson brackets

$$\{\phi_k, \pi_{k'}\} = \delta_{kk'} \tag{4.159}$$

replacing the field-theory Poisson brackets $\{\phi(x), \pi(y)\} = \delta(x-y)$ in the position representation. Each mode with fixed k is then described by an independent canonical pair (ϕ_k, π_k), which can easily be quantized to a pair $(\hat{\phi}_k, \hat{\pi}_k)$ of operators.

The classical reality condition implies the adjointness relations

$$\hat{\phi}_k^\dagger = \hat{\phi}_{-k} \quad , \quad \hat{\pi}_k^\dagger = \hat{\pi}_{-k} \,. \tag{4.160}$$

The Hamilton operator can therefore be expressed as

$$\hat{H} = \frac{1}{2} \sum_{k=-\infty}^{\infty} \left(\hat{\pi}_k \hat{\pi}_k^\dagger + \omega_k^2 \hat{\phi}_k \hat{\phi}_k^\dagger \right) \tag{4.161}$$

with $\omega_k = \sqrt{m^2 + k^2}$. A further transformation,

$$\hat{\phi}_k = \frac{1}{2} \left(\hat{\phi}_k^{\mathrm{R}} - i \hat{\phi}_k^{\mathrm{L}} \right) \quad , \quad \hat{\pi}_k = \frac{1}{2} \left(\hat{\pi}_k^{\mathrm{R}} + i \hat{\pi}_k^{\mathrm{L}} \right) , \tag{4.162}$$

explicitly decouples left and right-moving modes, $\hat{\phi}_k^{\mathrm{L}}$ and $\hat{\phi}_k^{\mathrm{R}}$, respectively. The Hamilton operator then reads

$$\hat{H} = \frac{1}{2} \sum_{k=-\infty}^{\infty} \left(\left(\hat{\pi}_k^{\mathrm{R}} \right)^2 + \left(\hat{\pi}_k^{\mathrm{L}} \right)^2 + \frac{1}{4} \omega_k^2 \left(\hat{\phi}_k^{\mathrm{R}} \right)^2 + \frac{1}{4} \omega_k^2 \left(\hat{\phi}_k^{\mathrm{L}} \right)^2 \right) . \tag{4.163}$$

4.3.1.1 Partition function

Since all the modes decouple and have harmonic Hamiltonians, the mapping for a single degree of freedom at the second order provides an exact effective description in any state in which cross-correlations between different modes vanish. In the absence of interaction terms in the Hamiltonian, the latter condition is satisfied in the ground state. More generally, we can also consider ensemble averages in finite-temperature states. Since cross-correlations do not contribute the the energy of our non-interacting system, they will not be affected by a turning on a finite temperature. Moreover, correlations in harmonic systems have oscillatory solutions around zero and therefore vanish in an ensemble average.

Mode fluctuations parameterized by the canonical variable s_k with momentum p_k and Casimir U_k, by contrast, are bounded from below by the uncertainty relation and do not average to zero. For every fixed mode and at finite temperature T, we can compute the partition function

$$\mathcal{Z}(\beta,\omega_k,\lambda)=\int_0^\infty\int_{-\infty}^\infty\int_{U_{\min}}^\infty \mathrm{d}s_k\,\mathrm{d}p_k\,\mathrm{d}U_k\exp\left(-\beta\left(\frac{1}{2}p_k^2+\lambda\frac{U_k}{2s_k^2}+\frac{1}{8}\omega_k^2s_k^2\right)\right), \tag{4.164}$$

where $\beta=1/k_{\mathrm{B}}T$ and $U_{\min}=\hbar^2/4$ and we have restricted s_k to positive values. We have inserted the auxiliary parameter λ in anticipation of an application below in which a λ-derivative of $\mathcal{Z}$ will give us the ensemble average of the quantum uncertainty U_k. For all other purposes, we use the physical value $\lambda=1$. If we perform the U_k-integral before the s_k-integral, the partition function

$$\mathcal{Z}(\beta,\omega_k,\lambda)=4\pi\lambda^{-1}\omega_k^{-3}\beta^{-3}\left(2+\beta\omega_k\sqrt{U_{\min}\lambda}\right)\exp\left(-\frac{1}{2}\beta\omega_k\sqrt{U_{\min}\lambda}\right) \tag{4.165}$$

can be obtained in closed form.

A derivative by ω_k (at $\lambda=1$) results in the ensemble averages

$$\langle(s_k^{\mathrm{R}})^2\rangle_{\mathrm{E}}=\langle(s_k^{\mathrm{L}})^2\rangle_{\mathrm{E}}=\frac{12}{\omega_k^2\beta}+\frac{U_{\min}\beta}{1+\frac{1}{2}\sqrt{U_{\min}}\omega_k\beta}. \tag{4.166}$$

of dispersions in a thermal state. Moreover, the average energy per mode is

$$\langle E_k\rangle_{\mathrm{E}}=-\frac{\partial\log\mathcal{Z}}{\partial\beta}=\frac{12+\beta\omega_k\left(6\sqrt{U_{\min}}+U_{\min}\omega_k\beta\right)}{2\beta\left(2+\beta\sqrt{U_{\min}}\omega_k\right)}. \tag{4.167}$$

In the limit $T\to 0$, the value

$$\langle E_k\rangle_E=\sqrt{U_{\min}}\frac{\omega_k}{2} \tag{4.168}$$

agrees with the ground-state energy if we use $U_{\min}=\hbar^2/4$, noting that a single mode used here appears with frequency $\omega_k/2$ in (4.163). (The combination of ϕ_k^{R} and ϕ_k^{L} has the standard harmonic-oscillator energy $\frac{1}{2}\hbar\omega_k$ on average.) Finally, the ensemble average of the quantum uncertainty in a thermal state can be determined

as

$$\langle U_k\rangle_E = \frac{8}{\beta^2\omega_k}\frac{1}{\mathcal{Z}}\left.\frac{\partial^2\mathcal{Z}}{\partial\omega_k\partial\lambda}\right|_{\lambda=1} = U_{\min} + \frac{24}{\beta^2\omega_k^2} + \frac{4U_{\min}}{2+\sqrt{U_{\min}}\beta\omega_k}\,, \tag{4.169}$$

which approaches $U_{\min}$ as $T \to 0$. For $T \neq 0$, $\langle U_k\rangle_{\mathrm{E}} > U_{\min}$ in a mixed, finite-temperature state. The difference $U - U_{\min}$ is therefore an impurity parameter in this situation, which is in agreement with our discussion in Sec. 4.2.2 and the fact that the Casimir U only appears in the second-order moment $\Delta(\pi^2)$.

We see that canonical variables for semiclassical truncations can give easy access to thermodynamical quantities by rewriting a quantum statistical system in the form of a classical system. The canonical nature of variables parameterizing quantum moments makes it possible to determine the correct phase-space volume for the partition function.

4.3.1.2 Two-point function

We extend the definition of moments to our field theory by applying the quantum-mechanics definition to each mode ϕ_k. Introducing $\widehat{\delta\phi}_k = \hat{\phi}_k - \langle\hat{\phi}_k\rangle_{\mathrm{Q}}$, we then have $\Delta(\phi_k\phi_{k'}) = \langle\widehat{\delta\phi}_k\widehat{\delta\phi}_{k'}\rangle_{\mathrm{Q}}$, from which we can obtain correlations in the position representation by Fourier transformation. In these definitions, we have explicitly indicated that expectation values $\langle\cdot\rangle_{\mathrm{Q}}$ refer to a quantum state as opposed to the ensemble average used in (4.166).

The two-point function

$$\begin{aligned}\langle\Delta\left(\phi(x)\phi(y)\right)\rangle_{\mathrm{E}} &= \sum_{kk'}\langle\langle\widehat{\delta\phi}_k\widehat{\delta\phi}_{k'}\rangle_{\mathrm{Q}}\rangle_{\mathrm{E}}e^{ikx}e^{ik'y}\\ &= \frac{1}{4}\sum_{kk'}\left\langle\left\langle\left(\widehat{\delta\phi}^{\mathrm{R}}_k - i\widehat{\delta\phi}^{\mathrm{L}}_k\right)\left(\widehat{\delta\phi}^{\mathrm{R}}_{k'} - i\widehat{\delta\phi}^{\mathrm{L}}_{k'}\right)\right\rangle_{\mathrm{Q}}\right\rangle_{\mathrm{E}}e^{ikx}e^{ik'y}\end{aligned}$$

combines both types of averages. We can simplify the double summation using $\widehat{\delta\phi}^{\mathrm{L}}_{-k} = -\widehat{\delta\phi}^{\mathrm{L}}_k$, which follows from the adjointness relation for $\hat{\phi}_k$. Using zero cross-covariances between the modes as well as the fact that the fluctuations only depend on the wave number k but not on whether the mode is left or right-moving,

the double summation is then reduced to

$$\langle \Delta\left(\phi(x)\phi(y)\right)\rangle_{\mathrm{E}} = \frac{1}{2}\sum_k \langle\langle \widehat{\delta\phi}_k^{\mathrm{R}} \widehat{\delta\phi}_k^{\mathrm{R}}\rangle_{\mathrm{Q}}\rangle_{\mathrm{E}} \cos\left(k(x-y)\right). \tag{4.170}$$

Inserting (4.166), we obtain

$$\langle \Delta\left(\phi(x)\phi(y)\right)\rangle_{\mathrm{E}} = \frac{1}{2}\sum_k \left(\frac{12}{\omega_k^2\beta} + \frac{U_{\min}\beta}{1+\frac{1}{2}\sqrt{U_{\min}}\omega_k\beta}\right)\cos\left(k(x-y)\right). \tag{4.171}$$

In the limit in which the radius of the circle goes to infinity, we can replace $\sum_k$ by $(2\pi)^{-1}\int \mathrm{d}k$, such that

$$\langle \Delta\left(\phi(x)\phi(y)\right)\rangle_{\mathrm{E}} = \frac{1}{2}\int \frac{\mathrm{d}k}{2\pi} \left(\frac{12}{\omega_k^2\beta} + \frac{U_{\min}\beta}{1+\frac{1}{2}\sqrt{U_{\min}}\omega_k\beta}\right)\cos\left(k(x-y)\right). \tag{4.172}$$

It is instructive to consider the low-temperature limit $\beta \to \infty$. Restoring $\hbar$; the result is,

$$\begin{aligned} \lim_{\beta\to\infty} \langle \Delta\left(\phi(x)\phi(y)\right)\rangle_{\mathrm{E}} &= \hbar \int \frac{\mathrm{d}k}{4\pi\omega_k} \cos\left(k(x-y)\right) \\ &= \frac{\hbar}{2\pi} K_0(m|x-y|) \end{aligned} \tag{4.173}$$

with a Bessel function K_0, agrees exactly with the equal-time two-point function obtained using path integral methods.

We can also consider the case where the temperature is nonzero but still small enough for the semi-classical approximation to be valid. Taylor expanding the integrand about $\beta = \infty$, the first-order temperature correction to the two-point function is:

$$\langle \Delta\left(\phi(x)\phi(y)\right)\rangle_{\mathrm{E}} = \frac{\hbar}{2\pi} K_0(m|x-y|) + \frac{9kT}{4m}\hbar \exp\left(-m|x-y|\right) + O(T^2). \tag{4.174}$$

The asymptotic behavior $K_0(z) \sim \sqrt{\frac{1}{2}\pi/z}\, e^{-z}$ for large z shows that the term linear in the temperature decreases more slowly with the distance than the temperature-independent term. For large-distance correlations, this correction from a non-zero temperature may therefore be relevant.

4.3.2 Closure conditions

Our third and fourth order mappings suggest new closure conditions (in the sense of [101]) that can be used to describe moments by a small number of parameters. In particular, we may assume that the second-order fluctuation parameter s contributes to higher-order moments such that $\Delta(q^n) = s^n$, at least for even n. For the third-order moments $\Delta(q^3)$ in the fourth-order truncation, we have seen that the cubic dependence on s_i is multiplied by a free parameter, given by the Casimir variable C, which is lacking in even-order moments $\Delta(q^2)$ and $\Delta(q^4)$. Since odd-order moments are often sub-dominant, for instance in the family of Gaussian states, we can set $C = 0$ and assume that this behavior extends to higher orders. These considerations suggest the closure conditions

$$\Delta(q^n) = \begin{cases} s^n & \text{for even } n \\ 0 & \text{for odd } n \end{cases} \tag{4.175}$$

for all moments, replacing a truncation to finite order. In an effective Hamiltonian, we then obtain the *all-orders effective potential*

$$V_{\text{all-orders}}(q,s) = V(q) + \frac{U}{2ms^2} + \sum_n \frac{1}{(2n)!} \frac{\mathrm{d}^{2n}V(q)}{\mathrm{d}q^{2n}} s^{2n} = \frac{U}{2ms^2} + \frac{1}{2}\left(V(q+s) + V(q-s)\right) \tag{4.176}$$

for a classical potential $V(q)$. The Casimir variable U may be set equal to the minimum value $\hbar^2/4$ allowed by the uncertainty relation.

4.3.2.1 Non-differentiable potentials

Semiclassical physics is usually based on an expansion which requires a smooth potential. Our all-orders effective potential, by contrast, explicitly sums up a perturbative series and expresses quantum effects via finite shifts of the classical potential. It can therefore be applied to potentials that are not smooth or not even differentiable.

As an example, consider the potential $V(q) = |q|$. In particular, we can check the ground state energy. In the static case of zero momentum (and using atomic

units in which $\hbar = 1$ and $m = 1$), we have

$$V_{\text{all-orders}}(q, s) = \frac{1}{8s^2} + \frac{1}{2}\left(|q + s| + |q - s|\right) . \tag{4.177}$$

This function has a minimum at $q = 0$ and $s = 2^{-2/3}$, and the minimum value is $E_{\text{ground}} = 0.94$. We can calculate the exact value of the ground state energy using a truncated oscillator basis. The result is $E^{\text{exact}}_{\text{ground}} = 0.81$.

It is possible obtain this non-differentiable potential as a limit of a differentiable one. To this end, consider the Hamiltonian

$$H = \sqrt{1 + \pi^2} + \frac{1}{2}q^2 \tag{4.178}$$

which can be interpreted as describing a relativistic particle with position-dependent mass $\sqrt{H^2 - \pi^2} = \sqrt{1 + \frac{1}{2}q^2}$. After a simple canonical transformation $(q, \pi) \mapsto (-\pi, q)$ the Hamiltonian

$$H = \frac{\pi^2}{2} + \sqrt{1 + q^2} \tag{4.179}$$

appears in standard form for a non-relativistic system. Now the all-orders effective potential with $U = 1/4$ is given by

$$V_{\text{all-orders}}(q, s) = \frac{1}{8s^2} + \frac{1}{2}\left(\sqrt{1 + (q + s)^2} + \sqrt{1 + (q - s)^2}\right) \tag{4.180}$$

and minimized when $q = 0$. Minimizing

$$V_{\text{all-orders}}(0, s) = \frac{1}{8s^2} + \sqrt{1 + s^2} \tag{4.181}$$

with respect to s, we find the minimum value

$$E_{\text{ground}} = 1.47 . \tag{4.182}$$

The exact ground state energy is

$$E^{\text{exact}}_{\text{ground}} = 1.44. \tag{4.183}$$

The agreement here is better than in the preceding example, which can be interpreted as a limit of a potential in which $\sqrt{1 + q^2}$ is replaced by $\lim_{d\to 0}\sqrt{d + q^2}$.

4.3.2.2 Canonical tunneling in polynomial potentials

The regimes of validity of the all-orders potential can be tested in the case of tunneling escape. For this purpose, we consider a fourth-order polynomial potential in order to describe tunneling escape from a metastable state:

$$V_{\text{poly}}(q) = \frac{27}{4} V_{\text{top}} \gamma q^2 \left(q - 1\right) \left(q - \frac{1}{\gamma}\right) , \tag{4.184}$$

where V_{top} is a parameter that controls the height of the barrier and γ controls the location of the global minimum of this potential. When γ is small, this potential has the following approximate critical points with the corresponding potential values: The top of the barrier is characterized by

$$q_{\text{top}} \approx \frac{2}{3} \quad , \quad V_{\text{poly}}(q_{\text{top}}) = V_{\text{top}} \tag{4.185}$$

and the global minimum is characterized by

$$q_{\text{min}} \approx \frac{3}{4\gamma} \quad , \quad V_{\text{poly}}(q_{\text{min}}) \approx -\frac{729\, V_{\text{top}}}{1024 \gamma^3} . \tag{4.186}$$

In addition to the global minimum, there is a local minimum at $q = 0$ with $V_{\text{poly}}(0) = 0$.

Classically, if the particle starts close to the local minimum at $q = 0$ with an energy less than V_{top}, the particle will remain confined. However if quantum degrees of freedom are taken into account, we know that the particle can tunnel through the barrier and into the lower basin. We can account for this modified dynamics using second-order variables if the barrier is sufficiently small. If the barrier is large, higher-order corrections need to be taken into account in order to see tunneling. The all-orders effective potential, given by

$$V_{\text{all-orders}}(q, s) = \frac{U}{2ms^2} + \frac{1}{2} \left(V_{\text{poly}}(q + s) + V_{\text{poly}}(q - s)\right) \tag{4.187}$$

includes some of the terms that result from higher-order moments.

For escape from a metastable state, the particle is initially at the local minimum at $q = 0$, around which

$$V_{\text{poly}}(q) \approx \frac{27}{4} V_{\text{top}} q^2 . \tag{4.188}$$

For this quadratic approximation, the effective potential is

$$V_{\text{eff}}(q,s) \approx \frac{27}{4} V_{\text{top}} \left(q^2 + s^2\right) + \frac{U}{2s^2} \,. \tag{4.189}$$

This potential has a minimum at

$$q = 0 \quad , \quad s = \left(\frac{2U}{27 V_{\text{top}}}\right)^{1/4} \tag{4.190}$$

which give the approximate ground state energy

$$V_0 \approx \frac{3}{8}\sqrt{\frac{3U}{V_{\text{top}}}}\left(V_{\text{top}} + 2\right) \,. \tag{4.191}$$

Given the initial conditions (4.190) we can track the particle dynamics numerically; see Fig. 4.1. If the parameter V_{top} becomes large the particles no longer tunnels if one only considers the second-order canonical mapping. Second-order dynamics can provide good approximations in certain regimes, but for deep tunneling we need an extension to higher orders. The all-orders effective potential is then useful for understanding the escape from a local minimum in deep tunneling situations.

Using the all-orders potential, we estimate the tunneling time as a function of the tunnel exit position of the particle, which corresponds to the particle position around the critical point $q_{\text{top}} \approx 2/3$. Figures 4.2 and 4.3 show numerical comparison of the canonical tunneling time and the exit momentum of the particle, using the all-orders potential and exact solutions, respectively.

In [95] we used the all-orders effective potential for atomic systems, based on the all-orders closure condition. In a further approximation, it was possible to eliminate some of the basic variables such that $s \approx q$ inside the barrier. For the polynomial potential we can test the same behavior by computing the evolution of the expectation value q and its fluctuation s. As shown Fig. 4.4, the approximate relationship between q and s during tunneling is maintained also here.

Finally, it is interesting to note that the tunneling time can be sensitive to the parameter γ which specifies the location of the global minimum of the classical potential (4.184). We estimate the tunneling time in terms of γ, starting with $\gamma = 0.1$, as shown in Fig. 4.5.

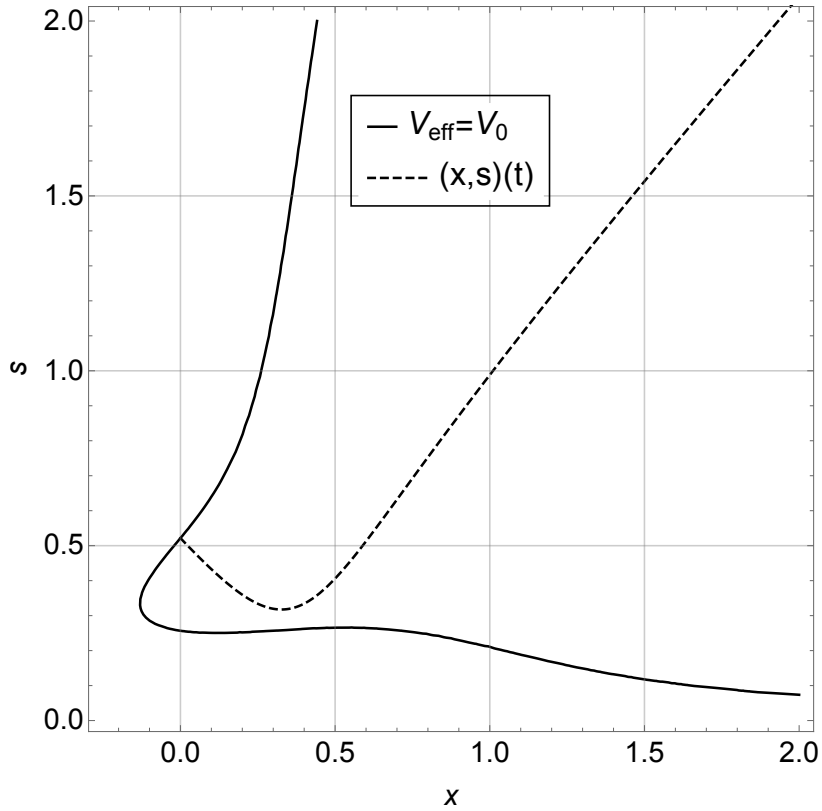

Figure 4.1. Dynamics in the all-orders effective potential (4.187): The potential is represented by its ground-state equipotential curve $V_{\text{eff}} = V_0$ (solid line), together with a tunneling trajectory starting from the local minimum (dashed line). For this plot we chose the parameters $V_{\text{top}} = 1$, $\gamma = 0.1$, $U = 1/4$. The "extra dimension" given by the fluctuation parameter s provides the particle with an escape route around the classical barrier, without violating energy conservation.

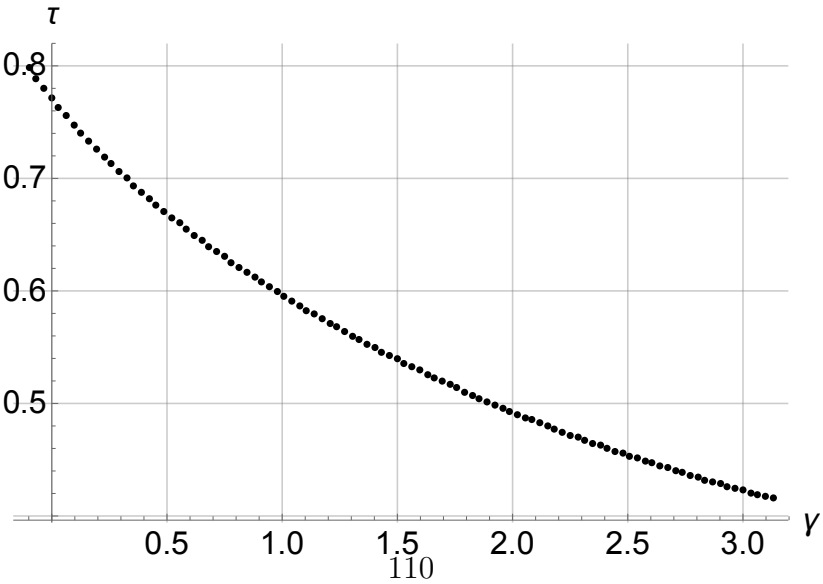

Figure 4.5. The tunneling time as a function of γ in the potential (4.184).

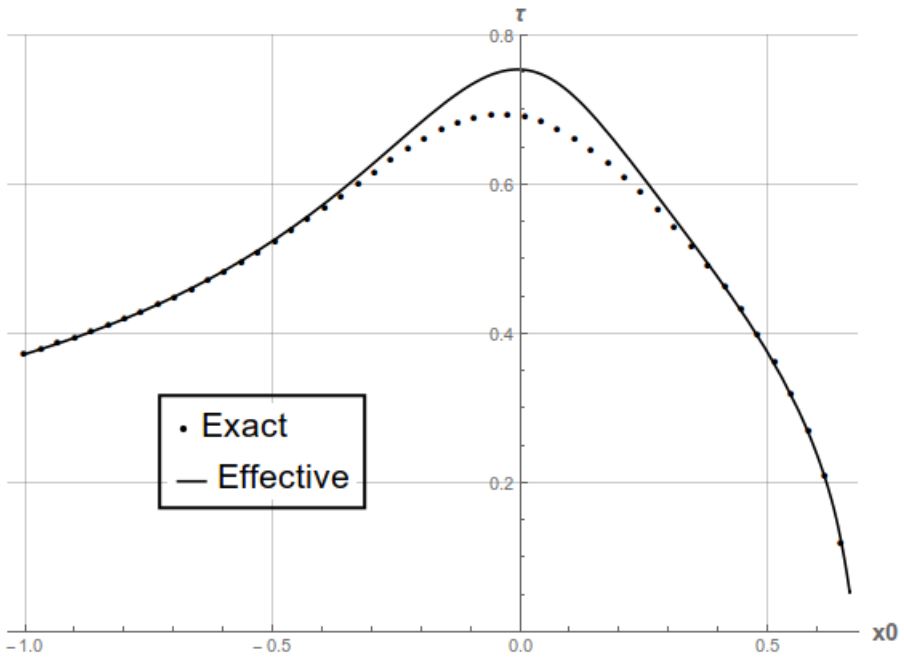

Figure 4.2. Tunneling times as a function of the starting position, for an exact calculation and the all-orders potential, respectively. There is good agreement, with larger discrepancies close to the origin where we have deep tunneling.

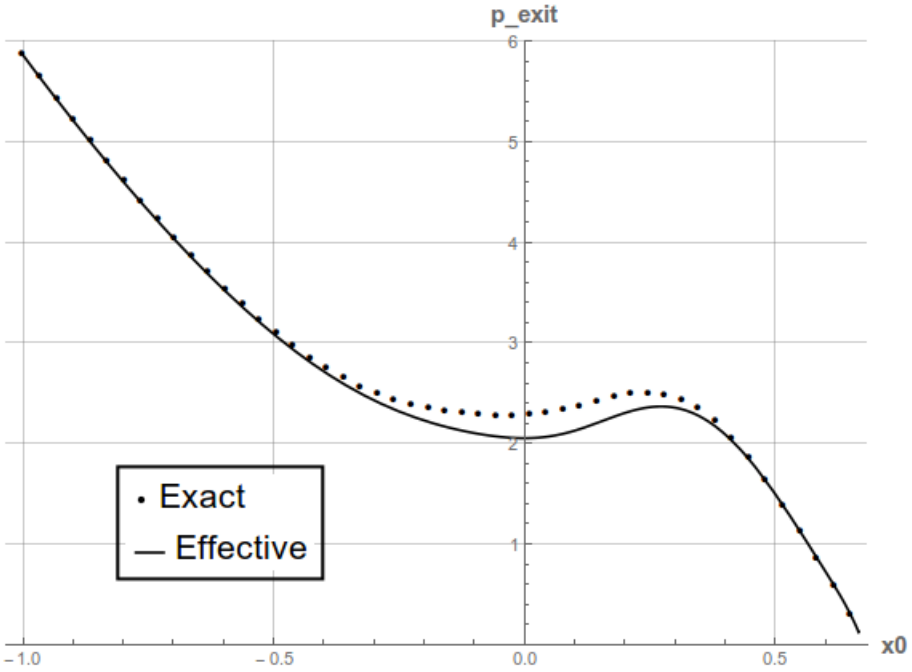

Figure 4.3. The exit momentum of the particle as a function of the initial position.

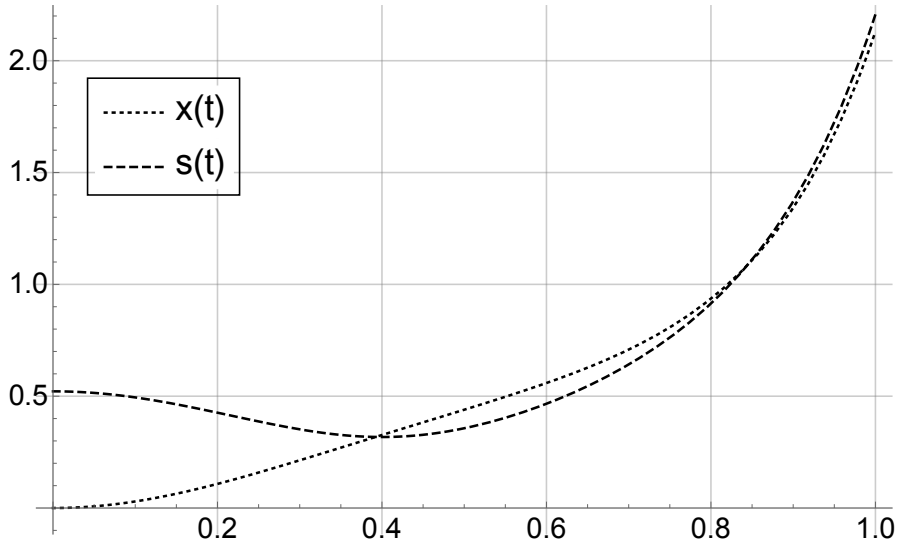

Figure 4.4. Trajectories of the tunneling coordinate q and its fluctuation s for the all-orders effective potential (4.187).

4.3.3 Effective potentials

Casimir–Darboux coordinates for moments, in combination with the effective Hamiltonian (4.6), allow us to identify the dynamics of a semiclassical truncation with a dynamical canonical system. The classical momentum π (derived from the momentum expectation value) is then accompanied by one or more new momenta that parameterize fluctuations, correlations, and higher moments.

For a single classical pair of degrees of freedom to second semiclassical order, the moments are quadratic in the new momentum p_s with constant coefficients. A dynamical system with standard kinetic term is therefore obtained [100]:

$$\begin{aligned}\langle\hat{H}\rangle &= \frac{\langle\hat{\pi}^2\rangle}{2m} + V(\hat{q}) = \frac{\pi^2+\Delta(\pi^2)}{2m} + V(q) + \frac{1}{2}V''(q)\Delta(q^2) + \cdots \\ &= \frac{\pi^2}{2m} + \frac{p_s^2}{2m} + \frac{U}{2ms^2} + V(q) + \frac{1}{2}V''(q)s^2 + \cdots \end{aligned} \tag{4.192}$$

with effective potential

$$V_{\rm eff}(q,s) = \frac{U}{2ms^2} + V(q) + \frac{1}{2}V''(q)s^2\,. \tag{4.193}$$

Our third-order moments provide an extension to the next order, now with three

non-classical momenta. The first version, (4.61), is quadratic in momenta but with coefficients depending on the configuration variables s_i. The second version, (4.71), results in a simplified system with constant coefficients in the extended kinetic term.

However, for two pairs of degrees of freedom, it is not possible to have momentum fluctuations which are quadratic in Darboux momenta with constant coefficients [115]. The resulting effective theories are therefore more involved in such cases. Nevertheless, it is possible to extract an effective potential. Using the Taylor expansion (4.6) of the effective Hamiltonian $\langle\hat{H}\rangle$ and setting all canonical momenta equal to zero, we obtain an expression depending only on the canonical coordinates. We do not require that the momenta vanish for all solutions of interest, which would then be adiabatic, but rather extract a term from the effective Hamiltonian that serves as an effective potential. For this purpose, canonical variables are required in order to know which functions of the moments should be considered momenta.

For two classical degrees of freedom to second semiclassical order, this procedure leads to the effective potential

$$\begin{aligned} V^{(1)}_{\rm eff}(q_1,q_2,s_1,s_2,\alpha,\beta,U_1,U_2) &= V(q_1,q_2) \\ &+\frac{1}{4\sin^2(\beta)}\left(\frac{U_1-\sqrt{U_2}\sin(\alpha+\beta)}{s_1^2}+\frac{U_1-\sqrt{U_2}\sin(\alpha-\beta)}{s_2^2}\right) \\ &+\frac{1}{2}V_{11}(q_1,q_2)s_1^2+V_{12}(q_1,q_2)s_1s_2\cos(\beta)+\frac{1}{2}V_{22}(q_1,q_2)s_2^2 \end{aligned} \tag{4.194}$$

We have used the notation $V_{ij}=\partial^2 V/\partial q_i\partial q_j$, and $V(q_1,q_2)$ is the classical potential. The two Casimir coordinates U_1 and U_2 are constants of motion for any classical dynamics and can be considered (state-dependent) parameters of the effective potential, while the remainder in the effective Hamiltonian is a non-standard kinetic term.

We define the low-energy effective potential $V_{\rm low}(q_1,q_2)$ as the effective potential $V_{\rm eff}$ restricted to values of the moments (that is, s_1, s_2, α, β, U_1 and U_2) obtained in the ground state of the interaction system. We therefore determine the moments by minimizing the effective potential with respect to s_1, s_2, α, β and the two Casimir coordinates while keeping the classical-type variables q_1 and q_2 free.

In this process, we have to respect the boundaries imposed by uncertainty relations. Since W is linear in U_1 and $\sqrt{U_2}$, minimization sends these two values to

the boundary. (From (4.135), we know that $U_2 > 0$ for $p_4 = 0$ to be possible.) The relevant boundary components, at zero momenta, can be obtained from Heisenberg's uncertainty relation applied to each canonical pair:

$$\Phi(\beta, 0, \alpha, 0) = \frac{1}{2\sin(\beta)^2}\left(U_1 - \sqrt{U_2}\sin(\alpha+\beta)\right) \geq \frac{\hbar^2}{4} \tag{4.195}$$

$$\Gamma(\beta, 0, \alpha, 0) = \frac{1}{2\sin(\beta)^2}\left(U_1 - \sqrt{U_2}\sin(\alpha-\beta)\right) \geq \frac{\hbar^2}{4}\,. \tag{4.196}$$

For fixed U_1 and U_2, these two relations must be true for all α and β. Moreover, for any choice of U_1 and U_2 there must be solutions of α and β such that both relations are saturated: If the coupling between the two degrees of freedom is turned off adiabatically we expect saturation in the ground state. Since U_1 and U_2 are constants of motion for any Hamiltonian, their values do not change during this adiabatic decoupling. Therefore, any choice of U_1 and U_2 must allow some solutions of α and β such that the uncertainty relations are saturated.

At saturation, we can subtract (4.195) and (4.196) and obtain

$$-\frac{1}{2}\sqrt{U_2}\frac{\cos(\alpha)}{\sin(\beta)} = 0\,, \tag{4.197}$$

and thus $U_2 = 0$ or $\cos(\alpha) = 0$. In the latter case, the U_2-dependent term in the effective potential,

$$V_{U_2} = -\frac{\sqrt{U_2}\cos(\beta)}{4\sin^2(\beta)}\left(\frac{1}{s_1^2} + \frac{1}{s_2^2}\right)\,, \tag{4.198}$$

is, for any classical potential, unbounded from below in $\sqrt{U_2}$ for any β such that $\cos(\beta) > 0$. This solution of (4.197) is therefore ruled out by the condition that a stable ground state must exist for a large class of classical potentials. We conclude that $U_2 = 0$.

Given this solution, the smallest value of U_1 for which (4.195) can be fulfilled is $U_1 = \hbar^2/2$. Therefore,

$$\Phi|_{p_3=p_4=U_2=0,U_1=\hbar^2/2} = \frac{\hbar^2}{4\sin\beta^2} = \Gamma_{p_3=p_4=U_2=0,U_1=\hbar^2/2} \tag{4.199}$$

from (4.151) and (4.152). The effective potential then reads

$$\begin{aligned} V^{(2)}_{\rm eff}(q_1,q_2,s_1,s_2,\beta) &= V(q_1,q_2) \\ &\quad + \frac{\hbar^2}{8\sin(\beta)^2 s_1^2} + \frac{\hbar^2}{8\sin(\beta)^2 s_2^2} + \frac{1}{2}V_{11}s_1^2 \\ &\quad + V_{12}s_1 s_2\cos(\beta) + \frac{1}{2}V_{22}s_2^2\,. \end{aligned} \tag{4.200}$$

Although we have not minimized the potential in the direction of α, the α-dependence has disappeared. There should, however, be a unique pure state that corresponds to the ground state where the effective potential has its minimum. Since minimization does not determine α, it must be the pure-state condition that fixes its value. This conclusion is in agreement with our earlier discussion of impurity parameters: In the mapping (4.149)–(4.156), α appears only in moments of the form $\Delta(\pi_i\pi_j)$ which are not required to reconstruct a pure state in the position representation.

Minimization by s_1, s_2 and β gives us three equations:

$$0 = \frac{\partial V^{(2)}_{\rm eff}}{\partial s_1} = -\frac{\hbar^2}{4s_1^3\sin^2\beta} + V_{11}s_1 + V_{12}s_2\cos\beta \tag{4.201}$$

$$0 = \frac{\partial V^{(2)}_{\rm eff}}{\partial s_2} = -\frac{\hbar^2}{4s_2^3\sin^2\beta} + V_{22}s_2 + V_{12}s_1\cos\beta \tag{4.202}$$

$$0 = \frac{\partial V^{(2)}_{\rm eff}}{\partial \beta} = -\frac{\hbar^2(s_1^2+s_2^2)\cos\beta}{4s_1^2s_2^2\sin^2\beta} - V_{12}s_1s_2\sin\beta\,. \tag{4.203}$$

Subtracting s_2 times (4.202) from s_1 times (4.201), we obtain

$$\sin^2\beta = \frac{\hbar^2}{4s_1^2s_2^2}\frac{s_2^2-s_1^2}{V_{11}s_1^2 - V_{22}s_2^2}\,. \tag{4.204}$$

Using the sum of s_2 times (4.202) and s_1 times (4.201), we derive

$$4V_{12}^2s_1^2s_2^2\cos^2\beta = \left(\frac{\hbar^2(s_1^2+s_2^2)}{4s_1^2s_2^2\sin^2\beta} - (V_{11}s_1^2+V_{22}s_2^2)\right)^2 \tag{4.205}$$

$$= \left(\frac{s_1^2+s_2^2}{s_1^2-s_2^2}(V_{11}s_1^2 - V_{22}s_2^2) + (V_{11}s_1^2+V_{22}s_2^2)\right)^2 \tag{4.206}$$

$$= 4\frac{(V_{11}s_1^4 - V_{22}s_2^4)^2}{(s_1^2-s_2^2)^2}\,. \tag{4.207}$$

Alternatively, we can derive $4V_{12}^2 s_1^2 s_2^2 \cos^2\beta$ as follows: The sum of $s_1 \sin^2\beta$ times (4.201) and $\cos\beta \sin\beta$ times (4.203) implies

$$\begin{aligned} 0 &= -\frac{\hbar^2(s_1^2+s_2^2)}{4s_1^2 s_2^2 \sin^2\beta} + \frac{\hbar^2}{4s_2^2} + V_{11} s_1^2 \sin^2\beta && (4.208) \\ &= \frac{s_1^2+s_2^2}{s_1^2-s_2^2}(V_{11}s_1^2 - V_{22}s_2^2) + \frac{\hbar^2}{4}\frac{V_{11}-V_{22}}{V_{11}s_1^2 - V_{22}s_2^2} && (4.209) \end{aligned}$$

using (4.204). This equation together with (4.204) also gives us

$$\begin{aligned} 4V_{12}^2 s_1^2 s_2^2 \cos^2\beta &= 4V_{12}^2 s_1^2 s_2^2 \left(1 - \frac{2\hbar^2}{s_1^2 s_2^2}\frac{s_2^2 - s_1^2}{V_{11}s_1^2 - V_{22}s_2^2}\right) && (4.210) \\ &= 4V_{12}^2 \left(s_1^2 s_2^2 + (s_1^2+s_2^2)\frac{V_{11}s_1^2 - V_{22}s_2^2}{V_{11}-V_{22}}\right) && (4.211) \\ &= 4V_{12}^2 \frac{V_{11}s_1^4 - V_{22}s_2^4}{V_{22}-V_{11}}\,. && (4.212) \end{aligned}$$

Equating (4.205) and (4.210), we have

$$V_{11}s_1^4 - V_{22}s_2^4 = \frac{V_{12}^2}{V_{22}-V_{11}}(s_1^2 - s_2^2)^2 \tag{4.213}$$

which can be interpreted as a quadratic equation for s_1^2/s_2^2 with solution

$$\frac{s_1^2}{s_2^2} = \frac{(V_{22}-V_{11})\sqrt{V_{11}V_{22}-V_{12}^2} - V_{12}^2}{V_{11}(V_{22}-V_{11}) - V_{12}^2}\,. \tag{4.214}$$

(There is a unique sign choice implied by $s_1^2/s_2^2 > 0$.)

This solution implies

$$\begin{aligned} \frac{s_1^2+s_2^2}{s_1^2-s_2^2} &= \frac{(V_{22}-V_{11})\left(\sqrt{V_{11}V_{22}-V_{12}^2}+V_{11}\right) - 2V_{12}^2}{(V_{22}-V_{11})\left(\sqrt{V_{11}V_{22}-V_{12}^2}-V_{11}\right)} && (4.215) \\ V_{11}\frac{s_1^2}{s_2^2} - V_{22} &= (V_{22}-V_{11})\sqrt{V_{11}V_{22}-V_{12}^2}\frac{V_{11}-\sqrt{V_{11}V_{22}-V_{12}^2}}{V_{11}(V_{22}-V_{11})-V_{12}^2} && (4.216) \end{aligned}$$

which can be used in (4.208) to obtain

$$s_2^4 = \frac{\hbar^2}{4}\frac{V_{11}V_{22} - V_{12}^2 - V_{11}^2}{V_{11}V_{22} - V_{12}^2}\frac{V_{11} + \sqrt{V_{11}V_{22} - V_{12}^2}}{(V_{22} - V_{11})\sqrt{V_{11}V_{22} - V_{12}^2} + V_{11}V_{22} - V_{11}^2 - 2V_{12}^2}\,. \tag{4.217}$$

We also have

$$\begin{aligned} s_1^4 &= s_2^4(V_{11} \leftrightarrow V_{22}) && (4.218)\\ &= \frac{\hbar^2}{4}\frac{V_{11}V_{22} - V_{12}^2 - V_{22}^2}{V_{11}V_{22} - V_{12}^2}\frac{V_{22} + \sqrt{V_{11}V_{22} - V_{12}^2}}{(V_{11} - V_{22})\sqrt{V_{11}V_{22} - V_{12}^2} + V_{11}V_{22} - V_{22}^2 - 2V_{12}^2} && (4.219) \end{aligned}$$

and the angle β can be obtained by (4.204).

If we insert these solutions in the effective potential, the results can be seen to equal the low-energy effective potential [102]

$$\begin{aligned} V_{\rm low}(q_1, q_2) &= V(q_1, q_2) + \frac{\hbar}{2}\sqrt{\frac{1}{2}\left(V_{11} + V_{22} + \sqrt{(V_{11} - V_{22})^2 + 4V_{12}^2}\right)} && (4.220)\\ &\quad + \frac{\hbar}{2}\sqrt{\frac{1}{2}\left(V_{11} + V_{22} - \sqrt{(V_{11} - V_{22})^2 + 4V_{12}^2}\right)}\,. && (4.221) \end{aligned}$$

although it initially appears in a rather different algebraic form. Our derivation automatically provides results for the ground-state variances and covariance at the minimum of the effective potential. For instance, while the actual expression for β is quite complicated and not given here, for small V_{12} we can use a Taylor expansion and obtain

$$\beta = \frac{\pi}{2} + \frac{V_{12}}{(V_{11}V_{22})^{1/4}\left(\sqrt{V_{11}} + \sqrt{V_{22}}\right)} + O(V_{12}^2)\,. \tag{4.222}$$

In the limit of weak coupling, the moment $\Delta(q_1 q_2)$ therefore goes to zero.

As a simple example, consider the Hamiltonian

$$H = \frac{1}{2}\pi_1^2 + \frac{1}{2}\pi_2^2 + \frac{\omega^2}{2}q_1^2 + \frac{\omega^2}{2}q_2^2 + \gamma\omega^2 q_1 q_2\,. \tag{4.223}$$

Its quantization has the exact ground-state energy

$$E = \frac{1}{2}\hbar\omega\left(\sqrt{1+\gamma}+\sqrt{1-\gamma}\right) \tag{4.224}$$

agreeing with what we get from (4.220).

4.4 Discussion

Our extensions of canonical variables for moments from second order for a single degree of freedom demonstrate several new features of semiclassical states and their dynamics. In particular, we have identified various parameters related to the impurity of a state, a result which also plays a role in the determination of semiclassical potentials. Canonical moment variables are therefore useful tools to understand features of the quantum state space.

Our other applications illustrate the fact that canonical mappings of the form derived here can be relevant in a large set of different physical fields. For instance, they allow one to rewrite quantum statistics in classical terms and thereby provide convenient access to new types of variables (Section 4.3.1). Interestingly, there is a well-defined partition function for second-order moments even though these variables are subject to a non-invertible Poisson structure. For a derivation of the correct phase-space volume element it is therefore crucial to identify Casimir–Darboux variables. Casimir variables do not have momenta and therefore do not contribute the usual $2\pi\hbar$-volume to a partition function. Nevertheless, in our example we saw that we have to integrate over them in order to obtain the correct thermodynamical results for fluctuations.

In tunneling situations, canonical moment variables demonstrate a new heuristic picture of tunneling in which an external field literally opens up a tunnel through a higher-dimensional extension of the classical potential (Fig. 4.1). During tunneling, higher than second-order moments are crucial, which we have captured by the new all-orders effective potential (4.176) defined here for any classical potential. A separate paper [95] provides a detailed application to tunneling ionization in atoms with a successful comparison with recent discussions of experimental results, for which the closure conditions discussed here provide the foundation.

Chapter 5
Equivalence of models in loop quantum cosmology and group field theory

5.1 Introduction

In this chapter we use the idea of faithful realizations in order to define a notion of equivalence that can be used to link a model of group field cosmology with loop quantum cosmology. This link is interesting because it suggests new directions on the group field side of the equivalence. In particular, the link suggests singularities might be more common than currently expected in group field cosmology. Additionally, the link suggests possible generalized group field Hamiltonians based on a quantization ambiguity in harmonic cosmology.

Consider a dynamical system given by a real variable, V, and a complex variable, J, with Poisson brackets

$$\{V, J\} = i\delta J \quad , \quad \{V, \bar{J}\} = -i\delta \bar{J} \quad , \quad \{J, \bar{J}\} = 2i\delta V \tag{5.1}$$

for a fixed real δ. If we identify $H^{\delta}_{\varphi} = \delta^{-1}\mathrm{Im}J = -i(2\delta)^{-1}(J - \bar{J})$ as a Hamiltonian generating evolution in some parameter φ, the equations of motion are solved by

$$V(\varphi) = A\cosh(\delta\varphi) - B\sinh(\delta\varphi) \tag{5.2}$$

$$\mathrm{Re}J(\varphi) = A\sinh(\delta\varphi) - B\cosh(\delta\varphi)\,. \tag{5.3}$$

The brackets (5.1) belong to the Lie algebra $\mathrm{su}(1,1)$ and have the Casimir $R = V^2 - |J|^2$. If R is required to be zero, we obtain $A^2 - B^2 - (\delta H^\delta_\varphi)^2 = 0$ and therefore there is some φ_0 such that $A/(\delta H^\delta_\varphi) = \cosh(\delta\varphi_0)$ and $B/(\delta H^\delta_\varphi) = -\sinh(\delta\varphi_0)$. The solution (5.2) then reads

$$V(\varphi) = \delta H^\delta_\varphi \cosh(\delta(\varphi - \varphi_0)) \tag{5.4}$$

and displays the paradigmatic behavior of the volume of a bouncing universe model. This construction defines harmonic cosmology [103, 104]; see also [105] for further properties related to $\mathrm{su}(1,1)$, in particular group coherent states.

The bouncing behavior can also be inferred from an effective Friedmann equation that describes modified evolution of the scale factor giving rise to the volume V. To do so, we should provide a physical interpretation to the time parameter φ used so far. A temporal description, shared by some models of loop quantum cosmology [106, 107] and group field cosmology [108–112], is a so-called internal time [113]: The parameter φ is proportional to the value of a scalar field ϕ as a specific matter contribution devised such that ϕ is in one-to-one correspondence with some time coordinate such as proper time τ. The scalar ϕ itself can then be used as a global time. Its dynamics must be such that its momentum p_ϕ never becomes zero — "time" ϕ then never stops. With a standard isotropic scalar Hamiltonian

$$h_\phi = \frac{1}{2}\frac{p_\phi^2}{V} + VW(\phi)\,, \tag{5.5}$$

this condition is fulfilled only for vanishing potential $W(\phi)$, such that p_ϕ is conserved. The scalar should therefore be massless and without self-interactions. With these conditions, the conserved momentum p_ϕ generates "time" translations in ϕ, and can therefore be identified with the evolution generator H^δ_φ introduced above. In order to match with coefficients in the Friedmann equation derived below, we set

$$p_\phi = \sqrt{12\pi G} H^\delta_\varphi\,. \tag{5.6}$$

The Hamiltonian (5.5) also allows us to derive a relationship between ϕ and proper time τ, measured by co-moving observers in an isotropic cosmological model. Proper-time equations of motion are determined by Poisson brackets with the

Hamiltonian constraint, to which (5.5) provides the matter contribution. Therefore,

$$\frac{\mathrm{d}\phi}{\mathrm{d}\tau} = \{\phi, h_\phi\} = \frac{p_\phi}{V}\,. \tag{5.7}$$

Writing proper-time derivatives with a dot and using $V = a^3$ to introduce the scale factor a, the chain rule then implies

$$\left(\frac{\dot{a}}{a}\right)^2 = \left(\frac{\dot{\phi}}{3V}\frac{\mathrm{d}V}{\mathrm{d}\phi}\right)^2 = \frac{p_\phi^2}{9V^4}\left(\frac{\mathrm{d}V}{\mathrm{d}\phi}\right)^2 \tag{5.8}$$

in which

$$\frac{1}{V^2}\left(\frac{\mathrm{d}V}{\mathrm{d}\phi}\right)^2 = \frac{1}{V^2}\{V, p_\phi\}^2 = 12\pi G\frac{(\mathrm{Re}J)^2}{V^2} = 12\pi G\left(1 - \frac{\delta^2 p_\phi^2}{12\pi G V^2}\right) \tag{5.9}$$

follows from the ϕ-equations of motion, the zero Casimir $R = 0$, and the identification (5.6) with $H^\delta_\varphi = \delta^{-1}\mathrm{Im}J$. Putting everything together,

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{4\pi G}{3}\frac{p_\phi^2}{V^2}\left(1 - \frac{\delta^2 p_\phi^2}{12\pi G V^2}\right) = \frac{8\pi G}{3}\rho_\phi\left(1 - \frac{\delta^2\rho_\phi}{6\pi G}\right) \tag{5.10}$$

with the energy density $\rho_\phi = \frac{1}{2}p_\phi^2/a^6$ of the free, massless scalar. Upon rescaling $\delta = 4\pi G\tilde{\delta}$, this effective Friedmann equation agrees with what has been derived in loop quantum cosmology, following [114].

Harmonic cosmology can be obtained as a deformation of a certain model of classical cosmology. In the limit of vanishing δ, $H^0_\varphi = \lim_{\delta\to 0} H^\delta_\varphi$ has Poisson bracket

$$\{V, H^0_\varphi\} = \lim_{\delta\to 0}\mathrm{Re}J\,. \tag{5.11}$$

For finite H^0_φ, we must have $\lim_{\delta\to 0}\mathrm{Im}J = 0$, such that the vanishing Casimir implies $\lim_{\delta\to 0}\mathrm{Re}J = V$. Therefore,

$$\{V, H^0_\varphi\} = V \tag{5.12}$$

with an exponential solution $V(\phi) = \exp(\sqrt{12\pi G}\phi)$ that no longer exhibits a bounce. Moreover, noticing that

$$\{V, V^{-1}H^0_\varphi\} = 1\,, \tag{5.13}$$

we can identify $H^0_\varphi/V = P$ with the momentum canonically conjugate to V in the limit of $\delta \to 0$. Therefore,

$$H^0_\varphi = VP \tag{5.14}$$

is quadratic. Squaring this equation, we find

$$P^2 = \frac{(H^0_\varphi)^2}{V^2} = \frac{p_\phi^2}{12\pi G V^2} \tag{5.15}$$

which, upon relating $P = \dot{a}/(4\pi G a)$ to the Hubble parameter and V with the scale factor cubed, is equivalent to the Friedmann equation of an isotropic, spatially flat model sourced by a free, massless scalar field with momentum p_ϕ:

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3}\rho_\phi\,. \tag{5.16}$$

5.2 Loop quantum cosmology as a canonical realization of harmonic cosmology

It is of interest to construct a canonical momentum P of V also in the case of non-zero δ. The pair (V, P) will then be Darboux coordinates on symplectic leaves of the Poisson manifold defined by (5.1), and the full (real) three-dimensional manifold will have Casimir–Darboux coordinates (V, P, R). Following the methods of [115], we can construct such a momentum directly from the brackets (5.1).

Suppose we already know the momentum P. The Poisson bracket of any function on our manifold with V then equals the negative derivative by P. In particular,

$$\frac{\partial \mathrm{Im}J}{\partial P} = -\{\mathrm{Im}J, V\} = \delta \mathrm{Re}J \tag{5.17}$$

$$\frac{\partial \mathrm{Re}J}{\partial P} = -\{\mathrm{Re}J, V\} = -\delta \mathrm{Im}J \tag{5.18}$$

while $\partial V/\partial P = 0$. Up to a crucial sign, these equations are very similar to our equations of motion in the preceding section, and the same is true for their solutions:

$$\mathrm{Im}J(V,P) = A(V)\cos(\delta P) - B(V)\sin(\delta P) \tag{5.19}$$

$$\mathrm{Re}J(V,P) = -A(V)\sin(\delta P) - B(V)\cos(\delta P)\,. \tag{5.20}$$

Since we are now dealing with partial differential equations, the previous constants A and B are allowed to depend on V.

Given these solutions, we can evaluate the Casimir

$$R = V^2 - |J|^2 = V^2 - A(V)^2 - B(V)^2 \,. \tag{5.21}$$

If it equals zero, we have $A(V)^2 + B(V)^2 = V^2$, and there is a P_0 such that $A(V)/V = -\sin(\delta P_0)$ and $B(V)/V = -\cos(\delta P_0)$. Thus,

$$\mathrm{Im}J(V,P) = V\sin(\delta(P-P_0)) \tag{5.22}$$

$$\mathrm{Re}J(V,P) = V\cos(\delta(P-P_0)) \tag{5.23}$$

or

$$J(V,P) = V\exp(i\delta(P-P_0)) \,. \tag{5.24}$$

The canonical realization of (5.1), given by Casimir–Darboux coordinates (V,P,R), identifies J as a "holonomy modification" of the classical Hamiltonian (5.14), in which the Hubble parameter represented by the momentum P is replaced by a periodic function of P. The vanishing Casimir, $R=0$, then appears as a reality condition for P in (5.24).

We conclude that the paradigmatic bounce model of loop quantum cosmology, analyzed numerically in [116], is a canonical realization of harmonic cosmology.

5.3 Group field theory as a bosonic realization of harmonic cosmology

The canonical realization constructed in the preceding section is faithful: the number of Darboux coordinates agrees with the rank of the Poisson tensor given by (5.1), and the number of Casimir coordinates agrees with the co-rank. If one drops the condition of faithfulness, inequivalent realizations can be constructed which even locally are not related to the original system by a canonical transformations. We will call "realization equivalent" any two systems that are realizations of the same model. This notion of equivalence therefore generalizes canonical equivalence. As we will show now, this generalization is crucial in relating loop quantum cosmology

to group field theory.

5.3.1 Bosonic realizations

Instead of canonical realizations, one may consider bosonic realizations, replacing canonical variables, (q, p) such that $\{q, p\} = 1$, with classical versions of creation and annihilation operators, $(z, \bar{z})$ such that $\{\bar{z}, z\} = i$. The map $z = 2^{-1/2}(q + ip)$ defines a bijection between canonical and bosonic realizations.

The brackets (5.1) correspond to the Lie algebra $\mathrm{su}(1, 1)$. A different real form of this algebra, $\mathrm{sp}(2, \mathbb{R})$, has a large number of (non-faithful) bosonic realizations given by the special case of $N = 1$ in the family of realizations

$$A_{ij}^{(n)} = \sum_{\alpha=1}^{n} \bar{z}_{i\alpha}\bar{z}_{j\alpha} \quad , \quad B_{ij}^{(n)} = \sum_{\alpha=1}^{n} z_{i\alpha}z_{j\alpha} \quad , \quad C_{ij}^{(n)} = \frac{1}{2}\sum_{\alpha=1}^{n} (\bar{z}_{i\alpha}z_{j\alpha} + z_{j\alpha}\bar{z}_{i\alpha}) \tag{5.25}$$

of $\mathrm{sp}(2N, \mathbb{R})$ [117–120] with relations

$$[A_{ij}, A_{i'j'}] = 0 = [B_{ij}, B_{i'j'}] \tag{5.26}$$

$$[B_{ij}, A_{i'j'}] = C_{j'j}\delta_{ii'} + C_{i'j}\delta_{ij'} + C_{j'i}\delta_{ji'} + C_{ii'}\delta_{jj'} \tag{5.27}$$

$$[C_{ij}, A_{i'j'}] = A_{ij'}\delta_{ji'} + A_{ii'}\delta_{jj'} \tag{5.28}$$

$$[C_{ij}, B_{i'j'}] = -B_{jj'}\delta_{ii'} - B_{ji'}\delta_{ij'} \tag{5.29}$$

$$[C_{ij}, C_{i'j'}] = C_{ij'}\delta_{i'j} - C_{i'j}\delta_{ij'} \, . \tag{5.30}$$

The indices take values in the ranges $\alpha = 1, \ldots, n$ and $i, j = 1, \ldots, N$, where $i \leq j$ in A_{ij} and B_{ij}. There are $2nN$ real degrees of freedom in the bosonic coordinates $z_{i\alpha}$, while $\mathrm{sp}(2N, \mathbb{R})$ has dimension $N(2N + 1)$.

For $N = 1$, we have three generators

$$A^{(n)} = \sum_{\alpha=1}^{n} \bar{z}_\alpha\bar{z}_\alpha \quad , \quad B^{(n)} = \sum_{\alpha=1}^{n} z_\alpha z_\alpha \quad , \quad C^{(n)} = \frac{1}{2}\sum_{\alpha=1}^{n} (\bar{z}_\alpha z_\alpha + z_\alpha\bar{z}_\alpha) \tag{5.31}$$

with relations

$$[A^{(n)}, B^{(n)}] = C^{(n)} \quad , \quad [A^{(n)}, C^{(n)}] = -2A^{(n)} \quad , \quad [B^{(n)}, C^{(n)}] = 2B^{(n)} \, . \tag{5.32}$$

For any n, the identification

$$A^{(n)} = i\bar{J}/\delta \quad , \quad B^{(n)} = iJ/\delta \quad , \quad C^{(n)} = 2iV/\delta \tag{5.33}$$

relates these brackets to (5.1).

5.3.2 Model of group field theory

In [121], a toy model of group field theory has been derived that produces bouncing cosmological dynamics for the number observable of certain microscopic degrees of freedom. Starting with a tetrahedron, the model assigns annihilation and creation operators to the sides, which change the area in discrete increments. For an isotropic model, the four areas should be identical, and their minimal non-zero value is determined by a quantum number $j = 1/2$, modelling the discrete nature through a spin system following the loop paradigm [122]. Each isotropic excitation has the "single-particle" Hilbert space $(1/2)^{\otimes 4}$ which contains a unique spin-2 subspace. Since this subspace consists of totally symmetric products of the individual states, it is preferred by the condition of isotropy. Restriction to the spin-2 subspace then implies a 5-dimensional single-particle Hilbert space with complex-valued bosonic variables A_i.

A simple non-trivial dynamics is then proposed [121] by the action

$$S = \int \mathrm{d}\phi \left(\frac{1}{2} i \left(A_i^* \frac{\mathrm{d}A^i}{\mathrm{d}\phi} - \frac{\mathrm{d}A_i^*}{\mathrm{d}\phi} A^i \right) - \mathcal{H}(A^i, A_j^*) \right) \tag{5.34}$$

in internal time ϕ. The first term indeed implies bosonic Poisson brackets $\{A_i^*, A^j\} = i\delta_i^J$. The second term is fixed by proposing a squeezing Hamiltonian

$$\mathcal{H}(A^i, A_j^*) = \frac{1}{2} i\lambda \left(A_i^* A_j^* g^{ij} - A^i A^j g_{ij} \right) \tag{5.35}$$

with a coupling constant λ and a constant metric g_{ij} with inverse g^{ij}. The metric is defined through an identification of the spin-2 index i with all totally symmetric combinations of four indices $B_I \in \{1, 2\}$ taking two values, such that

$$g_{(B_1 B_2 B_3 B_4)(C_1 C_2 C_3 C_4)} = \epsilon_{(B_1 (C_1 \epsilon_{B_2 C_2} \epsilon_{B_3 C_3} \epsilon_{B_4) C_4)}} \tag{5.36}$$

with separate total symmetrizations of $\{B_1, B_2, B_3, B_4\}$ and $\{C_1, C_2, C_3, C_4\}$, respectively, and the usual totally antisymmetric ϵ_{BC}. Ordering index combinations as

$$i \in (1,2,3,4,5) = (1111, (1112), (1122), (1222), (2222)) \,, \tag{5.37}$$

the metric can be determined explicitly as the matrix

$$g = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix} . \tag{5.38}$$

A second crucial observable, in addition to the Hamiltonian, is the excitation number,

$$V = \frac{1}{2}\left(A_i^* A^i + A^i A_i^*\right) , \tag{5.39}$$

identified with the cosmological volume following group field cosmology. This volume evolves in internal time ϕ according to the Hamiltonian $\mathcal{H}$. Solutions for $V(\phi)$, derived in [121], show bouncing behavior (5.4) that can be modeled by the effective Friedmann equation (5.10).

We can now readily show that this behavior is not a coincidence: The metric (5.38) has eigenvalues $+1$ with three-fold degeneracy and -1 with two-fold degeneracy. Diagonalizing it by an orthogonal matrix gives linear combinations z_α of the A^i and A_i^* that preserve the bosonic bracket $\{A_i^*, A^j\} = i\delta_i^j$, defining a bosonic transformation:

$$z_1 = \frac{1}{\sqrt{2}}(A^1 + A^5) \quad , \quad z_2 = \frac{1}{\sqrt{2}}(A^2 - A^4) \quad , \quad Z_3 = A^3 \tag{5.40}$$

for eigenvalue $+1$, and

$$z_4 = \frac{1}{\sqrt{2}}(A^1 - A^5) \quad , \quad z_5 = \frac{1}{\sqrt{2}}(A^2 + A^4) \tag{5.41}$$

for eigenvalue -1.

We can deal with the negative eigenvalues in two ways. First, multiplication of z_4 and z_5 with i preserves the bosonic bracket and leads to a metric $g'_{ij} = \delta_{ij}$. We

then have $\mathcal{H} = \frac{1}{2}i\lambda(A^{(5)} - B^{(5)})$ for (5.35) and $V = C^{(5)}$ for (5.39). Alternatively, using only diagonalization by an orthogonal matrix, we have

$$\mathcal{H} = \frac{1}{2}i\lambda\left(A^{(3)} - B^{(3)} - (A^{(2)} - B^{(2)})\right) \tag{5.42}$$

and

$$V = C^{(3)} + C^{(2)} \tag{5.43}$$

where z_1, z_2 and z_3 contribute to the $n = 3$ realization, and z_4 and z_5 to $n = 2$. Observing (5.33) and the fact that the relations (5.1) are invariant under changing the sign of J, the volumes and Hamiltonians in both loop quantum cosmology and group field theory are identified with the same generators in harmonic cosmology. The models of loop quantum cosmology and group field theory are therefore realization equivalent.

5.4 Implications and further directions

There is an immediate application of our result to the appearance of singularities in the model [121] of group field cosmology. As argued in this paper, because the volume is derived from the positive number operator of microscopic excitations A^i, it can be zero only at a local minimum, which requires $V(\phi_{\min}) = 0$ and $\mathrm{d}V/\mathrm{d}\phi = 0$ at some internal time $\phi_{\min}$. The combination of these two conditions is quite restrictive, and [121] concludes that a singularity (zero volume) can be reached only for a small number of initial conditions.

However, our identification of the model of [121] as a bosonic realization of harmonic cosmology suggests a more cautious approach to the singularity problem. In $\mathrm{su}(1,1)$, there is no positivity condition on the generator that corresponds to the volume V. The bosonic realization in terms of microscopic excitations A^i is therefore local, in the sense that the A^i are local coordinates on the Poisson manifold that realizes harmonic cosmology, and $V = 0$ is at the boundary of a local chart. Accompanying $V(\phi_{\min}) = 0$ with $\mathrm{d}V/\mathrm{d}\phi = 0$ is therefore unjustified unless one can show that evolution never leaves a local chart. The condition $V(\phi_{\min}) = 0$ is not as restrictive as the combination, and it leaves more room for solutions that reach zero volume. (These solutions may still be considered non-singular if there is a unique Hamiltonian that evolves solutions through zero volume. In loop quantum

cosmology, evolving through $V = 0$ is interpreted as changing the orientation of space [123, 124].)

In harmonic cosmology, further generalizations of the model used here have already been explored in some detail. The new relationship with group field theory suggests similar generalizations also on the group-field side of the equivalence. For instance, harmonic cosmology can be defined for any power-law $Q = a^p$ replacing $V = a^3$, describing a quantization ambiguity that corresponds to lattice refinement of an underlying discrete geometry [125, 126]. The same algebra, with arbitrary exponent p, can then be realized bosonically, suggesting related group-field models. (While the power-law $V = a^3$ is preferred at large volume because it avoids an expansion of the discrete scale to macroscopic size, a different power low may well be relevant near a spacelike singularity.)

Another parameter related to the relation $V = a^3$ is the averaging volume V_0 used to define the isotropic model. We have implicitly assumed $V_0 = 1$ in order to focus on algebraic properties; in general, we have $V = V_0 a^3$ where V_0 is computed as the coordinate volume of the averaging region. Classical equations do not depend on V_0, but quantum corrections do, as can be seen here from the fact that in the action (5.34) the Hamiltonian $\mathcal{H}$ is proportional to V_0, but the symplectic term is not. The microcopic action is then not invariant under changing V_0. Implications of a relation between V_0 and the infrared scale of an underlying field theory [127] are of importance for the interpretation of quantum cosmology [128], and similar conclusions should hold true in group-field cosmology.

In classical harmonic cosmology, the Casimir $R = 0$ is exactly zero, but this value usually changes in the presence of quantum corrections [103, 104, 129]. The bouncing behavior (5.2) is no longer guaranteed if $R < 0$ and $|R| > (\delta H_\varphi^\delta)^2$, because $V(\phi)$ behaves like a sinh under these conditions. These conditions require large quantum corrections, greater than the matter density related to p_ϕ^2. They are therefore unlikely to be fulfilled in a macroscopic universe. However, as pointed out in [128], an appeal to the BKL scenario [130] near a spacelike singularity shows that a homogeneous model is a good approximation only if it has small co-moving volume, given by the averaging volume V_0 mentioned above. Such a tiny region does not contain much matter energy, which can then easily be surpassed by quantum corrections in a high-curvature regime: $p_\phi \propto V_0$ is suppressed for small V_0, while volume fluctuations ΔV are not proportional to V_0 because they are bounded

from below by the V_0-independent $\hbar$ in uncertainty relations. The genericness of bouncing solutions in loop quantum cosmology or group-field cosmology is then not guaranteed.

Finally, a large class of microscopic models can be constructed from the bosonic realizations of harmonic cosmology with arbitrary n in (5.31). The question of whether these are related to group field cosmology in some way appears to be of interest.

Chapter 6
Summary

Semi-classical methods are generally considered useful owing to the scarcity of exact solutions in quantum mechanics. However, standard semi-classical methods such as the effective action, or the time dependent variational principle have their own domains of validity and may not help for all problems one is interested in. Canonical effective methods provides a more general recourse for such situations. However, this approach is more technically involved owing to a non-linear Poisson bracket, and constraints stemming from the Cauchy-Schwartz inequality. These problems can be overcome by a change of coordinates, from the moments to a set of variables that obey a canonical Poisson bracket. This direction was explored in this dissertation: A general method for constructing canonical coordinate systems was constructed, canonical coordinate systems were constructed for several specific examples, and several physical applications were explored.

The method developed for constructing faithful canonical realizations of semi-classical truncations is a good step towards making canonical effective methods available to a wider set of problems, which in turn can open the door to exploring semi-classical problems in a broader range of validity. Since the canonical coordinate systems are independent of the Hamiltonian used, once our method has been used to construct a canonical coordinate system for a given problem, the work spent finding this coordinate system can be spent in many problems. Also, since the coordinates obey a canonical Poisson bracket, many of the powerful canonical transformation techniques developed for classical mechanics can be applied in the semi-classical regime. This was seen in the example of parametric resonance of two coupled oscillators, where we used a canonical transformation to make contact with the problem of parametric resonance in the literature. Furthermore, our study of

semi-classical truncations led us to identifying the algebraic structure of the second order moments as the Lie algebra $sp(2N, \mathbb{R})$. This implies that the the Casimirs of this algebra are semi-classical constants of motion, this in turn can be used to simplify calculations by the introduction of extra conserved quantities.

The method of canonical realizations also allows one to more intuitively grasp quantum mechanical processes such as quantum tunneling. This is because the usage of a canonical coordinate system not subject to any constraints allows one to use ordinary phase space visualization methods, as we have in chapters three and four. In particular this allows us to see the path the electron takes in the quantum phase space as the atom is ionized.

Using the canonical effective methods and the faithful canonical realizations developed in chapter two, we give new clarity to the problem of tunneling times in chapter 3. Several new ingredients were needed for this. The ground states of most atoms are not semiclassical, so to make headway one needs to move beyond the semiclassical approximation. This was done by choosing a closure of moments. Motivated by results from chapters two and four, we choose the closure $\Delta(x^{2n}) = s^{2n}$ and zero for odd moments. Given a classical Hamiltonian of the form $H = \frac{1}{2}p^2 + V(x)$, this leads to the interesting effective potential $V_{\text{eff}} = \frac{U}{2s^2} + \frac{1}{2}\left(V(x+s) + V(x-s)\right)$. Where U is the Heisenberg uncertainty and s^2 is the variance of the wave function. Heuristically, the particle "feels" around itself at a distance s to decide where to move next. One interesting feature of this potential is that it was derived without a derivative expansion, allowing for the consideration of non-adiabatic states. When applied to tunneling, this effective potential provides much intuition. For example, inspection of the equipotential line of the ground state energy, allows one to see the tunneling channel open and close as the laser pulse passes over the atom. In addition to presenting a tunneling time definition based on these methods in chapter three, we also extract a wide range of physical data, such as: tunneling times for a given laser intensity, fluctuation sizes, offset angles and exit momenta. We were also able to compare with two existing definitions of tunneling times; The Bohmian tunneling time, and the tunneling time defined by classical backpropagation.

Beyond using the canonical variables to aid in calculations or visualization of quantum processes, they can also be used in order to better understand the properties of a quantum state space. For example, in chapter four we were able

to identify several parameters arising in our canonical realization as impurity parameters. Thus the canonical parametrization of the moments can give one some insight into the purity of the state. Furthermore, the canonical parametrization of the phase space allowed us to perform apply methods from statistical physics to semi-classical problems. Calculation of thermodynamic parameters with just the ordinary moments is difficult because one has to use a very inconvenient integration region due to the non-holonomic constraints on the moments and also because it is not clear what the phase space volume element should be for the moments, owing to their complicated Poisson bracket. Canonical coordinate systems thus alleviate these issues by trivializing the constraints and transforming the phase space volume element to standard one.

The framework created for defining and analyzing realizations was also useful for drawing links between different theories by way of realization equivalence. In chapter five we were able to link loop quantum cosmology and a model of group field cosmology by way of realization equivalence. This is significant because these two models of quantum cosmology were derived within the context of two different theories of quantum gravity, giving confidence in the predictions of either theory. Furthermore this link is useful because it implies several generalizations on the group field side of the equivalence. For one, the quantization ambiguity of harmonic cosmology suggests the use of a more general group field Hamiltonian. Also, this link has implications for the formation of singularities in group field cosmology.

The method of faithful realizations has demonstrated a broad range of applicability, from problems in quantum optics to quantum cosmology. This method is especially useful in situations where standard effective techniques can't be relied on, such as non-adiabatic scenarios or for systems without ground states. However there is still work to do. While we have a procedure for finding faithful canonical realizations for semi-classical truncations in general and several worked examples, there are still many truncations that need to have the method applied to them. In particular, a faithful canonical realization of the second order truncation for a system with N degrees of freedom remains to be completed. This would be significant because it would open the door to analyzing quantum field theories and many body systems in situations where an adiabatic effective potential can't be relied on.

Bibliography

[1] M. Peskin and D Schroeder in: *An Introduction to Quantum Field Theory*,(Westview Press, Colorado, 1995) pp 364-383

[2] S. Coleman and E. Weinberg, Radiative Corrections as the Origin of Spontaneous Symmetry Breaking, *Phys. Rev. D*, 7, 1888 (1973)

[3] G. Dunne, The Heisenberg-Euler Effective Action:75 years on, arXiv:1202.1557 [hep-th]

[4] V. Branchina et al., Effective action and the quantum equation of motion, arXiv:hep-th/0306050

[5] L. Dolan and R. Jackiw, Gauge Invariant Signal for Gauge Symmetry Breaking, *Phys. Rev. D*, 9, 2904 (1974)

[6] F. Dyson, Divergence of Perturbation Theory in Quantum Electrodynamics, *Phys. Rev.*, 85, 631 (1952)

[7] G. Dunne and T. Hall, Borel Summation of the Derivative Expansion and Effective Actions, arXiv:hep-th/9902064

[8] D. Boyansky et al., Non-Equillibrium Evolution of Scalar Fields in FRW Cosmologies I, arXiv:hep-ph/9310319

[9] F. Cooper et al., Quantum Dynamics in a time dependent variational approximation, *Phys. Rev. D*, 34, 3832 (1986)

[10] S. Pi and M. Samiullah, Renormalizability of the time dependent variational equations in quantum field theory, *Phys. Rev. D*, 36, 3128 (1987)

[11] M. Bojowald, Quantum Cosmology: Effective Theory, arXiv:1209.3403 [gr-qc]

[12] M. Bojowald, *Quantum Cosmology a Fundamental Description of the Universe*, ISBN: 978-1-4419-8275-9

[13] M. Bojowald, H. Hernandez, and A. Skirzewski Effective equations for isotropic quantum cosmology including matter, *Phys. Rev. D* 76(2007) 063511

[14] O. Prezhdo, Quantized Hamiltonian Dynamics, *Theor. Chem. Acc.* 116 (2006) 206

[15] M. Bojowald, Quantum cosmology: a review, *Rep. Prog. Phys.* 78 (2015) 023901, [arXiv:1501.04899]

[16] E. Pahl and O. Prezhdo, Extension of quantized Hamilton dynamics to higher orders, *J. Chem. Phys.* 116 (2002) 8704–8712

[17] M. Bojowald and A. Skirzewski, Effective Equations of Motion for Quantum Systems, *Rev. Math. Phys.* 18 (2006) 713–745, [math-ph/0511043]

[18] M. Bojowald and A. Skirzewski, Quantum Gravity and Higher Curvature Actions, *Int. J. Geom. Meth. Mod. Phys.* 4 (2007) 25–52, [hep-th/0606232], Proceedings of "Current Mathematical Topics in Gravitation and Cosmology" (42nd Karpacz Winter School of Theoretical Physics), Ed. Borowiec, A. and Francaviglia, M.

[19] M. Bojowald and S. Brahma, Canonical derivation of effective potentials, [arXiv:1411.3636]

[20] F. Arickx, J. Broeckhove, W. Coene, and P. van Leuven, Gaussian Wave-packet Dynamics, *Int. J. Quant. Chem.: Quant. Chem. Symp.* 20 (1986) 471–481

[21] T. Holstein and H. Primakoff, Field dependence of the intrinsic domain magnetization of a ferromagnet, *Phys. Rev.* 58 (1940) 1098–1113

[22] G. Rosensteel and D. J. Rowe, Nuclear sp$(3, R)$ model, *Phys. Rev. Lett.* 38 (1977) 10–14

[23] G. Rosensteel and D. J. Rowe, On the algebraic formulation of collective models III. The symplectic shell model of collective motion, *Ann. Phys.* 126 (1980) 343–370

[24] J. Deenen and C. Quesne, Dynamical group of microscopic collective states. I. One-dimensional case, *J. Math. Phys.* 23 (1982) 878–889

[25] D. J. Rowe, Coherent state theory of the noncompact symplectic group, *J. Math. Phys.* 25 (1984) 2662–2671

[26] O. Castaños, E. Chacón, M. Moshinsky, and C. Quesne, Boson realization of sp(4). I. The matrix formulation, *J. Math. Phys.* 28 (1985) 2107–2123

[27] M. Moshinsky, Boson realization of symplectic algebras, *J. Phys. A* 18 (1985) L1–L6

[28] N. Mukunda, Dynamical symmetries and classical mechanics, *Phys. Rev.* 155 (1967) 1383–1386

[29] N. Mukunda, Realizations of Lie algebras in classical mechanics, *J. Math. Phys.* 8 (1967) 1069–1072

[30] P. Chand, C. L. Mehta, N. Mukunda, and E. C. G. Sudarshan, Realization of Lie algebras by analytic functions of generators of a given Lie algebra, *J. Math. Phys.* 8 (1967) 2048–2059

[31] J. Rosen, On realizations of Lie algebras and symmetries in classical and quantum mechanics, *Il Nuovo Cim.* IL A (1967) 614–621

[32] M. Iosifescu and H. Scutaro, Poisson bracket realizations of Lie algebras and subrepresentations of $(\mathrm{ad}^{\otimes k})_s$, *J. Math. Phys.* 25 (1984) 2856–2962

[33] R. Haag, *Local Quantum Physics*, Springer-Verlag, Berlin, Heidelberg, New York, 1992

[34] A. Tsobanjan, Semiclassical states on Lie algebras, *J. Math. Phys.* 56 (2015) 033501, [arXiv:1410.0704]

[35] M. Bojowald, D. Brizuela, H. H. Hernandez, M. J. Koop, and H. A. Morales-Técotl, High-order quantum back-reaction and quantum cosmology with a positive cosmological constant, *Phys. Rev. D* 84 (2011) 043514, [arXiv:1011.3022]

[36] A. Cannas da Silva and A. Weinstein, *Geometric models for noncommutative algebras*, volume 10 of *Berkeley Mathematics Lectures*, Am. Math. Soc., Providence, 1999

[37] S. Goshen and H. J. Lipkin, A simple independent-particle system having collective properties, *Ann. Phys.* 6 (1959) 301–309

[38] V. I. Arnold, *Mathematical Methods of Classical Mechanics*, Springer, 1997

[39] P. A. M. Dirac, *Lectures on Quantum Mechanics*, Yeshiva Press, 1969

[40] P. G. Bergmann, Observables in General Relativity, *Rev. Mod. Phys.* 33 (1961) 510–514

[41] B. Dittrich, Partial and Complete Observables for Hamiltonian Constrained Systems, *Gen. Rel. Grav.* 39 (2007) 1891–1927, [gr-qc/0411013]

[42] P. Eckle, A. N. Pfeiffer, C. Cirelli, et al., Attosecond Ionization and Tunneling Delay Time Measurements in Helium, *Science* 322 (2009) 1525–1529

[43] N. Camus, E. Yakaboylu, L. Fechner, et al., Experimental Evidence for Quantum Tunneling Time, *Phys. Rev. Lett.* 119 (2017) 023201

[44] U. S. Sainadh, H. Xu, X. Wang, et al., Attosecond angular streaking and tunnelling time in atomic hydrogen, [arXiv:1707.05445]

[45] E. H. Hauge and J. A. Stovneng, Tunneling times: a critical review, *Rev. Mod. Phys.* 61 (1989) 917–936

[46] R. Landauer and Th. Martin, Barrier interaction time in tunneling, *Rev. Mod. Phys.* 66 (1994) 217–228

[47] T. Zimmermann, S. Mishra, B. R. Doran, et al., Tunneling Time in Weak Measurements in Strong Field Ionization, *Phys. Rev. Lett.* 116 (2016) 233603

[48] A. S. Landsman, M. Weger, J. Maurer, R. Boge, A. Ludwig, S. Heuser, C. Cirelli, L. Gallmann, and U. Keller, Ultrafast resolution of tunneling delay time, *Optica* 1 (2014) 343

[49] L. Torlina, F. Morales, J. Kaushal, et al., Interpreting attoclock measurements of tunnelling times, *Nature Physics* 11 (2015) 503–508

[50] A. N. Pfeiffer, C. Cirelli, M. Smolarski, et al., Attoclock reveals natural coordinates of the laser-induced tunneling current flow in atoms, *Nat. Phys.* 8 (2012) 76–80

[51] N. Eicke and M. Lein, Trajectory-free ionization times in strong field ionization, *Phys. Rev. A.* 97 (2018) 031402

[52] N. Teeny, E. Yakaboylu, H. Bauke, and C. Keitel, Ionization Time and Exit Momnetum in Strong Field Tunnel Ionization, *Phys. Rev. Lett.* 116 (2016) 063003

[53] H. Ni, U. Saalmann, and J.-M. Rost, Tunneling Ionization Time Resolved by Backpropagation, *Phys. Rev. Lett.* 117 (2016) 023002

[54] H. Ni, U. Saalmann, and J.-M. Rost, Tunneling exit characteristics from classical backpropagation of an ionized electron wave packet, *Phys. Rev. A* 97 (2018) 013426

[55] H. Ni, N. Eicke, C. Ruiz, J. Cai, F. Oppermann, N. I. Shvetsov-Shilovski, and L.-W. Pi, Tunneling criteria and a nonadiabatic term for strong-field ionization, *Phys. Rev. A* 98 (2018) 013411

[56] D. Bohm, A Suggested Interpretation of the Quantum Theory in Terms of "Hidden" Variables; I, *Phys. Rev.* 85 (1952) 166–179

[57] D. Bohm, A Suggested Interpretation of the Quantum Theory in Terms of "Hidden" Variables; II, *Phys. Rev.* 85 (1952) 180–193

[58] N. Douguet and K. Bartschat, Dynamics of tunneling ionization using Bohmian mechanics, *Phys. Rev. A* 97 (2018) 013402

[59] F. Arickx, J. Broeckhove, W. Coene, and P. van Leuven, Gaussian Wave-packet Dynamics, *Int. J. Quant. Chem.: Quant. Chem. Symp.* 20 (1986) 471–481

[60] O. Prezhdo, Quantized Hamiltonian Dynamics, *Theor. Chem. Acc.* 116 (2006) 206

[61] M. Bojowald and A. Skirzewski, Effective Equations of Motion for Quantum Systems, *Rev. Math. Phys.* 18 (2006) 713–745, [math-ph/0511043]

[62] M. Bojowald and A. Skirzewski, Quantum Gravity and Higher Curvature Actions, *Int. J. Geom. Meth. Mod. Phys.* 4 (2007) 25–52, [hep-th/0606232], Proceedings of "Current Mathematical Topics in Gravitation and Cosmology" (42nd Karpacz Winter School of Theoretical Physics), Ed. Borowiec, A. and Francaviglia, M.

[63] B. Baytaş, M. Bojowald, and S. Crowe, Faithful realizations of semiclassical truncations, arXiv:1810.12127

[64] C. Kühn, Moment ClosureâĂŤA Brief Review, In *Control of Self Organizing Non-Linear Systems*, pages 253–271, Springer International Publishing, 2016

[65] B. Baytaş, M. Bojowald, and S. Crowe, Effective potentials from canonical realizations of semiclassical truncations, [to appear]

[66] E. Wigner, The transition state method, *Trans. Faraday Soc.* 34 (1938) 29–41

[67] L. V. Keldysh, *Zh. Eksp. Teor. Fiz.* 47 (1964) 1945, Sov. Phys. JETP 20 (1965) 1307

[68] V. S. Popov, Tunnel and multiphoton ionization of atoms and ions in a strong laser field (Keldysh theory), *Phys.-Usp.* 47 (2004) 855–885

[69] P. Eckle *et al.*, Science **322**, 1525 (2009).

[70] N. Camus *et al.*, Phys. Rev. Lett. **119**, 023201 (2017).

[71] E. H. Hauge and J. A. Stovneng, Rev. Mod. Phys. **61**, 917 (1989).

[72] R. Landauer and T. Martin, Rev. Mod. Phys. **66**, 217 (1994).

[73] T. Zimmermann, S. Mishra, R. B. Doran, D. F. Gordon and A. S. Landsma *Tunneling Time and Weak Measurement in Strong Field Ionization*, Phys. Rev. Lett. **116**, 233603 (2016)

[74] A. S. Landsman, M. Weger, J. Maurer, R. Boge, A. Ludwig, S. Heuser, C. Cirelli, L. Gallmann, and U. Keller *Ultrafast resolution of tunneling delay time* Optica **1**, 343 (2014)

[75] N. Camus, E. Yakaboylu, L. Fechner, M. Klaiber, M. Laux, Y. Mi, K. Z. Hatsagortsyan, T. Pfeifer, C. H. Keitel, and R. Moshammer *Experimental Evidence for Quantum Tunneling Time* Phys. Rev. Lett. **119**, 023201 (2017)

[76] L. Torlina *et al.*, Nat. Phys. **11**, 503 (2015)

[77] H. Ni, U. Saalmann, and J. M. Rost Phys. Rev. Lett. **117**, 023002 (2016)

[78] U. S. Sainadh *et al.*, arXiv: 1707.05445

[79] N. Douguet and K. Bartschat, *Dynamics of tunneling ionization using Bohmian mechanics*, Phys. Rev. A **97**, 013402 (2018)

[80] H. Ni, U. Saalmann, and J. Rost, *Tunneling exit characteristics from classical backpropagation of an ionized electron wave packet*, Phys. Rev. A **97**, 013426 (2018)

[81] F. Arickx, J. Broeckhove, W. Coene, and P. van Leuven, Int. J. Quant. Chem.: Quant. Chem. Symp. **20**, 471 (1986).

[82] O. Prezhdo, Theor. Chem. Acc. **116**, 206 (2006).

[83] M. Bojowald and A. Skirzewski, Rev. Math. Phys. **18**, 713 (2006), math-ph/0511043.

[84] M. Bojowald *et al.*, Phys. Rev. D **84**, 043514 (2011), arXiv:1011.3022.

[85] A. Cannas da Silva and A. Weinstein, *Geometric models for noncommutative algebras*, Vol. 10 of *Berkeley Mathematics Lectures* (Am. Math. Soc., Providence, 1999).

[86] V. I. Arnold, *Mathematical Methods of Classical Mechanics*, (Springer, 1997).

[87] C. Kühn, in *Control of Self Organizing Non-Linear Systems* (Springer International Publishing, 2016), pp. 253–271.

[88] A. Pfeiffer, C. Cirelli, M. Smolarski, D. Dimitrovski, M. Abu-samha, L. Madsen, U. Keller *Attoclock reveals natural coordinates of the laser induced tunneling current flow in atoms* Phys. Rev. Lett. **8**, 76 (2012)

[89] N. Eicke and M. Lein *Trajectory-free ionization times in strong field ionization* Phys. Rev. A. **97**, 031402 (2018)

[90] H. Ni, N. Eicke, C. Ruiz, J. Cai, F. Oppermann, N. Shvetsov-Shilovski, L. Pi *Tunneling criteria and a nonadiabatic term for strong field ionization* Phys. Rev. A. **98**, 013411 (2018)

[91] N. Teeny, E. Yakaboylu, H. Bauke and C. Keitel *Ionization Time and Exit Momnetum in Strong Field Tunnel Ionization* Phys. Rev. Lett. **116**, 063003(2016)

[92] M. Bojowald and A. Skirzewski, Effective Equations of Motion for Quantum Systems, *Rev. Math. Phys.* 18 (2006) 713–745, [math-ph/0511043]

[93] M. Bojowald and A. Skirzewski, Quantum Gravity and Higher Curvature Actions, *Int. J. Geom. Meth. Mod. Phys.* 4 (2007) 25–52, [hep-th/0606232]

[94] B. Baytaş, M. Bojowald, and S. Crowe, Faithful realizations of semiclassical truncations, [arXiv:1810.12127]

[95] B. Baytaş, M. Bojowald, and S. Crowe, Canonical Tunneling Time in Ionization Experiments, [arXiv:1810.12804]

[96] A. Tsobanjan, Semiclassical states on Lie algebras, *J. Math. Phys.* 56 (2015) 033501, [arXiv:1410.0704]

[97] M. Bojowald, D. Brizuela, H. H. Hernandez, M. J. Koop, and H. A. Morales-Técotl, High-order quantum back-reaction and quantum cosmology with a positive cosmological constant, *Phys. Rev. D* 84 (2011) 043514, [arXiv:1011.3022]

[98] V. I. Arnold, *Mathematical Methods of Classical Mechanics*, Springer, 1997

[99] F. Arickx, J. Broeckhove, W. Coene, and P. van Leuven, Gaussian Wave-packet Dynamics, *Int. J. Quant. Chem.: Quant. Chem. Symp.* 20 (1986) 471–481

[100] O. Prezhdo, Quantized Hamiltonian Dynamics, *Theor. Chem. Acc.* 116 (2006) 206

[101] C. Kühn, Moment ClosureâĂŤA Brief Review, In *Control of Self Organizing Non-Linear Systems*, pages 253–271, Springer International Publishing, 2016

[102] F. Cametti, G. Jona-Lasinio, C. Presilla, and F. Toninelli, Comparison between quantum and classical dynamics in the effective action formalism, In *Proceedings of the International School of Physics "Enrico Fermi", Course CXLIII*, pages 431–448, Amsterdam, 2000. IOS Press, [quant-ph/9910065]

[103] M. Bojowald, Large scale effective theory for cosmological bounces, *Phys. Rev. D* 75 (2007) 081301(R), [gr-qc/0608100]

[104] M. Bojowald, Harmonic cosmology: How much can we know about a universe before the big bang?, *Proc. Roy. Soc. A* 464 (2008) 2135–2150, [arXiv:0710.4919]

[105] E. R. Livine and M. Martín-Benito, Group theoretical Quantization of Isotropic Loop Cosmology, *Phys. Rev. D* 85 (2012) 124052, [arXiv:1204.0539]

[106] M. Bojowald, Loop Quantum Cosmology, *Living Rev. Relativity* 11 (2008) 4, [gr-qc/0601085], `http://www.livingreviews.org/lrr-2008-4`

[107] M. Bojowald, Quantum cosmology: a review, *Rep. Prog. Phys.* 78 (2015) 023901, [arXiv:1501.04899]

[108] G. Calcagni, S. Gielen, and D. Oriti, Group field cosmology: a cosmological field theory of quantum geometry, *Class. Quantum Grav.* 29 (2012) 105005, [arXiv:1201.4151]

[109] S. Gielen, D. Oriti, and L. Sindoni, Cosmology from Group Field Theory Formalism for Quantum Gravity, *Phys. Rev. Lett.* 111 (2013) 031301, [arXiv:1303.3576]

[110] S. Gielen, D. Oriti, and L. Sindoni, Homogeneous cosmologies as group field theory condensates, *JHEP* 1406 (2014) 013, [arXiv:1311.1238]

[111] S. Gielen and D. Oriti, Quantum cosmology from quantum gravity condensates: cosmological variables and lattice-refined dynamics, *New J. Phys.* 16 (2014) 123004, [arXiv:1407.8167]

[112] S. Gielen, Perturbing a quantum gravity condensate, *Phys. Rev. D* 91 (2015) 043526, [arXiv:1411.1077]

[113] P. A. M. Dirac, Generalized Hamiltonian dynamics, *Can. J. Math.* 2 (1950) 129–148

[114] K. Vandersloot, On the Hamiltonian Constraint of Loop Quantum Cosmology, *Phys. Rev. D* 71 (2005) 103506, [gr-qc/0502082]

[115] B. Baytaş, M. Bojowald, and S. Crowe, Faithful realizations of semiclassical truncations (2018), [arXiv:1810.12127]

[116] A. Ashtekar, T. Pawlowski, and P. Singh, Quantum Nature of the Big Bang: An Analytical and Numerical Investigation, *Phys. Rev. D* 73 (2006) 124038, [gr-qc/0604013]

[117] S. Goshen and H. J. Lipkin, A simple independent-particle system having collective properties, *Ann. Phys.* 6 (1959) 301–309

[118] J. Deenen and C. Quesne, Dynamical group of microscopic collective states. I. One-dimensional case, *J. Math. Phys.* 23 (1982) 878–889

[119] O. Castaños, E. Chacón, M. Moshinsky, and C. Quesne, Boson realization of sp(4). I. The matrix formulation, *J. Math. Phys.* 28 (1985) 2107–2123

[120] M. Moshinsky, Boson realization of symplectic algebras, *J. Phys. A* 18 (1985) L1–L6

[121] E. Adjei, S. Gielen, and W. Wieland, Cosmological evolution as squeezing: a toy model for group field cosmology, *Class. Quantum Grav.* 35 (2018) 105016, [arXiv:1712.07266]

[122] C. Rovelli and L. Smolin, Discreteness of Area and Volume in Quantum Gravity, *Nucl. Phys. B* 442 (1995) 593–619, [gr-qc/9411005], Erratum: *Nucl. Phys. B* 456 (1995) 753

[123] M. Bojowald, Absence of a Singularity in Loop Quantum Cosmology, *Phys. Rev. Lett.* 86 (2001) 5227–5230, [gr-qc/0102069]

[124] M. Bojowald, Isotropic Loop Quantum Cosmology, *Class. Quantum Grav.* 19 (2002) 2717–2741, [gr-qc/0202077]

[125] M. Bojowald, Loop quantum cosmology and inhomogeneities, *Gen. Rel. Grav.* 38 (2006) 1771–1795, [gr-qc/0609034]

[126] M. Bojowald, The dark side of a patchwork universe, *Gen. Rel. Grav.* 40 (2008) 639–660, [arXiv:0705.4398]

[127] M. Bojowald and S. Brahma, Minisuperspace models as infrared contributions, *Phys. Rev. D* 92 (2015) 065002, [arXiv:1509.00640]

[128] M. Bojowald, The BKL scenario, infrared renormalization, and quantum cosmology (2018), [arXiv:1810.00238]

[129] M. Bojowald, How quantum is the big bang?, *Phys. Rev. Lett.* 100 (2008) 221301, [arXiv:0805.1192]

[130] V. A. Belinskii, I. M. Khalatnikov, and E. M. Lifschitz, A general solution of the Einstein equations with a time singularity, *Adv. Phys.* 13 (1982) 639–667

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- B. Baytas, M. Bojowald and S. Crowe, Faithful realizations of semiclassical truncations, [arXiv:1810.12127]
- B. Baytas, M. Bojowald and S. Crowe, *Canonical tunneling times in ionization experiments,* Phys. Rev. A **97**, 013426 (2018)
- B. Baytas, M. Bojowald and S. Crowe, *Effective potentials from semiclassical* truncations, Phys. Rev. A **99**, 042114 (2019)
- B. Baytas, M. Bojowald and S. Crowe, *Equivalence of models in loop quantum cosmology and group field theory*, Universe 2019, 5(2), 41