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Thimble regularization of Quantum Field Theory as a solution to the sign problem

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"It is dangerous business, Frodo, going out of your door.
You step into the road and if you don't keep your feet,
there is no knowing where you might be swept off to."

(Bilbo Baggins)

Contents

1   Agenda and motivations

In the last years much effort has been put into studying non-perturbative properties of strongly coupled quantum field theories. In this context, a fundamental role has been played by Monte Carlo techniques, which rely on a Markov chain to compute expectation values of observables [1]. Despite being such a powerful tool, Monte Carlo has failed to work for a large class of important models, namely those featuring a *complex* action. This situation is referred to as the *sign problem* and has so far prevented an accurate solution of *e.g.* real-time quantum field theories [2], systems of electrons occurring in low-energy physics such as the Hubbard model [3, 4], models for nuclear physics [5], the Yang-Mills theory in presence of a θ-term [6, 7] and finite density QCD [8, 9]. In particular, a complete knowledge of the QCD phase diagram is still missing (especially in the high density region) because of the sign problem, even though many techniques have been put at work to a success in some regions of parameters. These approaches include reweighting [10], Taylor expansion [11], analytical continuation to imaginary chemical potential [12, 13], complex Langevin [14, 15, 16, 17], the fermion bag algorithm [18], effective 3d theories [19], the histogram method [20], density of states approach [21, 22], fugacity expansion [23], dimensional reduction [24] and large N_c limit [25]. To this day, there is not a single approach which is both rigorously justified and applicable to every part of the QCD phase diagram. As a consequence, a new approach was recently proposed [26], that is *thimble regularization* of a quantum field theory. This method is promising as it is based on a quite general mathematical framework and thus is expected to work in principle for any model in any regime. Being the approach both quite young and promising, yet challenging from a theoretical as well as a numerical point of view, it is worth a detailed study. In this respect, the present work covers the foundations of the method as well as its first applications, starting from simple toy models and then moving towards gauge theories. For a recent review on the subject, refer to [27].

The work is laid out as follows: in Section 2 we review the general formalism regarding the introduction of temperature and chemical potential in a quantum field theory, both in the continuum and on the lattice; in particular, we focus on the rise of the sign problem for free fermions. In Section 3 we discuss the general framework of Morse theory and Lefschetz thimble decomposition. We will make use of a language the theoretical physicist is expected to be familiar with, leaving the (involved) mathematical details to the references. In Section 4 we set up the basics of thimble regularization for theories involving gauge symmetry. In Section 5 we discuss the issue of performing actual Monte Carlo simulations on thimbles; a new parametrization is introduced, along with a Monte Carlo algorithm. In Section 6 a simple one-dimensional model will be discussed in detail within the framework of Morse theory. Although quite simple, this model provides valuable insights to become familiar with the formalism, while at the same time addressing the issue of the relevance of more than one thimble. In Section 7 a chiral random matrix model is solved by thimble decomposition in a region of parameters which was shown to be affected by a severe sign problem. In Section 8 the simplest examples of gauge theories are studied, that is $\mathrm{SU}(N)$ one-link models. Despite their obvious simplicity, these models provide a non trivial setting to test the thimble formalism for gauge theories. In Section 9 QCD in $0+1$ dimensions is studied at various numbers of quark flavours. This theory is interesting because the origin of its sign problem lies in the presence of a quark chemical potential, as in real QCD. The model can be solved analytically, thus providing exact results to compare with. Numerical simulations of thimble regularization for the theory are performed and their results compared with exact ones. The issue of the relevance of multiple thimbles is discussed as well. In Section 10 we set up the basic formalism to tackle Yang-Mills theory in 2 dimensions with the thimble formalism. Exact results are available for this model, in which the sign problem is put in by hand by means of a complex coupling. Although in some sense "unphysical", this model is useful to study issues which are there also in more realistic situations (such as Yang-Mills with a θ-term or QCD). One of this issue is the presence of toronic modes. There is also the problem of numerically integrating on a gauge-symmetric thimble. These issues are discussed in detail, although actual numerical computations for this model are left for future study.

2 Genesis of the sign problem

The study of quantum field theories such as QCD at zero density, that is in vacuum, has made it possible to compute many cross-sections in particle scattering experiments with increasingly higher precision. However, in extreme conditions, such as the collisions between heavy ions, it becomes necessary to explicitly introduce temperature and matter density in the theory. A similar situation occurs in models for the extremely dense matter in neutron stars or in the study of the interactions between quarks and gluons just after the Big-Bang. From the point of view of statistical mechanics (which a quantum field theory resembles in its Euclidean formulation) the introduction of temperature corresponds to going from the microcanonical ensemble to the canonical one, while the introduction of a chemical potential corresponds to the grandcanonical ensemble. In the next paragraphs, we shall refer to [28, 29, 30, 31].

2.1 The introduction of temperature and density

Let us consider the canonical partition function of a quantum mechanical system whose dynamics is governed by the Hamiltonian $\hat{H}$ in a heat bath at temperature T

$$Z(T) = \mathrm{Tr}\left[e^{-\beta \hat{H}}\right] \tag{2.1}$$

with $\beta = 1/(k_B T)$, where k_B is Boltzmann constant and we shall put $k_B = 1$. It is easy to derive a relation with the quantum field theory described by $\hat{H}$ in its Euclidean path-integral formulation. Let us consider a generic field theory consisting in a collection of fields $\Phi(x)$ on a D-dimensional spacetime. The trace in (2.1) forces periodic boundary conditions on bosonic fields and antiperiodic boundary conditions on fermionic fields. Then the path-integral expression for the partition function becomes

$$Z(T) = \int \mathcal{D}\Phi \, e^{-S_E[\Phi]}$$

$$\mathcal{D}\Phi = \prod_x \mathrm{d}\Phi(x)$$

The path-integral is understood with the appropriate boundary conditions for the fields and $S_E[\Phi]$ is the Euclidean action of the theory resulting from an integration of the Lagrangian density $\mathcal{L}_E$ on the whole $(D-1)$-dimensional space and on a finite time interval with extent β

$$S_E[\Phi] = \int_0^\beta \mathrm{d}t \int_{\mathbb{R}^{D-1}} \mathrm{d}^{D-1}x \, \mathcal{L}_E[\Phi(t,\vec{x}), \partial_\mu \Phi(t,\vec{x})]$$

Here $t = 0$ and $t = \beta$ are understood to be identified, thus going from an Euclidean spacetime $\mathbb{R}^D$ to $S^1 \times \mathbb{R}^{D-1}$. When discretizing the field theory on a lattice, we will consider a spatial extension Na along each axis, where a is the lattice spacing and N is the number of spatial lattice sites. For the time direction, instead, we will have

$$\beta = \frac{1}{T} = N_T a$$

where N_T is the number of temporal lattice sites. This lattice field theory is a system of finite spatial volume $(Na)^{D-1}$ at finite temperature T. The limit $\beta \to \infty$, that is $N_T \to \infty$ with fixed a corresponds to the system at zero temperature. The continuum limit corresponds to taking $a \to 0$ while keeping Na and $N_T a$ fixed. To keep finite size effects under control, one should in principle ensure that N/N_T is large enough.

In vacuum, the net number of particles is zero; conversely, in matter it is often necessary to consider a non-vanishing number density and thus a chemical potential is introduced in the theory [32]. The grandcanonical partition function takes the form

$$Z(T, \mu) = \text{Tr} \left[e^{-\beta(\hat{H} - \mu\hat{N})} \right]$$

where $\hat{N}$ is the particle number operator and μ is the chemical potential. The particle number density can be readily computed by

$$n = \frac{1}{V}\langle \hat{N} \rangle = \frac{T}{V}\frac{\partial}{\partial\mu} \ln Z(T, \mu)$$

where V is the spacetime volume. Let us now consider the continuum Euclidean action for free Dirac fermions in 4 dimensions[1]

$$S_E[\psi, \bar{\psi}] = \int_0^\beta \mathrm{d}t \int_{\mathbb{R}^3} \mathrm{d}^3x \left[\frac{1}{2}\bar{\psi}(x)\gamma^\mu \overleftrightarrow{\partial}_\mu \psi(x) + m\bar{\psi}(x)\psi(x) \right] \tag{2.2}$$

Invariance under *global* U(1) transformations

$$\psi \to e^{i\alpha}\psi$$

$$\bar{\psi} \to e^{-i\alpha}\bar{\psi}$$

(with α a real, constant parameter) yields, by Noether's theorem, charge conservation: the particle number operator is given by the space integral of the temporal component of the conserved vector current, that is

$$\partial^\mu J_\mu = 0 \quad \Leftrightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^3} \mathrm{d}^3x\, J_0(t, \vec{x}) = 0$$

Here $J_\mu = \bar{\psi}\gamma_\mu\psi$ and so, in the Euclidean formulation, the conserved charge (particle number) is

$$\int_{\mathbb{R}^3} \bar{\psi}(t, \vec{x})\gamma_4\psi(t, \vec{x})$$

This is precisely the quantity that should be coupled to the chemical potential in the action, which then becomes

$$S_E[\psi, \bar{\psi}] = \int_0^\beta \mathrm{d}t \int_{\mathbb{R}^3} \mathrm{d}^3x \left[\frac{1}{2}\bar{\psi}(x)\gamma^\mu \overleftrightarrow{\partial}_\mu \psi(x) + m\bar{\psi}(x)\psi(x) + \mu\bar{\psi}(x)\gamma_4\psi(x) \right] \tag{2.3}$$

We now want to compute the energy density

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[1]A more usual form for the fermion kinetic term is $\bar{\psi}(x)\gamma^\mu\partial_\mu\psi(x) = \bar{\psi}(x)\displaystyle{\not}\partial\psi(x)$, which can be recovered from (2.2) after an integration by parts. The reader will also notice that, for the sake of simplicity, we have considered only a single fermion flavour.

$$\varepsilon(\mu) = \frac{1}{V_3} \langle \hat{H} \rangle = -\frac{1}{V_3} \frac{\partial}{\partial \beta} \ln Z(T, \mu)$$

where V_3 is the spatial volume. To this purpose, we start by rewriting the partition function ($\bar{\psi} = \psi^\dagger \gamma_4$)

$$Z(T, \mu) = \int \mathcal{D}\psi \mathcal{D}\psi^\dagger \, e^{-\int dt \, d^3x \, \psi^\dagger(x)[\gamma_4(\slashed{\partial} + m + \mu\gamma_4)]\psi(x)} = \det\left[\gamma_4(\slashed{\partial} + m + \mu\gamma_4)\right]$$

with $\psi(\beta, \vec{x}) = -\psi(0, \vec{x})$ and $\psi^\dagger(\beta, \vec{x}) = -\psi^\dagger(0, \vec{x})$. We will follow the treatment given in [30]. Using $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$, and $\alpha_i \equiv \gamma_4\gamma_i$, we have

$$\det\left[\gamma_4(\slashed{\partial} + m + \mu\gamma_4)\right] = \det\left[\partial_4 + \mu + \vec{\alpha} \cdot \vec{\nabla} + \gamma_4 m\right] \tag{2.4}$$

The sought-after determinant is better computed in momentum space; we therefore introduce the Fourier representation

$$\psi(t, \vec{x}) = \frac{1}{\sqrt{V_3}} \sum_{n \in \mathbb{Z}} \sum_{\vec{p}} e^{i(\omega_n t + \vec{p} \cdot \vec{x})} \tilde{\psi}_n(\vec{p})$$

where $\omega_n = \frac{(2n+1)\pi}{\beta} = (2n+1)\pi T$ are the fermionic Matsubara frequencies. For simplicity of notation, we have omitted spinor indices and employed a discrete sum for the momenta. This choice of normalization for ψ ensures that $\tilde{\psi}_n(\vec{p})$ is dimensionless. Before computing the determinant (2.4) we write

$$S[\psi, \psi^\dagger] = \int_0^\beta dt \int_{\mathbb{R}^3} d^3x \, \psi^\dagger(x) \left[\partial_4 + \mu + \vec{\alpha} \cdot \vec{\nabla} + \gamma_4 m\right] \psi(x)$$

$$= \frac{1}{V_3} \sum_{n,m} \sum_{\vec{p}, \vec{q}} \int_0^\beta dt \, e^{i(\omega_m - \omega_n)t} \int_{\mathbb{R}^3} d^3x \, e^{i(\vec{q} - \vec{p}) \cdot \vec{x}} \, \tilde{\psi}_n^\dagger(\vec{p}) \left[i\,\omega_m + \mu + i\,\vec{\alpha} \cdot \vec{q} + \gamma_4 m\right] \tilde{\psi}_m(\vec{q})$$

$$= \sum_{n \in \mathbb{Z}} \sum_{\vec{p}} \tilde{\psi}_n^\dagger(\vec{p}) \left[\beta(i\,\omega_n + \mu + i\,\vec{\alpha} \cdot \vec{p} + \gamma_4 m)\right] \tilde{\psi}_n(\vec{p})$$

where the temporal extent β comes from

$$\frac{1}{\beta} \int_0^\beta dt \, e^{i(\omega_m - \omega_n)t} = \delta_{m,n}$$

The operator whose determinant we want to compute is diagonal in momentum space, therefore all that is left is a determinant in Dirac space. Using the so called *chiral representation* for the gamma matrices, that is

$$\gamma_i = \begin{pmatrix} 0 & -i\,\sigma_i \\ i\,\sigma_i & 0 \end{pmatrix} \quad i = 1, 2, 3$$

$$\gamma_4 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$$

(where σ_i are the Pauli matrices), we have

$$Z(T,\mu) = \det\left[\beta(i\,\omega_n + \mu + i\,\vec{\alpha}\cdot\vec{p} + \gamma_4 m)\right] = \prod_{n\in\mathbb{Z}}\prod_{\vec{p}}\det\left[\beta\begin{pmatrix} i\,\omega_n + \mu - \vec{\sigma}\cdot\vec{p} & m \\ m & i\,\omega_n + \mu + \vec{\sigma}\cdot\vec{p} \end{pmatrix}\right]$$

$$= \prod_{n\in\mathbb{Z}}\prod_{\vec{p}}\beta^4\det\left[(i\,\omega_n + \mu - \vec{\sigma}\cdot\vec{p})(i\,\omega_n + \mu + \vec{\sigma}\cdot\vec{p}) - m^2\mathbb{1}_{2\times2}\right]$$

$$= \prod_{n\in\mathbb{Z}}\prod_{\vec{p}}\beta^4\det\left[(i\,\omega_n + \mu)^2 - (\vec{\sigma}\cdot\vec{p})^2 - m^2\mathbb{1}_{2\times2}\right] = \prod_{n\in\mathbb{Z}}\prod_{\vec{p}}\beta^4\det\left[(-(\omega_n - i\,\mu)^2 - \vec{p}^2 - m^2)\mathbb{1}_{2\times2}\right]$$

$$= \prod_{n\in\mathbb{Z}}\prod_{\vec{p}}\left[\beta^2\left((\omega_n - i\,\mu)^2 + E(\vec{p})^2)\right)\right]^2$$

where we have used $(\vec{\sigma}\cdot\vec{p})^2 = \vec{p}^2$ and $E(\vec{p}) = \sqrt{\vec{p}^2 + m^2}$. Since we are interested in the logarithm of the partition function, we have

$$\ln Z(T,\mu) = 2\sum_{n\in\mathbb{Z}}\sum_{\vec{p}}\ln\left[\beta^2\left((\omega_n - i\,\mu)^2 + E(\vec{p})^2)\right)\right]$$

Now we compute the energy density

$$\varepsilon(\mu,T) = -\frac{1}{V_3}\frac{\partial}{\partial\beta}\ln Z(T,\mu)\Big|_{\beta\mu\text{ fixed}}$$

$$= -\frac{2}{V_3}\sum_{n\in\mathbb{Z}}\sum_{\vec{p}}\frac{2\beta\left((\omega_n - i\,\mu)^2 + E(\vec{p})^2\right) + 2\beta^2(\omega_n - i\,\mu)\frac{\partial}{\partial\beta}(\omega_n - i\,\mu)}{\beta^2\left((\omega_n - i\,\mu)^2 + E(\vec{p})^2\right)}\Bigg|_{\beta\mu\text{ fixed}}$$

$$= -4\frac{1}{\beta}\sum_{n\in\mathbb{Z}}\frac{1}{V_3}\sum_{\vec{p}}\frac{(\omega_n - i\,\mu)^2 + E(\vec{p})^2 - (\omega_n - i\,\mu)^2}{(\omega_n - i\,\mu)^2 + E(\vec{p})^2}$$

$$= -4\frac{1}{\beta}\sum_{n\in\mathbb{Z}}\frac{1}{V_3}\sum_{\vec{p}}\frac{\vec{p}^2 + m^2}{(\omega_n - i\,\mu)^2 + \vec{p}^2 + m^2}$$

where we have used

$$\frac{\partial\omega_n}{\partial\beta} = \frac{\partial}{\partial\beta}\frac{(2n+1)\pi}{\beta} = -\frac{1}{\beta^2}(2n+1)\pi = -\frac{\omega_n}{\beta}$$

$$\frac{\partial\mu}{\partial\beta} = \frac{1}{\beta}\left(\frac{\partial}{\partial\beta}(\beta\mu) - \mu\right) = -\frac{\mu}{\beta}$$

So far we have considered a system of fermions inside a box of spatial volume V_3. Going to the thermodynamic limit means making the substitution

$$\frac{1}{V_3} \sum_{\vec{p}} \rightarrow \int_{\mathbb{R}^3} \frac{\mathrm{d}^3 p}{(2\pi)^3}$$

and we are interested in the energy density at zero temperature, that is $\varepsilon(\mu) \equiv \varepsilon(\mu, T = 0)$, which means taking the limit $\beta \rightarrow \infty$ with the substitution

$$\frac{1}{\beta} \sum_{n \in \mathbb{Z}} f(\omega_n) \rightarrow \int_{-\infty}^{+\infty} \frac{\mathrm{d}p_4}{2\pi} f(p_4)$$

so that we have

$$\varepsilon(\mu) = -\frac{4}{(2\pi)^4} \int_{\mathbb{R}^4} \mathrm{d}^4 p \, \frac{\vec{p}^2 + m^2}{(p_4 - i\,\mu)^2 + \vec{p}^2 + m^2}$$

which is manifestly divergent, as it includes the (vacuum) energy density at $\mu = 0$, which should be subtracted. Let us perform the integral in the p_4 complex plane: there are two poles at $p_4^\pm = i(\mu \pm \sqrt{\vec{p}^2 + m^2})$ (see Figure 2.1).
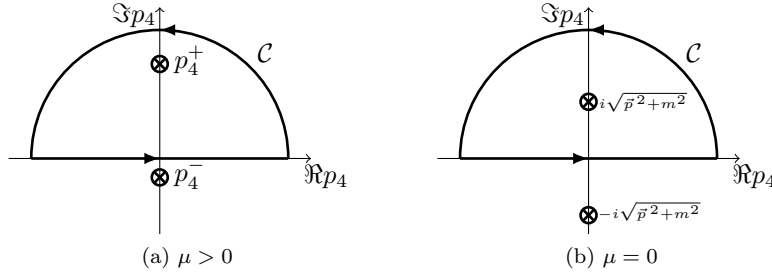
Figure 2.1: $f(p_4, \mu)$ pole structure in the complex p_4 plane for different values of μ.

Let us set

$$f(p_4, \mu) \equiv \frac{1}{(p_4 - p_4^+)(p_4 - p_4^-)}$$

In this notation what we are looking for is

$$\varepsilon(\mu) = -\frac{4}{(2\pi)^4} \int_{\mathbb{R}^3} \mathrm{d}^3 p \, (\vec{p}^2 + m^2) \left(\oint_{\mathcal{C}} \mathrm{d}p_4 \, f(p_4, \mu) - \oint_{\mathcal{C}} \mathrm{d}p_4 \, f(p_4, 0) \right)$$

where $\mathcal{C}$ is the contour depicted in Figure 2.1 (being $f(p_4, \mu) \sim 1/p_4^2$ for $|p_4| \rightarrow \infty$, the contribution from the semicircle vanishes). In Figure 2.1b we see that the only pole inside $\mathcal{C}$ for $\mu = 0$ is $i\sqrt{\vec{p}^2 + m^2}$. From Figure 2.1a, instead, we see that, for $\mu > 0$, only p_4^+ is inside $\mathcal{C}$ unless $\mu > \sqrt{\vec{p}^2 + m^2}$, in which case p_4^- is inside $\mathcal{C}$ as well. Collecting all these considerations, we have

$$\oint_{\mathcal{C}} \mathrm{d}p_4\, f(p_4, \mu) - \oint_{\mathcal{C}} \mathrm{d}p_4\, f(p_4, 0)$$

$$= 2\pi i \left[\mathrm{Res}\left(f, p_4^+\right) + \theta\left(\mu - \sqrt{\vec{p}^2 + m^2}\right) \mathrm{Res}\left(f, p_4^-\right) - \mathrm{Res}\left(f\big|_{\mu=0}, i\sqrt{\vec{p}^2 + m^2}\right) \right]$$

$$= 2\pi i \left[\frac{1}{p_4^+ - p_4^-} + \theta\left(\mu - \sqrt{\vec{p}^2 + m^2}\right) \frac{1}{p_4^- - p_4^+} - \frac{1}{i\sqrt{\vec{p}^2 + m^2} - \left(-i\sqrt{\vec{p}^2 + m^2}\right)} \right]$$

$$= 2\pi i \left[\frac{1}{2i\sqrt{\vec{p}^2 + m^2}} - \theta\left(\mu - \sqrt{\vec{p}^2 + m^2}\right) \frac{1}{2i\sqrt{\vec{p}^2 + m^2}} - \frac{1}{2i\sqrt{\vec{p}^2 + m^2}} \right]$$

$$= -\frac{\pi}{\sqrt{\vec{p}^2 + m^2}} \theta\left(\mu - \sqrt{\vec{p}^2 + m^2}\right)$$

so that

$$\varepsilon(\mu) = \frac{1}{4\pi^3} \int_{\mathbb{R}^3} \mathrm{d}^3 p\, \theta\left(\mu - \sqrt{\vec{p}^2 + m^2}\right) \sqrt{\vec{p}^2 + m^2}$$

For massless fermions, we can obtain the final result in closed form

$$\varepsilon(\mu)\big|_{m=0} = \frac{1}{\pi^2} \int_0^\infty \mathrm{d}l\, l^2 \theta(\mu - l) l = \frac{1}{\pi^2} \int_0^\mu \mathrm{d}l\, l^3 = \frac{1}{4\pi^2} \mu^4$$

and this is the correct (*finite*) result.

2.2   Finite density on the lattice

We have discussed the introduction of finite temperature as well as chemical potential in the continuum formulation of a free field theory of Dirac fermions. Let us now introduce a spacetime lattice Λ on which we discretize the action (2.3). We will follow [28] and see that the so called *naive* discretization for the chemical potential leads to divergences in the continuum limit. The action for free fermions becomes

$$S[\psi, \bar{\psi}] = a^3 a_T \sum_{n, m \in \Lambda} \bar{\psi}(n) D(n|m) \psi(m)$$

$$D(n|m) = \frac{1}{2a} \sum_{j=1}^3 \left(\delta_{n+\hat{j}, m} - \delta_{n-\hat{j}, m}\right) \gamma_j + \frac{1}{2a_T} \left(\delta_{n+\hat{4}, m} - \delta_{n-\hat{4}, m}\right) \gamma_4 + m\delta_{m,n} \mathbb{1} + \mu \delta_{m,n} \gamma_4 \qquad (2.5)$$

where spinor indices have been implied and for simplicity we have considered a single fermion of mass m. We have also introduced a different lattice spacing a_T for the temporal direction. After defining the (inverse) lattice Fourier transform[2]

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[2]With this choice of normalization, $\tilde{\psi}(p)$ holds the same dimensionality as $\psi(n)$.

$$\psi(n) = \frac{1}{\sqrt{|\Lambda|}} \sum_{p\in\tilde{\Lambda}} e^{i(\vec{p}\cdot\vec{n}a + p_4 n_4 a_T)} \tilde{\psi}(p)$$

with $|\Lambda| = N^3 N_T$ ($N = N_1 N_2 N_3$) the total number of lattice points, we rewrite the action in momentum space

$$S[\psi,\bar{\psi}] = a^3 a_T \sum_{n,m\in\Lambda} \bar{\psi}(n) D(n|m) \psi(m) = a^3 a_T \sum_{p,q\in\tilde{\Lambda}} \tilde{\bar{\psi}}(p) \tilde{D}(p|q) \tilde{\psi}(q)$$

with

$$\tilde{D}(p|q) = \frac{1}{|\Lambda|} \sum_{n,m\in\Lambda} e^{-i(\vec{p}\cdot\vec{n}a + p_4 n_4 a_T)} D(n|m) e^{i(\vec{q}\cdot\vec{m}a + q_4 m_4 a_T)}$$

$$= \frac{1}{|\Lambda|} \sum_{n,m\in\Lambda} e^{-i(\vec{p}\cdot\vec{n}a + p_4 n_4 a_T)} \left[\frac{1}{2a} \sum_{j=1}^{3} \left(\delta_{n+\hat{j},m} - \delta_{n-\hat{j},m} \right) \gamma_j \right.$$

$$\left. + \frac{1}{2a_T} \left(\delta_{n+\hat{4},m} - \delta_{n-\hat{4},m} \right) \gamma_4 + m\delta_{m,n}\mathbb{1} + \mu\delta_{m,n}\gamma_4 \right] e^{i(\vec{q}\cdot\vec{m}a + q_4 m_4 a_T)}$$

$$= \frac{1}{|\Lambda|} \sum_{n\in\Lambda} e^{-i(\vec{p}\cdot\vec{n}a + p_4 n_4 a_T)} \left[\frac{1}{2a} \sum_{j=1}^{3} \left(e^{i[\vec{q}\cdot(\vec{n}+\hat{j})a + q_4 n_4 a_T]} - e^{i[\vec{q}\cdot(\vec{n}-\hat{j})a + q_4 n_4 a_T]} \right) \gamma_j \right.$$

$$\left. + \frac{1}{2a_T} \left(e^{i[\vec{q}\cdot\vec{n}a + q_4(n_4+1)a_T]} - e^{i[\vec{q}\cdot\vec{n}a + q_4(n_4-1)a_T]} \right) \gamma_4 + (m\mathbb{1} + \mu\gamma_4) e^{i(\vec{q}\cdot\vec{n}a + q_4 n_4 a_T)} \right]$$

$$= \frac{1}{|\Lambda|} \sum_{n\in\Lambda} e^{i[(\vec{q}-\vec{p})\cdot\vec{n}a + (q_4-p_4)n_4 a_T]} \left[\frac{1}{2a} \sum_{j=1}^{3} \left(e^{i\vec{q}\cdot\hat{j}a} - e^{-i\vec{q}\cdot\hat{j}a} \right) \gamma_j \right.$$

$$\left. + \frac{1}{2a_T} \left(e^{iq_4 a_T} - e^{-iq_4 a_T} \right) \gamma_4 + m\mathbb{1} + \mu\gamma_4 \right] = \delta_{p,q} \tilde{D}(p)$$

where we have used the shortcut notation $(\vec{n} \pm \hat{j})_i = n_i \pm \delta_{ij}$ and

$$\tilde{D}(p) = \frac{1}{a_T} \left(\frac{a_T}{a} i \sum_{j=1}^{3} \sin(p_j a)\gamma_j + i\sin(p_4 a_T)\gamma_4 + a_T m\mathbb{1} + a_T \mu\gamma_4 \right) \tag{2.6}$$

The partition function is

$$Z(T,\mu) = \int \mathcal{D}\psi \mathcal{D}\bar{\psi}\, e^{-S[\psi,\bar{\psi}]} = \det\tilde{D} = \prod_{p\in\tilde{\Lambda}} \det{}_D \tilde{D}(p)$$

where the subscript D means that the determinant (or the trace) is to be taken in Dirac space. Now we want to compute the energy density (remember that $\beta = N_T a_T$)

$$\varepsilon(\mu, T) = -\frac{1}{V_3} \frac{\partial}{\partial\beta} \ln Z(T,\mu)\Big|_{\mu a_T \text{ fixed}} = -\frac{1}{(Na)^3 N_T} \frac{\partial}{\partial a_T} \sum_{p\in\tilde{\Lambda}} \text{Tr}_D \ln\tilde{D}(p)\Big|_{\mu a_T \text{ fixed}}$$

Using the useful relation[3]

$$\left(i\sum_{\mu=1}^{4} c_\mu \gamma_\mu + c_{\mathbb{1}}\mathbb{1}\right)^{-1} = \frac{-i\sum_{\mu=1}^{4} c_\mu \gamma_\mu + c_{\mathbb{1}}\mathbb{1}}{\sum_{\mu=1}^{4} c_\mu^2 + c_{\mathbb{1}}^2} \tag{2.7}$$

which holds for generic, real coefficients $c_{\mathbb{1}}$ and c_μ. In our derivative we have

$$\frac{\partial}{\partial a_T}\sum_{p\in\tilde\Lambda}\mathrm{Tr}_D \ln \tilde D(p)\Big|_{\mu a_T \text{ fixed}} = \sum_{p\in\tilde\Lambda}\mathrm{Tr}_D\left(\tilde D^{-1}(p)\frac{\partial}{\partial a_T}\tilde D(p)\Big|_{\mu a_T \text{ fixed}}\right)$$

$$= -\frac{1}{a_T}\sum_{p\in\tilde\Lambda}\mathrm{Tr}_D\mathbb{1} + \sum_{p\in\tilde\Lambda}\mathrm{Tr}_D\left[\left(a_T\tilde D(p)\right)^{-1}\frac{\partial}{\partial a_T}\left(\frac{a_T}{a}i\sum_{j=1}^{3}\sin(p_j a)\gamma_j + i\sin(p_4 a_T)\gamma_4 + a_T m\mathbb{1} + a_T\mu\gamma_4\right)\Big|_{\mu a_T \text{ fixed}}\right]$$

$$= -\frac{4|\Lambda|}{a_T} + \sum_{p\in\tilde\Lambda}\mathrm{Tr}_D\left[\left(i\sum_{j=1}^{3}\left(\frac{a_T}{a}\sin(p_j a)\right)\gamma_j + i\left(\sin(p_4 a_T) - ia_T\mu\right)\gamma_4 + a_T m\mathbb{1}\right)^{-1}\left(\frac{i}{a}\sum_{j=1}^{3}\sin(p_j a)\gamma_j + m\mathbb{1}\right)\right]$$

$$= -\frac{4N^3 N_T}{a_T} + \sum_{p\in\tilde\Lambda}\mathrm{Tr}_D\left[\left(\frac{-i\sum_{j=1}^{3}\left(\frac{a_T}{a}\sin(p_j a)\right)\gamma_j - i\left(\sin(p_4 a_T) - ia_T\mu\right)\gamma_4 + a_T m\mathbb{1}}{\sum_{j=1}^{3}\left(\frac{a_T}{a}\sin(p_j a)\right)^2 + \left(\sin(p_4 a_T) - ia_T\mu\right)^2 + (a_T m)^2}\right)\left(\frac{i}{a}\sum_{j=1}^{3}\sin(p_j a)\gamma_j + m\mathbb{1}\right)\right]$$

$$= -\frac{4N^3 N_T}{a_T} + 4\sum_{p\in\tilde\Lambda}\left(\frac{\frac{a_T}{a^2}\sum_{j=1}^{3}\sin^2(p_j a) + a_T m^2}{\sum_{j=1}^{3}\left(\frac{a_T}{a}\sin(p_j a)\right)^2 + \left(\sin(p_4 a_T) - ia_T\mu\right)^2 + (a_T m)^2}\right)$$

Now we set $a_T = a$ and get

$$\varepsilon(\mu, T) = \frac{4}{a^4} - \frac{4}{N^3 N_T a^4}\sum_{p\in\tilde\Lambda}\left(\frac{\sum_{j=1}^{3}\sin^2(p_j a) + (am)^2}{\left(\sin(p_4 a) - ia\mu\right)^2 + \sum_{j=1}^{3}\sin^2(p_j a) + (am)^2}\right)$$

As before, we are interested in the thermodynamic limit as well as the zero temperature case, that is we substitute

$$\frac{1}{N^3 N_T a^4}\sum_{p\in\tilde\Lambda} \to \int_{-\frac{\pi}{a}}^{+\frac{\pi}{a}}\frac{\mathrm{d}^4 p}{(2\pi)^4} = \frac{1}{a^4}\int_{-\pi}^{+\pi}\frac{\mathrm{d}^4(pa)}{(2\pi)^4}$$

from which it follows

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[3]Actually (2.7) still holds for $c_4 \in \mathbb{C}$.

$$\varepsilon(\mu) = -\frac{1}{4\pi^4 a^4} \int\limits_{-\pi}^{+\pi} \mathrm{d}^4 q \, \frac{\sum\limits_{j=1}^{3} \sin^2 q_j + (am)^2}{(\sin q_4 - ia\mu)^2 + \sum\limits_{j=1}^{3} \sin^2 q_j + (am)^2} - (\mu = 0)$$

where, as before, we have subtracted the $\mu = 0$ contribution. Besides the naive introduction of the chemical potential on the lattice, in (2.5) we have also used *naive* fermions, which are subject to *doubling* [29, 28]. It turns out that this is not a source of problems and merely contributes a factor of 16 to $\varepsilon(\mu)$ (which can be removed by using *e.g.* Wilson fermions). In order to perform the continuum limit, it is convenient to separate the contribution from the center of the Brillouin zone to that from its corners: for each momentum component we have

$$\int\limits_{-\pi}^{+\pi} \mathrm{d}p_\mu \, f(\sin p_\mu) = \int\limits_{-\pi}^{-\frac{\pi}{2}} \mathrm{d}p_\mu \, f(\sin p_\mu) + \int\limits_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} \mathrm{d}p_\mu \, f(\sin p_\mu) + \int\limits_{+\frac{\pi}{2}}^{+\pi} \mathrm{d}p_\mu \, f(\sin p_\mu)$$

$$= \int\limits_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} \mathrm{d}p_\mu \, f(\sin p_\mu) + \int\limits_{0}^{+\frac{\pi}{2}} \mathrm{d}p_\mu \, f(\sin(p_\mu + \pi)) + \int\limits_{-\frac{\pi}{2}}^{0} \mathrm{d}p_\mu \, f(\sin(p_\mu - \pi))$$

$$= \int\limits_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} \mathrm{d}p_\mu \, f(\sin p_\mu) + \int\limits_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} \mathrm{d}p_\mu \, f(-\sin p_\mu)$$

which is also true if we have $p_\mu \to p_\mu + \alpha$ for some α. In our case, for the spatial components we have a function of $\sin^2 p_j$, which is even in $\sin p_j$, whereas for the temporal component we have a function of $(\sin p_4 - ia\mu)^2$, which is even in $\sin p_4$ modulo a change of sign in μ. The conclusion is that we can make the substitution

$$\int\limits_{-\pi}^{+\pi} \mathrm{d}^4 q \to 16 \int\limits_{-\pi/2}^{+\pi/2} \mathrm{d}^3 q \left(\frac{1}{2} \int\limits_{-\pi/2}^{+\pi/2} \mathrm{d}q_4 + \frac{1}{2} \int\limits_{-\pi/2}^{+\pi/2} \mathrm{d}q_4 \, (\mu \to -\mu) \right)$$

After setting

$$\tilde{\tilde{p}} \equiv \sqrt{\sum\limits_{j=1}^{3} \sin^2(p_j a) + (am)^2}$$

we have

$$\varepsilon(\mu) = -\frac{4}{\pi^4} \int\limits_{-\frac{\pi}{2a}}^{+\frac{\pi}{2a}} \mathrm{d}^3 p \, \tilde{\tilde{p}}^2 \left(\frac{1}{2} \oint\limits_{\mathcal{C}} \mathrm{d}p_4 \, g(p_4, \mu) + \frac{1}{2} \oint\limits_{\mathcal{C}} \mathrm{d}p_4 \, g(p_4, -\mu) - \oint\limits_{\mathcal{C}} \mathrm{d}p_4 \, g(p_4, 0) \right)$$

with

$$g(p_4, \mu) \equiv \frac{1}{(\sin(p_4 a) - ia\mu)^2 + \tilde{\tilde{p}}^2}$$

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$\mathcal{C}$ is the same contour of Figure 2.1 extending from $-\frac{\pi}{2a}$ to $+\frac{\pi}{2a}$ on the real p_4 axis (we are already thinking of taking the continuum limit $a \to 0$ and the semicircle gives no contribution, since $g(p_4, \mu) \sim e^{-|p_4|}$ for $p_4 \to +i\infty$). Following the same reasoning of the continuum case, the conclusion is that

$$\oint_{\mathcal{C}} \mathrm{d}p_4\, g(p_4, \mu) + \oint_{\mathcal{C}} \mathrm{d}p_4\, g(p_4, -\mu) - \oint_{\mathcal{C}} \mathrm{d}p_4\, g(p_4, 0)$$

$$= 2\pi i \left[\frac{1}{2}\mathrm{Res}\left(g, p_4^+\right) + \frac{1}{2}\theta\left(\Im p_4^-\right)\mathrm{Res}\left(g, p_4^-\right) + \frac{1}{2}\theta\left(\Im p_4^+\big|_{-\mu}\right)\mathrm{Res}\left(g\big|_{-\mu}, p_4^+\big|_{-\mu}\right) - \mathrm{Res}\left(g\big|_{\mu=0}, p_4^+\big|_{\mu=0}\right) \right]$$

The poles are given by

$$\sin(p_4^{\pm} a) = i(a\mu \pm \tilde{p})$$

and the residues

$$\mathrm{Res}\left(g, p_4^{\pm}\right) = \pm \frac{1}{2i\tilde{p}a\sqrt{1 + \left(a\mu \pm \tilde{p}\right)^2}}$$

Now we see the main difference with respect to the continuum case: $\mathrm{Res}\left(g, p_4^+\right)$ is now μ-dependent and therefore cannot be cancelled by $\mathrm{Res}\left(g\big|_{\mu=0}, p_4^+\big|_{\mu=0}\right)$, so it gives rise to a μ-dependent divergence. We are left with the integral

$$\varepsilon(\mu) = -\frac{4}{\pi^3}\frac{1}{a}\int_{-\frac{\pi}{2a}}^{+\frac{\pi}{2a}} \mathrm{d}^3p\, \tilde{p} \left(\frac{1}{2}\frac{1}{\sqrt{1 + \left(a\mu + \tilde{p}\right)^2}} - \frac{1}{2}\frac{\theta\left(a\mu - \tilde{p}\right)}{\sqrt{1 + \left(a\mu - \tilde{p}\right)^2}} + \frac{1}{2}\frac{\theta\left(-a\mu + \tilde{p}\right)}{\sqrt{1 + \left(-a\mu + \tilde{p}\right)^2}} - \frac{1}{\sqrt{1 + \tilde{p}^2}} \right)$$

$$= -\frac{4}{\pi^3}\frac{1}{a}\int_{-\frac{\pi}{2a}}^{+\frac{\pi}{2a}} \mathrm{d}^3p\, \tilde{p} \left(\frac{1}{2}\frac{1}{\sqrt{1 + \left(\tilde{p} + a\mu\right)^2}} - \frac{1}{2}\frac{\theta\left(a\mu - \tilde{p}\right)}{\sqrt{1 + \left(\tilde{p} - a\mu\right)^2}} + \frac{1}{2}\frac{1 - \theta\left(a\mu - \tilde{p}\right)}{\sqrt{1 + \left(\tilde{p} - a\mu\right)^2}} - \frac{1}{\sqrt{1 + \tilde{p}^2}} \right)$$

$$= -\frac{4}{\pi^3}\frac{1}{a}\int_{-\frac{\pi}{2a}}^{+\frac{\pi}{2a}} \mathrm{d}^3p\, \tilde{p} \left(\frac{1}{2}\frac{1}{\sqrt{1 + \left(\tilde{p} + a\mu\right)^2}} + \frac{1}{2}\frac{1}{\sqrt{1 + \left(\tilde{p} - a\mu\right)^2}} - \frac{1}{\sqrt{1 + \tilde{p}^2}} - \frac{\theta\left(a\mu - \tilde{p}\right)}{\sqrt{1 + \left(\tilde{p} - a\mu\right)^2}} \right)$$

Being each integral performed in half of the Brillouin zone, we can easily set $\tilde{p} \underset{a\to 0}{\sim} a\sqrt{\vec{p}^2 + m^2}$, so that

$$\varepsilon(\mu)\big|_{m=0} = -\frac{16}{\pi^2}\int_0^\infty \mathrm{d}l\, l^3 \left(\frac{1}{2}\frac{1}{\sqrt{1 + a^2\left(l + \mu\right)^2}} + \frac{1}{2}\frac{1}{\sqrt{1 + a^2\left(l - \mu\right)^2}} - \frac{1}{\sqrt{1 + a^2 l^2}} - \frac{\theta\left(a\mu - al\right)}{\sqrt{1 + a^2\left(l - \mu\right)^2}} \right)$$

While the last integral is convergent thanks to the θ function, the first three terms give a divergence. Let us extract the leading term for $a \to 0$

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$$\varepsilon(\mu)\big|_{m=0} \sim -\int_0^\infty \mathrm{d}l\, l^3 \left[\frac{1}{2}\left(1 - \frac{1}{2}a^2\,(l+\mu)^2 + 1 - \frac{1}{2}a^2\,(l-\mu)^2\right) - \left(1 - \frac{1}{2}a^2 l^2\right) + \mathcal{O}\left(a^4\right)\right] + \mathcal{O}\left(1\right)$$

$$\sim -\int_0^\infty \mathrm{d}l\, l^3 \left(-\frac{1}{2}\mu^2 a^2 + \mathcal{O}\left(a^4\right)\right) + \mathcal{O}\left(1\right) \sim \left(\frac{1}{2}\mu^2 a^2 + \mathcal{O}\left(a^4\right)\right)\int_0^\infty \mathrm{d}l\, l^3 + \mathcal{O}\left(1\right)$$

$$\sim \left(\frac{1}{2}\mu^2 a^2 + \mathcal{O}\left(a^4\right)\right)\frac{1}{a^4} + \mathcal{O}\left(1\right) \sim \frac{\mu^2}{a^2} + \mathcal{O}\left(1\right)$$

where we have made use of the fact that l goes to infinity as $\sim 1/a$.

We have seen that the naive introduction of the chemical potential on the lattice gives rise to quadratic divergences in the continuum limit even for free fermions. One possible way out is to introduce non covariant terms in the action (2.5). Even though this is possible (for $\mu \neq 0$ the Euclidean symmetry is already broken), there is a better prescription which is more aware of what happens in the continuum formulation. The reason why the problem is not present in the continuum is that, in the Euclidean formulation, the chemical potential, being coupled to the temporal component of the conserved vector current, enters the action as the fourth component of an imaginary, constant gauge field, that is it plays the role of iA_4. Let us consider QED in the continuum. The chemical potential is introduced like a photon field: the consequence is that, in computing Feynman graphs, the n-th power of an expansion in μ is equivalent to the insertion of n external photon legs with zero momentum. It can be shown that renormalizability of $\Gamma^{(n+l,m)}$ (the graph with $n+l$ external photon legs and m external fermionic legs) implies the finiteness of the contribution $\sim \mu^l$ to $\Gamma^{(n,m)}$ (see Figure 2.2 for a graphical representation). The effect of μ is to substitute l factors of electric charge e (or, equivalently, the electromagnetic coupling constant α) with μ and to make l wave function renormalization factors disappear. As a consequence of gauge invariance, then, the missing factors "cancel" each other. See [32] and references therein for further details.
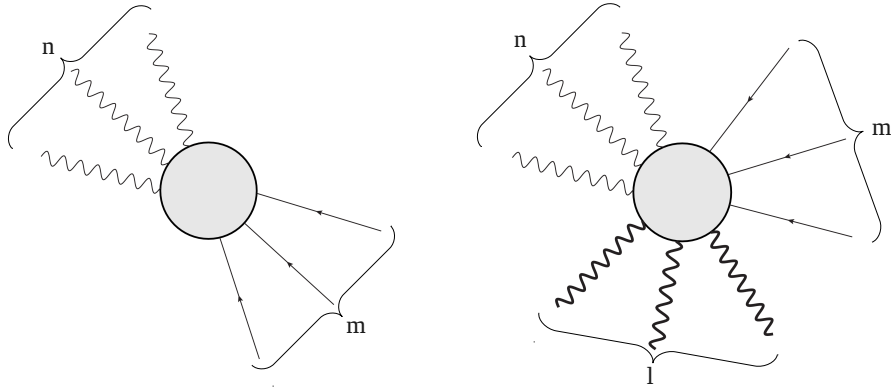
Figure 2.2: On the left, $\Gamma^{(n,m)}$, whose $\sim \mu^l$ contribution is equivalent to $\Gamma^{(n+l,m)}$ (on the right), where l zero momentum external photon legs have been inserted.

Going back to the lattice case, the problem lies in (2.5), where the chemical potential does not appear as the fourth component of a gauge field on the lattice, thus violating gauge invariance. Recall that in the lattice formulation of a gauge theory, the role of the gauge field is played by link variables $U_{\hat{\mu}}(n)$ that belong to the gauge group and are related to the continuum gauge field $A(x)$ (which belongs to the algebra of the gauge group) by

$$U_{\hat{\mu}}(n) = e^{iaA_\mu(na)}$$

This suggests that, in order for the chemical potential to act as the fourth component of a gauge field, it should be introduced in the fermionic action as an exponent, at the very same position of the *temporal* link variables in the action of the interacting theory (see [28, 29, 32] for details). The right prescription for the (naive) Dirac operator is thus

$$D(n|m) = \frac{1}{2a} \sum_{j=1}^{3} \left(\delta_{n+\hat{j},m} - \delta_{n-\hat{j},m} \right) \gamma_j + \frac{1}{2a_T} \left(e^{a_T \mu} \delta_{n+\hat{4},m} - e^{-a_T \mu} \delta_{n-\hat{4},m} \right) \gamma_4 + m \delta_{m,n} \mathbb{1}$$

and we immediately see that all the steps leading to (2.6) can be repeated in the very same way, but with the substitution $p_4 \to p_4 - i\mu$, which gives

$$\varepsilon(\mu) = -\frac{1}{4\pi^4 a^4} \int_{-\pi}^{+\pi} d^4q \, \frac{\sum_{j=1}^{3} \sin^2 q_j + (am)^2}{\sin^2(q_4 - ia\mu) + \sum_{j=1}^{3} \sin^2 q_j + (am)^2} - (\mu = 0)$$

As $\sin^2(q_4 - ia\mu \pm \pi) = \sin^2(q_4 - ia\mu)$, there is no need for a change of sign in μ like in the previous computations: the multiplicity due to the doublers (high momentum excitations on the corners of the Brillouin zone) simply yields a factor of 16 when integrating over half the Brillouin zone. The steps leading to the final result are pretty much the same, with a few differences. The function to integrate over $\mathcal{C}$ is

$$g(p_4, \mu) \equiv \frac{1}{\sin^2(p_4 a - ia\mu) + \tilde{\tilde{p}}^2}$$

whose poles are given by

$$\sin(p_4^{\pm} a - ia\mu) = \pm i \tilde{\tilde{p}}$$

from which it follows $\Im(p_4^{\pm} a - ia\mu) = \sinh^{-1}(\pm \tilde{\tilde{p}})$, or equivalently $\Im\left(p_4^{\pm} a \right) = a\mu \pm \sinh^{-1}(\tilde{\tilde{p}})$. The residues are

$$\operatorname{Res}\left(g, p_4^{\pm} \right) = \pm \frac{1}{2i\tilde{\tilde{p}} a \sqrt{1 + \tilde{\tilde{p}}^2}}$$

which are independent of μ and so ensure the cancellation of the diverging terms. Being

$$\oint_{\mathcal{C}} dp_4 \, g(p_4, \mu) - \oint_{\mathcal{C}} dp_4 \, g(p_4, 0) = 2\pi i \left[\operatorname{Res}\left(g, p_4^{+} \right) + \theta \left(\Im p_4^{-} \right) \operatorname{Res}\left(g, p_4^{-} \right) - \operatorname{Res}\left(g|_{\mu=0}, p_4^{+}|_{\mu=0} \right) \right]$$

$$= 2\pi i \left[\frac{1}{2i\tilde{\tilde{p}} a \sqrt{1 + \tilde{\tilde{p}}^2}} - \frac{\theta \left(a\mu - \sinh^{-1}(\tilde{\tilde{p}}) \right)}{2i\tilde{\tilde{p}} a \sqrt{1 + \tilde{\tilde{p}}^2}} - \frac{1}{2i\tilde{\tilde{p}} a \sqrt{1 + \tilde{\tilde{p}}^2}} \right] = -\frac{\pi \theta \left(a\mu - \log\left(\tilde{\tilde{p}} + \sqrt{1 + \tilde{\tilde{p}}^2} \right) \right)}{\tilde{\tilde{p}} a \sqrt{1 + \tilde{\tilde{p}}^2}}$$

$$= -\frac{\pi \theta \left(e^{a\mu} - \tilde{\tilde{p}} - \sqrt{1 + \tilde{\tilde{p}}^2} \right)}{\tilde{\tilde{p}} a \sqrt{1 + \tilde{\tilde{p}}^2}}$$

we have

$$\varepsilon(\mu) = -\frac{4}{\pi^4} \int\limits_{-\frac{\pi}{2a}}^{+\frac{\pi}{2a}} \mathrm{d}^3 p\, \tilde{\tilde{p}}^2 \left(\oint\limits_{\mathcal{C}} \mathrm{d}p_4\, g(p_4, \mu) - \oint\limits_{\mathcal{C}} \mathrm{d}p_4\, g(p_4, 0) \right) = \frac{4}{\pi^3} \frac{1}{a} \int\limits_{-\frac{\pi}{2a}}^{+\frac{\pi}{2a}} \mathrm{d}^3 p\, \theta \left(e^{a\mu} - \tilde{\tilde{p}} - \sqrt{1 + \tilde{\tilde{p}}^2} \right) \frac{\tilde{\tilde{p}}}{\sqrt{1 + \tilde{\tilde{p}}^2}}$$

In the continuum limit $e^{a\mu} \sim 1 + a\mu$, $\sqrt{1 + a^2 l^2} \sim 1 + \frac{1}{2}a^2 l^2$ and $\tilde{\tilde{p}} \sim a\,|\vec{p}|$ for massless fermions, so that our final result is

$$\varepsilon(\mu)\big|_{m=0} = \frac{16}{\pi^2} \int\limits_0^\infty \mathrm{d}l\, \frac{l^3}{\sqrt{1 + a^2 l^2}} \theta \left(1 + a\mu - al - \sqrt{1 + a^2 l^2} \right) \sim \frac{16}{\pi^2} \int\limits_0^\infty \mathrm{d}l\, \frac{l^3}{\sqrt{1 + a^2 l^2}} \theta \left(a\mu - al - \frac{1}{2}a^2 l^2 \right)$$

$$\sim \frac{16}{\pi^2} \int\limits_0^\infty \mathrm{d}l\, l^3 \left(1 - \frac{1}{2}a^2 l^2 \right) \theta \left(a\mu - al \right) \sim \frac{16}{\pi^2} \int\limits_0^\mu \mathrm{d}l\, l^3 = \frac{4}{\pi^2} \mu^4$$

which is precisely 16 times the continuum result (this factor of 16 may be removed by working *e.g.* with Wilson fermions [29]).

2.3   The sign problem

We have gone a long way to show all the calculations leading to the lattice implementation of the chemical potential. Now we will show in which sense such implementation gives rise to the sign problem. Let us consider the Dirac operator of an SU(N) lattice gauge theory

$$D(n|m) = \frac{1}{2a} \left[\sum_{j=1}^3 \left(U_{\hat{j}}(n)\delta_{n+\hat{j},m} - U_{-\hat{j}}(n)\delta_{n-\hat{j},m} \right) \gamma_j + \left(e^{a\mu} U_{\hat{4}}(n)\delta_{n+\hat{4},m} - e^{-a\mu} U_{-\hat{4}}(n)\delta_{n-\hat{4},m} \right) \gamma_4 \right] + m\delta_{m,n}\mathbb{1} \tag{2.8}$$

where $U_{\hat{\mu}}(n)$ are gauge link variables, belonging to the gauge group, with $U_{\hat{\mu}}^\dagger(n) = U_{\hat{\mu}}^{-1}(n) = U_{-\hat{\mu}}(n)$. By a suitable change of spacetime indices and using $\gamma_\mu^\dagger = \gamma_\mu$ as well as $\{\gamma_5, \gamma_\mu\} = 0$, it is easy to show that the following relation holds

$$\gamma_5\, D(\mu)\, \gamma_5 = D^\dagger(-\mu) \tag{2.9}$$

That is, with the introduction of the chemical potential, the Dirac operator is no more γ_5-Hermitian. While the *naive* Dirac operator in (2.8) is actually not very useful, as it yields *doublers* in the continuum limit, it is easy to show that (2.9) holds also for doubler-free fermion regularizations such as Wilson.

Being $(\det \gamma_5)^2 = 1$, one immediate consequence of (2.9) is that

$$\det D(\mu) = \overline{\det D(-\mu)}$$

so that the determinant of the Dirac operator is not real in presence of a chemical potential. Let us consider the action of an interacting lattice gauge theory such as QED or QCD

$$S[U, \psi, \bar{\psi}] = S_G[U] + S_F[U, \psi, \bar{\psi}]$$

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where S_G is the pure gauge action, dependent only on the link variables and the fermionic action is, analogously to (2.5), $S_F = \bar{\psi}D(U)\psi$. The partition function is

$$Z = \int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar{\psi}\,e^{-S[U,\psi,\bar{\psi}]} = \int \mathcal{D}U\,e^{-S_G[U]}\int \mathcal{D}\psi\mathcal{D}\bar{\psi}\,e^{-\bar{\psi}D(U)\psi} = \int \mathcal{D}U\,e^{-S_G[U]}\det D[U] = \int \mathcal{D}U\,e^{-S_{\text{eff}}[U]}$$

$$S_{\text{eff}}[U] = S_G[U] - \ln\det D[U]$$

The probability measure that Monte Carlo processes are expected to sample for non-perturbative evaluation of observables is

$$P[U] = \frac{1}{Z}e^{-S_{\text{eff}}[U]}$$

which gets complex in presence of a chemical potential. This is the so called *sign problem*[4], which plagues many lattice field theories, namely those referred to in Section 1. As already said, despite many attempts to tackle the sign problem with various approaches, a conclusive and general solution seems still far from being found. This is the reason why Lefschetz thimble regularization, which will be discussed in subsequent sections, was proposed.

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[4]The problem is actually a problem of *complex* terms in the action. The word "sign" comes from some models which lack a positive definite fermionic determinant in favour of one with an alternating sign, while still being real.

3   Morse theory and Lefschetz thimbles

In this section we give a lightweight mathematical introduction to Picard-Lefschetz theory, that is complex Morse theory. This presentation is by no means complete: for a more thorough treatment of the subject, the reader may refer to [33, 34, 35]. Algorithmic details as well as examples will be postponed to subsequent sections. The purpose of all the machinery that will be presented here is to rewrite the partition function of a generic lattice field theory with a complex action in such a way so that Monte Carlo sampling becomes feasible. We will follow the work of Witten [34] and the first two works [26, 36] which proposed this approach as a method for tackling the sign problem. Theoretical studies of different models with this method can be found in [37, 38, 39, 40, 41, 42].

3.1   One-dimensional integrals

As an invitation to the topic, let us first consider a simple one-dimensional integral (which can be regarded as a zero-dimensional field theory)

$$\mathcal{I}(\mu, \lambda) = \int\limits_{-\infty}^{+\infty} \mathrm{d}x \, e^{-\mu x^2 - \lambda x^4}$$

with $\mu \in \mathbb{C}$ and $\lambda \in \mathbb{R}^+$. In order to study the analytic properties of this integral, we go to the complex plane, that is $x \to z \in \mathbb{C}$. Any sensible integration contour on which evaluate $\mathcal{I}$ must end up as $|z| \to \infty$ in those regions of the complex z plane where $\Re(\mu z^2 + \lambda z^4) \to +\infty$, thus ensuring convergence. If we set $z = |z|e^{i\varphi}$, we see that the "good" regions are given by $\cos(4\varphi) > 0$. In Figure 3.1 we see the contours $\mathcal{C}_i$ connecting "good" regions at infinity: they are elements of the relative homology $H_1(\mathbb{C}, \mathbb{C}_T; \mathbb{Z})$, with $T \in \mathbb{R}$ large, so that their ends at infinity lie in $\mathbb{C}_T = \{z \in \mathbb{C} \mid \Re(\mu z^2 + \lambda z^4) > T\}$. However, the $\mathcal{C}_i$ are not all independent: being the integrand a holomorphic function, the sum of all the contours can be deformed to zero, so that we can write $\sum_i \mathcal{C}_i = 0$. As the original integration cycle $\mathcal{C} = \mathbb{R}$ connects two good regions, it is an element of the relative homology $H_1(\mathbb{C}, \mathbb{C}_T; \mathbb{Z})$ itself and therefore can be written as a linear combination of $\mathcal{C}_i$.
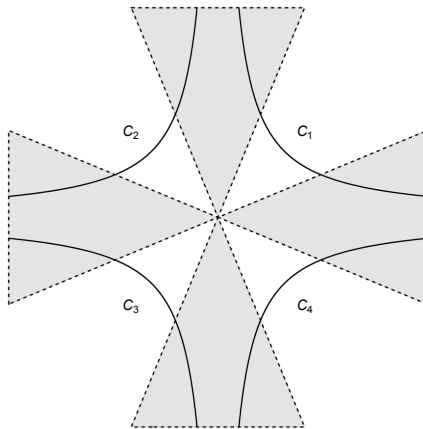
Figure 3.1: "Good" regions on which $\Re(\mu z^2 + \lambda z^4) \to +\infty$ for $|z| \to \infty$. Their union makes up $\mathbb{C}_T$. The four contours $\{\mathcal{C}_i\}$ connect the "good" regions.

An interesting point of view is that of Schwinger-Dyson equations for an integral analogous to $\mathcal{I}(\mu, \lambda)$ [43, 44, 45, 46]. Being the Schwinger-Dyson equation of third order, the number of linearly independent solutions is 3. Each independent solution in that context is an integral on a contour in the complex plane connecting two of the four disjoint regions making up $\mathbb{C}_T$. A one-dimensional integral similar to $\mathcal{I}(\mu, \lambda)$ will be subject of a thorough study in Section 6 within a more general framework, so that the previous, qualitative considerations should suffice.

Now let us come back to the problem of doing Monte Carlo sampling with the complex action $S(z) = \mu z^2 + \lambda z^4$. In elementary analysis, one technique that is often used is that of saddle point approximation, which consists of two steps. First, one deforms the integration contour to a curve in the complex plane which follows the direction of *steepest descent* of $\Re(S)$ around a stationary point. Holomorphicity ensures that, along this path, $\Im(S)$ is constant, hence the name *stationary phase*. The second step consists of a Taylor expansion of $\Re(S)$ around the stationary point, which provides an easy way of computing an approximation to $\mathcal{I}$. While we are interested in non-perturbative computations (and thus we do not want to Taylor expand), the first step is appealing: being $\Im(S)$ is constant, it can be factored out of the integrals and Monte Carlo sampling may then be performed with $e^{-\Re(S)}$ as a weight. In the next section we will discuss this approach in detail within the framework of Morse theory.

3.2 Decomposition in terms of thimbles

Let us consider a real n-dimensional manifold $\mathcal{Y}$ with a volume form $d\mathcal{V}$. Let $S : \mathcal{Y} \to \mathbb{C}$ be a complex function over $\mathcal{Y}$. We want to compute

$$\mathcal{I} = \int_{\mathcal{Y}} d\mathcal{V} \, e^{-S}$$

which may well be the partition function of an Euclidean lattice field theory whose dynamics is governed by the action S (the following considerations also hold if we are to compute the expectation value of an observable, provided that the original integral is convergent). Now let us assume that $\mathcal{Y}$ has a complexification $\mathcal{X}$ with an involution operator $\bar{\ }$ leaving $\mathcal{Y}$ fixed, so that $y = \bar{y} \; \forall y \in \mathcal{Y} \subset \mathcal{X}$. Let $z = (z^1, \cdots, z^n)$ be a set of local holomorphic coordinates on $\mathcal{X}$ (with $n = \dim_{\mathbb{C}} \mathcal{X}$). In the following we shall assume that $S(z)$ is holomorphic[5] and thus satisfies Cauchy-Riemann relations

$$\begin{cases} \frac{\partial S}{\partial \bar{z}^i} = 0 \\ \frac{\partial \bar{S}}{\partial z^i} = 0 \end{cases} \quad \Leftrightarrow \quad \begin{cases} \frac{\partial S_R}{\partial x^i} = \frac{\partial S_I}{\partial y^i} \\ \frac{\partial S_R}{\partial y^i} = -\frac{\partial S_I}{\partial x^i} \end{cases} \tag{3.1}$$

where we have set $z^i = x^i + i \, y^i$, $S_R = \Re(S)$, $S_I = \Im(S)$. Let us consider the function $S_R(x,y)$. First, we notice that the set of critical points of S_R coincides with the set of critical points of S thanks to (3.1), that is

$$\nabla_{(x^i, y^i)} S_R = 0 \quad \Leftrightarrow \quad \partial_{z^i} S = 0$$

We label $\Sigma = \{p_\sigma\} \subset \mathcal{X}$ the set of critical points of S, assuming that there are finitely many of them and they are all non degenerate[6], that is the matrix of the second derivatives (the Hessian) of S at p_σ has non-zero determinant. If this holds, S_R is said to be a *Morse function*. Let us call $H(S; p_\sigma)$ the Hessian of S at the critical point p_σ with coordinates $z_\sigma = (z_\sigma^1, \cdots, z_\sigma^n)$

$$[H(S; p_\sigma)]_{ij} \equiv \left. \frac{\partial^2 S}{\partial z^i \partial z^j} \right|_{z_\sigma}$$

$H(S; p_\sigma)$ is a *complex symmetric* $n \times n$ matrix. From (3.1), it follows that the $2n \times 2n$ Hessian matrix of S_R at p_σ has the structure (we set $(x, y) = (x^1, \cdots, x^n, y^1, \cdots, y^n)$ as variables on which S_R depends)

$$H(S_R; p_\sigma) = \begin{pmatrix} \Re\left(H(S; p_\sigma)\right) & -\Im\left(H(S; p_\sigma)\right) \\ -\Im\left(H(S; p_\sigma)\right) & -\Re\left(H(S; p_\sigma)\right) \end{pmatrix} \tag{3.2}$$

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[5]Actually, all subsequent statements hold also if S contains some logarithms, which is crucial for applications to theories with a term $\sim \log \det D$ coming from a fermionic Dirac operator D.

[6]This assumption will be released when we take symmetries into account.

$H(S_R; p_\sigma)$ has therefore n positive eigenvalues and n with opposite sign, so that the Morse index of p_σ is n for each critical point; S_R is said to be a *perfect* Morse function. As a consequence, S_R can be used to determine a basis of the relative homology group which the integration cycle we are interested in belongs to[7]. Define

$$\mathcal{X}_T \equiv \left\{ z \in \mathcal{X} \, \middle| \, S_R(z) \geq T \right\} \subset \mathcal{X} \qquad \mathbb{R}^+ \ni T \gg 1$$

that is $\mathcal{X}_T$ is the union of those regions in $\mathcal{X}$ in which S_R takes on arbitrarily large values. The relative homology group we are interested in is $H_n^+ \equiv H_n(\mathcal{X}, \mathcal{X}_T; \mathbb{Z})$ and we can find a basis of H_n^+ using the set Σ of critical points of S. Let us see how this is accomplished. After introducing a Kähler metric on $\mathcal{X}$

$$\mathrm{d}s^2 = \frac{1}{2} g_{i\bar{j}} \left(\mathrm{d}z^i \otimes \mathrm{d}\bar{z}^j + \mathrm{d}\bar{z}^j \otimes \mathrm{d}z^i \right)$$

we write the *steepest ascent* (SA) equations[8] for S

$$\frac{\mathrm{d}z^i}{\mathrm{d}t} = g^{i\bar{j}} \partial_{\bar{j}} \bar{S} \tag{3.3}$$

where $\partial_{\bar{j}} \equiv \frac{\partial}{\partial \bar{z}^j}$. The name "steepest ascent" comes from the fact that, along the flow $z(t)$ solution to (3.3), S_R is never decreasing

$$\frac{\mathrm{d}S_R}{\mathrm{d}t} = \left(\frac{\mathrm{d}z^j}{\mathrm{d}t} \partial_j + \frac{\mathrm{d}\bar{z}^j}{\mathrm{d}t} \partial_{\bar{j}} \right) \frac{1}{2} \left(S + \bar{S} \right) = \frac{1}{2} \left(\frac{\mathrm{d}z^j}{\mathrm{d}t} \partial_j S + \frac{\mathrm{d}\bar{z}^j}{\mathrm{d}t} \partial_{\bar{j}} \bar{S} \right)$$

$$= \frac{1}{2} \left(g^{j\bar{k}} \partial_{\bar{k}} \bar{S} \, \partial_j S + g^{\bar{j}k} \partial_k S \, \partial_{\bar{j}} \bar{S} \right) = g^{j\bar{k}} \partial_j S \, \partial_{\bar{k}} \bar{S} = g^{j\bar{k}} \left(\partial_j S \right) \overline{\left(\partial_k S \right)} \geq 0$$

where (3.1) has been used as well as (3.3) and the hermiticity of the metric. Given a critical point p_σ, the moduli space[9] of solutions to (3.3) with the boundary condition that the flow approaches p_σ for $t \to -\infty$, that is

$$\mathcal{J}_\sigma \equiv \left\{ z(0) \in \mathcal{X} \, \middle| \, \dot{z}^i = g^{i\bar{j}} \partial_{\bar{j}} \bar{S}, \, \lim_{t \to -\infty} z(t) = z_\sigma \right\} \subset \mathcal{X}$$

is a manifold of *real* dimension n. This can be seen from the fact that there are n independent directions along which one can leave p_σ with increasing S_R (the number of positive eigenvalues of $H(S_R; p_\sigma)$ is n). $\mathcal{J}_\sigma$ is called a *Lefschetz thimble* and can be seen as the union of all the SA curves starting from p_σ at $t \to -\infty$. It is important to notice that, apart from the *trivial flow* $z(t) = z_\sigma \, \forall\, t \in \mathbb{R}$, every flow belonging to $\mathcal{J}_\sigma$ has $S_R \to +\infty$ for $t \to +\infty$, hence $\mathcal{J}_\sigma$ is an element of the relative homology H_n^+. This statement can fail if there is a flow connecting two distinct critical points, that is $z(t) \to z_\tau$ for $t \to +\infty$ and $p_\tau \neq p_\sigma$. In such a case, we say that we are in presence of the *Stokes phenomenon* and $\mathcal{J}_\sigma$ is no more an element of H_n^+. In the following we shall assume that parameters on which S is dependent are sufficiently generic so that the Stokes phenomenon does not occur, postponing a more detailed discussion of it. We have seen that each $\mathcal{J}_\sigma$ is an element of the relative homology H_n^+; moreover, it can be shown that the thimbles generate the relative homology H_n^+ with *integer* coefficients. So any integration cycle $\mathcal{C} \in H_n^+$ can be decomposed as $\mathcal{C} = \sum_\sigma \mathfrak{n}_\sigma \mathcal{J}_\sigma$ with $\mathfrak{n}_\sigma \in \mathbb{Z}$. In our case, this translates into

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[7]We are assuming that the original integration cycle that we want to deform is a legitimate integration cycle connecting regions of convergence for the sought integral, in the spirit of the previous section.

[8]In references and in common literature on the subject, the reader will most likely be confronted with steepest *descent* equations (the sign in (3.3) is reversed) for $-S$; this is of course the same.

[9]Being (3.3) of first order in the flow time t, a solution is uniquely determined by giving the value of z at some t, say $t = 0$.

$$\mathcal{I} = \int_{\mathcal{Y}} \mathrm{d}\mathcal{V}\, e^{-S} = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \int_{\mathcal{J}_\sigma} \mathrm{d}\mathcal{V}\, e^{-S}$$

The fundamental feature of $\mathcal{J}_\sigma$, which is the very reason why this formalism was proposed to tackle the sign problem, is that S_I is *constant* on $\mathcal{J}_\sigma$. In fact, thanks to the SA equations (3.3)

$$\frac{\mathrm{d}S_I}{\mathrm{d}t} = \left(\frac{\mathrm{d}z^j}{\mathrm{d}t} \partial_j + \frac{\mathrm{d}\bar{z}^j}{\mathrm{d}t} \partial_{\bar{j}} \right) \frac{1}{2i} \left(S - \bar{S} \right) = \frac{1}{2i} \left(\frac{\mathrm{d}z^j}{\mathrm{d}t} \partial_j S - \frac{\mathrm{d}\bar{z}^j}{\mathrm{d}t} \partial_{\bar{j}} \bar{S} \right) = \frac{1}{2i}\, g^{j\bar{k}} \left(\partial_{\bar{k}} \bar{S}\, \partial_j S - \partial_j S\, \partial_{\bar{k}} \bar{S} \right) = 0$$

Thus S_I takes on the value at p_σ on the whole thimble, eliminating the sign problem[10] when one integrates on $\mathcal{J}_\sigma$, so that

$$\mathcal{I} = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma\, e^{-iS_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}\mathcal{V}\, e^{-S_R} = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma\, e^{-S(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}\mathcal{V}\, e^{-(S_R - S_R(z_\sigma))} \tag{3.4}$$

A more formal way of seeing the property of conservation of S_I is to regard the Kähler form $\Omega = \frac{i}{2} g_{i\bar{j}}\, \mathrm{d}z^i \wedge \mathrm{d}\bar{z}^j$ of $\mathcal{X}$ as a symplectic structure on $\mathcal{X}$; then the equations (3.3), along with (3.1) are the same as an Hamiltonian flow with S_I as Hamiltonian, which is then conserved [38]. Formula (3.4) suggests that one could perform Monte Carlo simulations using e^{-S_R} as a probability weight.

3.3 The coefficients $\mathfrak{n}_\sigma$

Now let us come to the issue of determining the coefficient $\mathfrak{n}_\sigma$. Consider the union of those regions in $\mathcal{X}$ in which S_R takes on arbitrarily small values

$$\mathcal{X}^{-T} \equiv \left\{ z \in \mathcal{X} \,\middle|\, S_R(z) \leq -T \right\} \subset \mathcal{X} \qquad \mathbb{R}^+ \ni T \gg 1$$

and the relative homology $H_n^- \equiv H_n(\mathcal{X}, \mathcal{X}^{-T}; \mathbb{Z})$. We now seek a basis of H_n^-. To each critical point p_σ we attach a *dual thimble*[11] $\mathcal{K}_\sigma$ defined by[12]

$$\mathcal{K}_\sigma \equiv \left\{ z(0) \in \mathcal{X} \,\middle|\, \dot{z}^i = -g^{i\bar{j}} \partial_{\bar{j}} \bar{S},\ \lim_{t \to -\infty} z(t) = z_\sigma \right\} \subset \mathcal{X}$$

that is the union of all the *steepest descent* (SD) curves starting at p_σ for $t \to -\infty$. Just as the $\mathcal{J}_\sigma$ form a basis of H_n^+, the $\mathcal{K}_\sigma$ form a basis of H_n^-. We introduce the bilinear form

$$\langle\, ,\, \rangle : H_n^+ \otimes H_n^- \to \mathbb{Z}$$

which gives the (oriented) *intersection number* between a cycle of H_n^+ and one of H_n^-. Since we are in the hypothesis of absence of the Stokes phenomenon, there are no flows connecting distinct critical points, so that $\langle \mathcal{J}_\sigma, \mathcal{K}_\tau \rangle = 0$ for $p_\sigma \neq p_\tau$. The only intersection between H_n^+ and H_n^- is the trivial flow $z(t) = z_\sigma\ \forall t$ so that, with a suitable choice of orientations, we have

$$\langle \mathcal{J}_\sigma, \mathcal{K}_\tau \rangle = \delta_{\sigma\tau}$$

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[10] There is actually a potential *residual sign problem* due to the complex volume element $\mathrm{d}\mathcal{V}$ appearing in the integrals over $\mathcal{J}_\sigma$. This issue will be discussed later.

[11] The dual thimble is often called *unstable* thimble, whereas $\mathcal{J}_\sigma$ is called *stable* thimble. This terminology comes from the fact that stable (unstable) thimbles connect regions of convergence (divergence) of the integral $\mathcal{I}$.

[12] A completely analogous definition of $\mathcal{K}_\sigma$ uses steepest ascent equations with $z(+\infty) = z_\sigma$ as boundary condition.

When applied to the decomposition of a cycle $\mathcal{C} \in H_n^+$, this gives

$$\langle \mathcal{C}, \mathcal{K}_\tau \rangle = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \langle \mathcal{J}_\sigma, \mathcal{K}_\tau \rangle = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, \delta_{\sigma\tau} = \mathfrak{n}_\tau$$

so $\mathfrak{n}_\sigma = \langle \mathcal{C}, \mathcal{K}_\sigma \rangle$ is the oriented intersection number between the original integration cycle $\mathcal{C}$ and the dual thimble $\mathcal{K}_\sigma$ attached to p_σ. In our case $\mathfrak{n}_\sigma = \langle \mathcal{Y}, \mathcal{K}_\sigma \rangle$.

3.4   The set of critical points

In the previous sections we have generically referred to Σ as the whole set of critical points of S. As for a realistic field theory a complete enumeration of its classical solutions (*i.e.* the critical points of the action) is likely to be unfeasible, it is of great importance to understand which critical points *actually* contribute to the expansion (3.4). Let us set

$$S_{\min} \equiv \min_{z \in \mathcal{C}} S_R(z)$$

that is the absolute minimum of S_R on the original manifold of integration $\mathcal{C}$. The set of critical points $\Sigma = \{p_\sigma\}$ can be decomposed as the disjoint union of three sets

$$\Sigma = \Sigma_0 \cup \Sigma_\leq \cup \Sigma_>$$

With the following definitions

$$\Sigma_0 \equiv \big\{ p_\sigma \in \Sigma \,\big|\, p_\sigma \in \mathcal{C} \big\}$$

$$\Sigma_\leq \equiv \big\{ p_\sigma \in \Sigma \,\big|\, p_\sigma \notin \mathcal{C}, S_R(z_\sigma) \leq S_{\min} \big\}$$

$$\Sigma_> \equiv \big\{ p_\sigma \in \Sigma \,\big|\, p_\sigma \notin \mathcal{C}, S_R(z_\sigma) > S_{\min} \big\}$$

All critical points belonging to $\Sigma_\leq$ give no contribution to (3.4); an explanation of this is as follows. Consider the unstable thimble $\mathcal{K}_\sigma$ associated to $p_\sigma \in \Sigma_\leq$: on $\mathcal{K}_\sigma$ S_R can only decrease, starting from a value $S_R(z_\sigma)$ that is already smaller than the smallest value of S_R on $\mathcal{C}$. The consequence is that any flow which is part of $\mathcal{K}_\sigma$ can never intersect $\mathcal{C}$, thus giving $\mathfrak{n}_\sigma = 0$. Now consider a critical point $p_\sigma \in \Sigma_>$, which can in principle (but does not necessarily have to) contribute to the decomposition in thimbles. The contribution of such a critical point is suppressed by a factor of $e^{-(S_R(z_\sigma)-S_{\min})}$ with respect to the thimble attached to the global minimum of S_R in $\mathcal{C}$. Any critical point $p_\sigma \in \Sigma_0$ automatically has $\mathfrak{n}_\sigma = 1$ (with a suitable choice of orientation) because $\mathcal{K}_\sigma$ intersects $\mathcal{C}$ just once, precisely at p_σ. The contribution of the latter class of critical points is exponentially suppressed for the same reasons given for $\Sigma_>$. It is expected that these suppressions become stronger in the *thermodynamic limit*. However, more complicated situations (such as an accumulation of critical points in a neighbourhood of the absolute minimum of S_R in $\mathcal{C}$) cannot be in principle excluded. In [26] an interacting scalar field theory at finite chemical potential is discussed. Let us call $\mathcal{J}_0$ the thimble attached to the global minimum of the action on the original domain of integration $\mathcal{C}$. It is shown that, considering only the integral over $\mathcal{J}_0$, one gets a field theory with the same degrees of freedom, symmetries, symmetry representations, perturbation theory and continuum limit as the original theory formulated on $\mathcal{C}$. Moreover, this is shown to hold at any value of μ. One is thus tempted to regard an integration over only $\mathcal{J}_0$ as a legitimate *regularization* of the original field theory. Of course, *universality* is not a theorem[13] and these statements are definitely not the last word on the matter; in particular, considerations from the subject of *resurgence* [47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58] may shed some light on the relation between perturbative and non-perturbative physics also in the framework of Morse theory and Lefschetz thimbles.

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[13]Moreover, this argument is supposed to hold in the thermodynamic limit.

3.5 The Stokes phenomenon

In order to ensure convergence of the integrals in (3.4), one requires that $S_R \to +\infty$ for $t \to +\infty$ along any given solution to (3.3) on $\mathcal{J}_\sigma$. However, if there is a flow such that $z(t) \to z_\tau$ for $t \to +\infty$, with $p_\tau \neq p_\sigma$, this requirement cannot be met and the decomposition in thimbles does not hold any more. This is the so-called *Stokes phenomenon*. Let us consider the space of parameters[14] on which the action S is dependent. To be more specific, let κ be a parameter on which S depends *continuously*. In general, there will be some curves (called *Stokes curves*) in the κ complex plane such that, when κ lies on one of them, the Stokes phenomenon occurs. Identifying the Stokes curves for a generic field theory can be highly non trivial and may require ad-hoc considerations. There is, however, a necessary (although not sufficient) condition for the Stokes phenomenon to occur. As S_I is conserved by any flow of SA or SD, for a flow to connect two distinct critical points p_σ and p_τ, one must have $S_I(z_\sigma) = S_I(z_\tau)$[15]. Therefore, if for a given value of κ and for each couple of critical points (p_σ, p_τ) one has $S_I(z_\sigma) \neq S_I(z_\tau)$, there cannot be any Stokes phenomenon. When κ goes through a Stokes curve, the coefficients $\mathfrak{n}_\sigma$ may jump. These discontinuities compensate the jump in shape of some thimbles (which in turn cause a sharp change in the integrals over the thimbles). This compensation occurs because the original integral $\mathcal{I}$ is continuous in κ, so the result of the decomposition (3.4) cannot undergo a discontinuity. In general, provided that Stokes curves are correctly identified, it is simple to compute the values of the $\mathfrak{n}_\sigma$ after a jump: one just imposes the continuity of the integral $\mathcal{I}$ before and after the jump. An example of this procedure will be given in Section 6.

3.6 Tangent space at a critical point

In the previous sections we have been rather generic; now let us consider a more concrete setting: we set $\mathcal{Y} = \mathbb{R}^n$ (and therefore $\mathcal{X} = \mathbb{C}^n$) along with the standard Euclidean metric. We also consider a scalar field theory with n real degrees of freedom $\{x^i\}$. The partition function is

$$\mathcal{Z} = \int_{\mathbb{R}^n} \mathrm{d}^n x \, e^{-S(x)}$$

We complexify the fields by taking $x^i \to z^i = x^i + i \, y^i$. Let us concentrate on a single critical point p_σ with coordinates z_σ. We introduce the vector notation

$$Z = \begin{pmatrix} z^1 \\ \vdots \\ z^n \end{pmatrix} \in \mathbb{C}^n \qquad V = \begin{pmatrix} x^1 \\ \vdots \\ x^n \\ y^1 \\ \vdots \\ y^n \end{pmatrix} \in \mathbb{R}^{2n}$$

and expand the action to second order around z_σ

$$S(z) \approx S(z_\sigma) + \frac{1}{2} Z^T H(S; p_\sigma) Z \tag{3.5}$$

where we have assumed $z_\sigma = 0$ for the sake of simplicity. Takagi's factorization theorem states that, given the *complex symmetric* matrix $H(S; p_\sigma)$, there exists a *unitary* $n \times n$ matrix W such that $W^T H(S; p_\sigma) W = \Lambda$, with $\Lambda = \mathrm{diag}(\lambda_1, \cdots, \lambda_n)$ and the λ_i (called *Takagi values*) are all real and non-negative. We assume that they are all positive (just as before we assumed $H(S; p_\sigma)$ to be invertible). The columns of W are n normalized *Takagi vectors* $v^{(i)}$, that is

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[14]The parameters are assumed to be complex in general.
[15]For a flow to connect p_σ and p_τ, one must also have $S_R(z_\sigma) \neq S_R(z_\tau)$, as any non-trivial flow cannot have constant S_R.

$$\sum_{k=1}^{n} v_k^{(i)} \bar{v}_k^{(j)} = \delta^{ij}$$

so that we can rephrase Takagi's theorem as

$$H(S;p_\sigma)v^{(i)} = \lambda_i \bar{v}^{(i)}$$

or, equivalently,

$$H(S;p_\sigma)W = \overline{W}\Lambda$$

Given the complex projector $\mathcal{P} = (\mathbb{1}_{n\times n} \; i\mathbb{1}_{n\times n}) \in \mathbb{C}^{n\times 2n}$, it is straightforward to show that, if $v_+ \in \mathbb{R}^{2n}$ is a normalized eigenvector of $H(S_R;p_\sigma)$ with (positive) eigenvalue λ, then $\mathcal{P}v_+ \in \mathbb{C}^n$ is a Takagi vector of $H(S;p_\sigma)$ with Takagi value λ. At the same time, if $v_- \in \mathbb{R}^{2n}$ is a normalized eigenvector of $H(S_R;p_\sigma)$ with eigenvalue $-\lambda$, then $\mathcal{P}v_- \in \mathbb{C}^n$ is a Takagi vector of $H(S;p_\sigma)$ with $-\lambda$ as Takagi value; this last statement holds for $i\mathcal{P}v_+$ as well. All this is discussed in Appendix A. The tangent space to $\mathcal{J}_\sigma$ at the critical point is spanned by the n complex vectors $v^{(i)}$, while the tangent space to $\mathcal{K}_\sigma$ at p_σ is spanned by the n complex vectors $iv^{(i)}$. Linear combinations of Takagi vectors are to be taken with *real* coefficients, to preserve the right dimensionality. These considerations are more transparent if one changes variables. We set $Z = W\zeta$ (or, equivalently, $\zeta = W^\dagger Z$). In general $\zeta_i = \eta_i + i\,\xi_i \in \mathbb{C}$; however, looking at the second order expansion of the action we have

$$S(z) \approx S(z_\sigma) + \frac{1}{2}\left(W\zeta\right)^T H(S;p_\sigma)\left(W\zeta\right) = S(z_\sigma) + \frac{1}{2}\zeta^T \left(W^T H(S;p_\sigma)W\right)\zeta = S(z_\sigma) + \frac{1}{2}\zeta^T \Lambda\zeta$$

$$= S(z_\sigma) + \frac{1}{2}\sum_{i=1}^{n}\lambda_i\zeta_i^2 = S(z_\sigma) + \frac{1}{2}\sum_{i=1}^{n}\lambda_i\left(\eta_i + i\,\xi_i\right)^2$$

so that

$$S_R(z) \approx S_R(z_\sigma) + \frac{1}{2}\sum_{i=1}^{n}\lambda_i\eta_i^2 - \frac{1}{2}\sum_{i=1}^{n}\lambda_i\xi_i^2$$

$$S_I(z) \approx S_I(z_\sigma) + \sum_{i=1}^{n}\lambda_i\eta_i\xi_i$$

This makes it manifest that, by taking $\xi_i = 0$, we stay on the stable thimble $\mathcal{J}_\sigma$ (where S_R increases), while by taking $\eta_i = 0$, we stay on the unstable thimble $\mathcal{K}_\sigma$ (where S_R decreases). This shows that linear combinations of Takagi vectors $v^{(i)}$ with real coefficients span $\mathcal{J}_\sigma$ at p_σ, whilst purely imaginary linear combinations of $v^{(i)}$ (that is real combinations of $iv^{(i)}$) span $\mathcal{K}_\sigma$ at p_σ. It is worth noting that the change of variables one needs to use to integrate on $\mathcal{J}_\sigma$ *close* to the critical point is $Z = W\eta$ (with real η), and the integration measure $\mathrm{d}^n z = \det W \mathrm{d}^n\eta$, with $\det W = e^{i\,\omega_\sigma}$, being W unitary.

3.7 Tangent space at a generic point

We have discussed the tangent space to $\mathcal{J}_\sigma$ at the critical point p_σ in detail. Unfortunately, we lack a local description for the tangent space at a generic point $z \in \mathcal{J}_\sigma$. Let us see how far we can go with respect to the characterization of $T_z\mathcal{J}_\sigma$. Consider the integral of a generic function over the thimble

$$\int_{\mathcal{J}_\sigma} \mathrm{d}^n z \, f(z) \tag{3.6}$$

where $\mathrm{d}^n z = \mathrm{d}z^1 \wedge \cdots \wedge \mathrm{d}z^n$ is the right form to integrate on the thimble[16], which is a manifold of *real* dimension n embedded in $\mathbb{C}^n$ (it can be thought as embedded in $\mathbb{R}^{2n}$ as well). Now, at a generic point $z \in \mathcal{J}_\sigma$, the form $\mathrm{d}^n z$ and the tangent space $T_z \mathcal{J}_\sigma$ are not parallel in general [59]. In order to express an integral over $\mathcal{J}_\sigma$ as an ordinary integral on $\mathbb{R}^n$, we have to change coordinates from the canonical basis of $\mathbb{C}^n$ (dual to the forms $\mathrm{d}z^i$) to a basis of $T_z \mathcal{J}_\sigma$. Let $\{U^{(i)}\}$ be a (local) basis of $T_z \mathcal{J}_\sigma$ which is orthonormal with respect to the standard Hermitian metric of $\mathbb{C}^n$; the matrix $U \in \mathbb{C}^{n \times n}$ whose columns are the $U^{(i)}$ is therefore unitary. Consider a neighbourhood $\Gamma_z \subset \mathcal{J}_\sigma$ of $z \in \mathcal{J}_\sigma$: on Γ_z, any point can be reached by a displacement $\delta z = \sum_i \delta y_i \, U^{(i)}$ with respect to z, where the δy_i are n *real* local coordinates in $T_z \mathcal{J}_\sigma$.[17] From the unitarity of U, it follows that $|\delta z|^2 = \delta y^2$. Now, let us introduce a local chart $\varphi : \Gamma_z \subset \mathcal{J}_\sigma \to \mathbb{R}^n$ defined by

$$\varphi \left(z + \sum_{i=1}^n \delta y_i \, U^{(i)} \right) = \delta y + \mathcal{O}\left(\delta y^2\right) \in \mathbb{R}^n \tag{3.7}$$

Using φ, we can rewrite the integral (3.6) in the following way[18]

$$\int_{\Gamma_z} \mathrm{d}^n z \, f(z) = \int_{\varphi(\Gamma_z)} \mathrm{d}^n \delta y \, f\left(\varphi^{-1}\left(\delta y\right)\right) \det U\left(\varphi^{-1}\left(\delta y\right)\right) \tag{3.8}$$

where $\det U = e^{i\,\omega}$ because U is unitary. $e^{i\,\omega}$ is what is often termed *residual phase*. The residual phase takes into account the (local) orientation of the thimble with respect to $\mathbb{C}^n$. Being complex, the residual phase has to be taken into account by reweighting observables when integrating over $\mathcal{J}_\sigma$. This can in principle give rise to a "residual sign problem". This residual sign problem is expected to be rather mild (with respect to the original one), nevertheless it is an issue which should be carefully checked for each theory one wants to study with the thimble approach. So far results have been quite encouraging in this respect [59, 60, 36, 61, 62]. We have traded the complex measure $\mathrm{d}^n z$ for $\mathrm{d}^n \delta y$, which is real, with the introduction of $\det U$ as a consequence. We now come to the problem of determining a local basis of $T_z \mathcal{J}_\sigma$, given the only tangent space to the thimble we know, the one at the critical point, *i.e.* $T_{p_\sigma} \mathcal{J}_\sigma$. First, consider the SA equations for an action S

$$\begin{aligned}
\frac{\mathrm{d}z_i}{\mathrm{d}t} &= \frac{\partial \bar{S}}{\partial \bar{z}^i} \\
\frac{\mathrm{d}\bar{z}_i}{\mathrm{d}t} &= \frac{\partial S}{\partial z^i}
\end{aligned} \tag{3.9}$$

Given the coordinates of $\mathbb{C}^n$, that is z^i and $\bar{z}^i$, any vector field V can be seen as a directional derivative operator acting on complex functions over $\mathbb{C}^n$. This yields the decomposition

$$V = V^i \partial_i + \bar{V}^i \partial_{\bar{i}}$$

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[16] We note that $\mathrm{d}^n z$ is different from the standard volume form of $\mathbb{C}^n$, which is $\mathrm{d}z^1 \wedge \mathrm{d}\bar{z}^1 \wedge \cdots \wedge \mathrm{d}z^n \wedge \mathrm{d}\bar{z}^n$. $\mathrm{d}^n z$ has precisely the right dimension to integrate on $\mathcal{J}_\sigma$ with $\dim_\mathbb{R} \mathcal{J}_\sigma = n$.

[17] As a consequence, we can change variables from δz to δy and we get the Jacobian $\det U$, that is (thinking of z as fixed) $\mathrm{d}^n z = \mathrm{d}^n \delta z = \det \left(\frac{\partial \delta z}{\partial \delta y}\right) \mathrm{d}^n \delta y = \det U \mathrm{d}^n \delta y$, because $\left(\frac{\partial \delta z}{\partial \delta y}\right)_{ij} = \frac{\partial \delta z_i}{\partial \delta y_j} = U_i^{(j)} = U_{ij}$.

[18] Here we are concentrating on Γ_z (all these statements hold in a neighbourhood of a given point z on the thimble). Any algorithm for numerical integration over $\mathcal{J}_\sigma$ should be able to integrate seamlessly over the whole thimble.

where V^i and $\bar{V}^i$ are functions of z and $\bar{z}$. As partial derivatives commute,[19] we have

$$0 = [W, V]_j = \left[W^i \partial_i + \bar{W}^i \partial_{\bar{i}} \, , \, V^i \partial_i + \bar{V}^i \partial_{\bar{i}} \right]_j = \left(W^i \partial_i + \bar{W}^i \partial_{\bar{i}} \right) V_j - \left(V^i \partial_i + \bar{V}^i \partial_{\bar{i}} \right) W_j$$

Now we set $W_i = \partial_{\bar{i}} \bar{S}$, that is the flow of steepest ascent and compute

$$0 = \left(\partial_{\bar{i}} \bar{S} \, \partial_i + \partial_i S \, \partial_{\bar{i}} \right) V_j - \left(V^i \partial_i + \bar{V}^i \partial_{\bar{i}} \right) \partial_{\bar{j}} \bar{S} = \left(\frac{\mathrm{d}z_i}{\mathrm{d}t} \partial_i + \frac{\mathrm{d}\bar{z}_i}{\mathrm{d}t} \partial_{\bar{i}} \right) V_j - V^i \partial_i \partial_{\bar{j}} \bar{S} - \bar{V}^i \partial_{\bar{i}} \partial_{\bar{j}} \bar{S} = \frac{\mathrm{d}V_j}{\mathrm{d}t} - \bar{V}^i \partial_{\bar{i}} \partial_{\bar{j}} \bar{S}$$

where we have used the holomorphicity of the action, the chain rule and equations (3.9). We end up with the *parallel transport* (PT) equation[20]

$$\frac{\mathrm{d}V_j}{\mathrm{d}t} = \sum_{i=1}^{n} \bar{V}_i \overline{\left(\frac{\partial^2 S}{\partial z^i \partial z^j} \right)} \tag{3.10}$$

which holds in particular for any tangent basis vector $U^{(i)}$. Thus, by solving (3.10) for each $U^{(i)}(t)$ along the flow given by (3.9), one gets the whole basis of $T_z \mathcal{J}_\sigma$, where $z = z(t)$ is a solution to SA equations with the appropriate boundary condition defining $\mathcal{J}_\sigma$. The right initial condition to solve the PT equations for the tangent vectors $U^{(i)}$ is that $U^{(i)}(t_0) \sim v^{(i)}$ at a time t_0 sufficiently small so that $z(t_0)$ is close to z_σ, at which the tangent basis consists of the set of Takagi vectors $v^{(i)}$. The matrix of second derivatives of S is the Hessian of the action computed along the flow at $z(t)$.[21] A numerical solution of (3.10) is by far the most computationally demanding task when integrating over $\mathcal{J}_\sigma$. It is instructive to look at another, "variational" derivation of (3.10). We can linearize (3.9) by considering an infinitesimal displacement δz. Making use of

$$\delta = \sum_{i=1}^{n} \left(\delta z_i \frac{\partial}{\partial z^i} + \overline{\delta z_i} \frac{\partial}{\partial \bar{z}^i} \right)$$

we work out a flow equation for δz

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\delta z_j \right) = \delta \left(\frac{\mathrm{d}z_j}{\mathrm{d}t} \right) = \sum_{i=1}^{n} \left(\delta z_i \frac{\partial}{\partial z^i} + \overline{\delta z_i} \frac{\partial}{\partial \bar{z}^i} \right) \frac{\partial \bar{S}}{\partial \bar{z}^j} = \sum_{i=1}^{n} \overline{\delta z_i} \overline{\left(\frac{\partial^2 S}{\partial z^i \partial z^j} \right)}$$

in which δz may well be a tangent space vector, *e.g.* $V^{(i)}$.

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[19]This will no longer be true when we consider Lie groups: in that case we will have to take into account the algebra of Lie derivatives.

[20]The name "parallel transport" comes from the fact that $[\overline{\partial S}, V] = \mathcal{L}_{\overline{\partial S}} V$, so equation (3.10) is a statement of parallel transporting the vector V along the flow given by $\overline{\partial S}$ by imposing that the Lie derivative of V along the flow $\overline{\partial S}$ be 0.

[21]It is important to understand that the eigenvectors of the Hessian at a generic configuration do *not* span the tangent space to the thimble at that configuration.

4 Gauge theories

In the previous section we have discussed the fundamentals of thimble decomposition for a scalar field theory. In this section we introduce the thimble formalism in the context of gauge theories. We will immediately see that new issues arise due to the Lie group structure. As a prototype for a gauge theory, the reader may think of one-link models with complex coupling, lattice Yang-Mills theory with complex gauge coupling or with a θ-term or full QCD with a sign problem due to finite chemical potential. In order to be sufficiently general with the formalism, in this section we will consider a theory ruled by an action $S(U)$ where $\{U_k\}$ is a collection of gauge variables (k is a generic multi-index, which may be in place of, *e.g.* link position and direction $(n, \hat{\mu})$), belonging to a certain *compact* Lie group, which we shall set to $\mathrm{SU}(N)$. An abridged version of these notions can be found in [63].

4.1 Complexification and Lie derivatives

Complexification of the fields boils down to complexifying the Lie algebra of $\mathfrak{su}(N)$, which then becomes $\mathfrak{sl}(N, \mathbb{C})$. Thus, for gauge variables U

$$\mathrm{SU}(N) \ni U = e^{ix_a T^a} \to e^{iz_a T^a} = e^{i(x_a + iy_a)T^a} \in \mathrm{SL}(N, \mathbb{C})$$

where sum is understood over colour indices $a = 1 \cdots N^2 - 1$. Notice that, after complexification, the gauge group is no more compact[22]. The Hermitian and traceless generators T^a of $\mathrm{SU}(N)$ (which are taken to be in the *fundamental* representation) satisfy the commutation relations

$$\left[T^a, T^b\right] = i f^{abc} T^c$$

and are normalized so that

$$\mathrm{Tr}\left(T^a T^b\right) = \frac{1}{2}\delta^{ab}$$

In going from $\mathrm{SU}(N)$ to $\mathrm{SL}(N, \mathbb{C})$, we have

$$\mathrm{SU}(N) \ni U^\dagger = e^{-ix_a T^a} \to e^{-iz_a T^a} = e^{-i(x_a + iy_a)T^a} = U^{-1} \in \mathrm{SL}(N, \mathbb{C})$$

which tells us that, whenever we wish to complexify a theory with an action that is function of U and $U^\dagger$ (as it usually happens), we have to replace $U^\dagger$ with U^{-1}. As *conjugate* field (which correspond to $\bar{z}$, conjugate to z of a scalar field theory) we take $\bar{U} \equiv \left(U^\dagger\right)^{-1}$. This conjugation operation corresponds to

$$\mathrm{SL}(N, \mathbb{C}) \ni U \mapsto \bar{U} \equiv \left[\left(e^{iz_a T^a}\right)^\dagger\right]^{-1} = \left(e^{-i\bar{z}_a T^a}\right)^{-1} = e^{i\bar{z}_a T^a}$$

which means $z \to \bar{z}$.[23] Notice that $\mathrm{SU}(N) \subset \mathrm{SL}(N, \mathbb{C})$ is left invariant by this conjugation, as it should. We now introduce the Lie derivatives ∇^a, $\bar{\nabla}^a$

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[22]Even though the gauge group is not compact, expectation values of observables are expected to remain finite, as convergence of these integrals is ensured by the thimble regularization.

[23]It is important to keep in mind that $\bar{U}$ refers to taking the complex conjugate in the algebra; one never takes the conjugate of T^a.

$$\nabla^a f(U) \equiv \frac{\partial}{\partial \alpha} f\left(e^{i\alpha T^a} U\right)\Bigg|_{\alpha=0}$$

$$\nabla^a f(\bar{U}) \equiv 0$$

$$\bar{\nabla}^a f(\bar{U}) \equiv \frac{\partial}{\partial \alpha} f\left(e^{i\alpha T^a} \bar{U}\right)\Bigg|_{\alpha=0}$$

$$\bar{\nabla}^a f(U) \equiv 0$$

acting on functions of U or $\bar{U}$ (we will be concerned with holomorphic actions, which depend only on U). We define the derivative operator ∇_k

$$\nabla_k f(\{U_l\}) \equiv T^a \nabla_k^a f(\{U_l\}) = T^a \frac{\partial}{\partial \alpha} f\left(e^{i\alpha T^a} U_k, \{U_{l \neq k}\}\right)\Bigg|_{\alpha=0}$$

and analogously for $\bar{\nabla}_k \equiv T^a \bar{\nabla}_k^a$. It is also convenient to introduce two "real" derivatives, $\nabla_\Re^a$ and $\nabla_\Im^a$, defined by

$$\nabla_\Re^a \equiv \nabla^a + \bar{\nabla}^a$$

$$\nabla_\Im^a \equiv i\left(\nabla^a - \bar{\nabla}^a\right)$$

or, equivalently

$$\nabla^a = \frac{1}{2}\left(\nabla_\Re^a - i\,\nabla_\Im^a\right)$$

$$\bar{\nabla}^a = \frac{1}{2}\left(\nabla_\Re^a + i\,\nabla_\Im^a\right)$$

It is straightforward to show that these derivatives satisfy the Cauchy-Riemann equations (analogous to (3.1)) for any function $S(U) = S_R(U) + i\,S_I(U)$

$$\begin{cases} \bar{\nabla}^a S(U) = 0 \\ \nabla^a \bar{S}(\bar{U}) = 0 \end{cases} \Leftrightarrow \begin{cases} \nabla_\Re^a S_R = \nabla_\Im^a S_I \\ \nabla_\Im^a S_R = -\nabla_\Re^a S_I \end{cases}$$

From these relations it follows

$$\nabla_k^a S = \nabla_{\Re,k}^a S_R - i\,\nabla_{\Im,k}^a S_R$$

$$\bar{\nabla}_k^a \bar{S} = \nabla_{\Re,k}^a S_R + i\,\nabla_{\Im,k}^a S_R$$

and

$$\nabla_{\Re,k}^a S^R = \frac{1}{2}\left(\nabla_k^a S + \bar{\nabla}_k^a \bar{S}\right)$$

$$\nabla_{\Im,k}^a S^R = -\frac{1}{2i}\left(\nabla_k^a S - \bar{\nabla}_k^a \bar{S}\right)$$

as well as

$$\nabla^a_{\Re,k} \nabla^{a'}_{\Re,k'} S^R = \frac{1}{2} \left(\nabla^a_k \nabla^{a'}_{k'} S + \bar{\nabla}^a_k \bar{\nabla}^{a'}_{k'} \bar{S} \right)$$

$$\nabla^a_{\Re,k} \nabla^{a'}_{\Im,k'} S^R = -\frac{1}{2i} \left(\nabla^a_k \nabla^{a'}_{k'} S - \bar{\nabla}^a_k \bar{\nabla}^{a'}_{k'} \bar{S} \right)$$

$$\nabla^a_{\Im,k} \nabla^{a'}_{\Re,k'} S^R = -\frac{1}{2i} \left(\nabla^a_k \nabla^{a'}_{k'} S - \bar{\nabla}^a_k \bar{\nabla}^{a'}_{k'} \bar{S} \right)$$

$$\nabla^a_{\Im,k} \nabla^{a'}_{\Im,k'} S^R = -\frac{1}{2} \left(\nabla^a_k \nabla^{a'}_{k'} S + \bar{\nabla}^a_k \bar{\nabla}^{a'}_{k'} \bar{S} \right)$$

The previous relations, along with $\bar{\nabla}^a_k \bar{S} = \overline{\nabla^a_k S}$ [24], ensure that the Hessian $H(S_R; U_\sigma)$ at a critical point U_σ (for which $\nabla^a_k S(U_\sigma) = 0$) has the same structure as (3.2). One should keep in mind that these derivatives do not commute in general, but they obey the $\mathfrak{su}(N)$ Lie algebra. In particular

$$\left[\nabla^a, \nabla^b \right] f(U) = \nabla^a \nabla^b f(U) - \nabla^b \nabla^a f(U) = \frac{\partial}{\partial \alpha} \frac{\partial}{\partial \beta} f \left(e^{i\alpha T^a} e^{i\beta T^b} U \right) \bigg|_{\alpha=\beta=0} - \frac{\partial}{\partial \beta} \frac{\partial}{\partial \alpha} f \left(e^{i\beta T^b} e^{i\alpha T^a} U \right) \bigg|_{\alpha=\beta=0}$$

$$= \frac{\partial^2}{\partial \alpha \partial \beta} \left[f \left(e^{i\alpha T^a + i\beta T^b - \frac{1}{2} \alpha\beta [T^a, T^b]} U \right) - f \left(e^{i\alpha T^a + i\beta T^b - \frac{1}{2} \alpha\beta [T^b, T^a]} U \right) \right] \bigg|_{\alpha=\beta=0}$$

$$= \frac{\partial^2}{\partial \alpha \partial \beta} \left[-\frac{1}{2} \alpha\beta f^{abc} \nabla^c f(U) + \frac{1}{2} \alpha\beta f^{bac} \nabla^c f(U) \right] \bigg|_{\alpha=\beta=0} = -f^{abc} \nabla^c f(U)$$

where the vanishing terms have been neglected and Taylor expansion as well as Baker-Campbell-Hausdorff formula has been used. The commutator for $\bar{\nabla}$ gives the very same result. Being U and $\bar{U}$ independent variables, we have $\left[\nabla^a, \bar{\nabla}^b \right] = 0$, so that the complete algebra of Lie derivatives is the following

$$\left[\nabla^a_k, \nabla^b_{k'} \right] = -\delta_{k,k'} f^{abc} \nabla^c_k$$

$$\left[\bar{\nabla}^a_k, \bar{\nabla}^b_{k'} \right] = -\delta_{k,k'} f^{abc} \bar{\nabla}^c_k \tag{4.1}$$

$$\left[\nabla^a_k, \bar{\nabla}^b_{k'} \right] = 0$$

An important consideration is due: although Lie derivatives do not commute in general, the Hessian matrix of S is still *symmetric* at any critical point U_σ, because $\nabla^a_k S(U_\sigma) = 0$, so the commutators (4.1) vanish at U_σ.

4.2 Steepest ascent and parallel transport equations

We seek a way of writing steepest ascent equations (3.9) with Lie derivatives. The natural way of doing this is [64, 65]

$$\frac{\mathrm{d}}{\mathrm{d}t} U_k(t) = \left(i T^a \bar{\nabla}^a_k \overline{S[U(t)]} \right) U_k(t) \tag{4.2}$$

where the infinitesimal "displacement" of U_k is $\mathrm{d}t \, \bar{\nabla}^a_k \bar{S} T^a \in \mathfrak{sl}(N, \mathbb{C})$ ($\mathrm{d}U U^{-1}$ lies in $\mathfrak{sl}(N, \mathbb{C})$ [29]). This flow equation automatically keeps $U(t)$ in $\mathrm{SL}(N, \mathbb{C})$, which can be readily seen by considering the expression

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[24]This holds for all the actions we will consider in this work, thanks to their gauge-invariant trace of products of U.

$$U_k(t + \mathrm{d}t) = e^{i\,\mathrm{d}t\,T^a\,\bar{\nabla}_k^a\bar{S}}U_k(t) \tag{4.3}$$

whose first order expansion in $\mathrm{d}t$ coincides with $(4.2)^{25}$. The chain rule along steepest ascent curves takes the form

$$\frac{\mathrm{d}}{\mathrm{d}t} = \bar{\nabla}_k^a\bar{S}\,\nabla_k^a + \nabla_k^a S\,\bar{\nabla}_k^a$$

where summation over both k and a is understood. Along the SA curve $U(t)$ solution to (4.2), $S_R = \Re(S)$ is always non-decreasing, while $S_I = \Im(S)$ is conserved

$$\frac{\mathrm{d}S_R}{\mathrm{d}t} = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(S + \bar{S}\right) = \frac{1}{2}\left(\bar{\nabla}_k^a\bar{S}\,\nabla_k^a S + \nabla_k^a S\,\bar{\nabla}_k^a\bar{S}\right) = \sum_{k,a}|\nabla_k^a S|^2 = \|\nabla S\|^2 \geq 0$$

$$\frac{\mathrm{d}S_I}{\mathrm{d}t} = \frac{1}{2i}\frac{\mathrm{d}}{\mathrm{d}t}\left(S - \bar{S}\right) = \frac{1}{2i}\left(\bar{\nabla}_k^a\bar{S}\,\nabla_k^a S - \nabla_k^a S\,\bar{\nabla}_k^a\bar{S}\right) = 0$$

which is why we call (4.2) a "steepest ascent" equation. We will now derive a generalization of parallel transport equations (3.10) for gauge theories. In the present case, vectors can be seen as directional derivatives which inherit the commutation relations of $\mathfrak{su}(N)$. The decomposition

$$V = V_{k,a}\nabla_k^a + \bar{V}_{k,a}\bar{\nabla}_k^a$$

allows us to write

$$[V, V'] = \left[V_{k,a}\nabla_k^a + \bar{V}_{k,a}\bar{\nabla}_k^a, V'_{k',b}\nabla_{k'}^b + \bar{V}'_{k',b}\bar{\nabla}_{k'}^b\right] = V_{k,a}V'_{k',b}\left[\nabla_k^a, \nabla_{k'}^b\right] + V_{k,a}\bar{V}'_{k',b}\left[\nabla_k^a, \bar{\nabla}_{k'}^b\right]$$

$$+ \bar{V}_{k,a}V'_{k',b}\left[\bar{\nabla}_k^a, \nabla_{k'}^b\right] + \bar{V}_{k,a}\bar{V}'_{k',b}\left[\bar{\nabla}_k^a, \bar{\nabla}_{k'}^b\right] = -f^{abc}V_{k,a}V'_{k',b}\nabla_k^c\,\delta_{k,k'} - f^{abc}\,\bar{V}_{k,a}\bar{V}'_{k',b}\bar{\nabla}_k^c\,\delta_{k,k'}$$

$$= \left(-f^{abc}V_{k,a}V'_{k,b}\right)\nabla_k^c + \overline{\left(-f^{abc}V_{k,a}V'_{k,b}\right)}\bar{\nabla}_k^c$$

which reads (in components)

$$[V, V']_{k,c} = -f^{abc}V_{k,a}V'_{k,b}$$

As before, we pick $V'_{k,c} = \bar{\nabla}_k^c\bar{S}$ in the commutator

$$-f^{abc}V_{k,a}\bar{\nabla}_k^b\bar{S} = \left[V, \bar{\nabla}\bar{S}\right]_{k,c} = \left(V_{k',a}\nabla_{k'}^a + \bar{V}_{k',a}\bar{\nabla}_{k'}^a\right)\bar{\nabla}_k^c\bar{S} - \left(\bar{\nabla}_{k'}^a\bar{S}\,\nabla_{k'}^a + \nabla_{k'}^a S\,\bar{\nabla}_{k'}^a\right)V_{k,c}$$

$$= V_{k',a}\nabla_{k'}^a\bar{\nabla}_k^c\bar{S} + \bar{V}_{k',a}\bar{\nabla}_{k'}^a\bar{\nabla}_k^c\bar{S} - \frac{\mathrm{d}V_{k,c}}{\mathrm{d}t}$$

which, using the holomorphicity of the action $(\nabla_{k'}^a\bar{S} = 0)$, becomes (explicit summation is restored for the sake of clarity)

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[25] Actually, an iteration of (4.3) gives a solution to (4.2) which is of first order in $\mathrm{d}t$. This is the *Euler* integration scheme.

$$\frac{\mathrm{d}}{\mathrm{d}t}V_{k,c}(t) = \sum_{k',a} \bar{V}_{k',a}(t)\,\bar{\nabla}^a_{k'}\bar{\nabla}^c_k\overline{S\,[U(t)]} + \sum_{a,b} f^{abc}\,V_{k,a}(t)\,\bar{\nabla}^b_k\overline{S\,[U(t)]} \tag{4.4}$$

The first term is the usual one with the Hessian of S computed at $U(t)$[26] and the second term comes from the non abelian nature of the (complexified) group. As for the case of a scalar theory, we can also derive (4.4) in a "variational" way. In order to do this, we proceed with the same spirit of Section 3.7, remembering that, within gauge theories, an infinitesimal displacement δz takes place in the algebra of the gauge group, that is

$$U_k \to U'_k = e^{i\,\delta z_{k,a}T^a}U_k$$

so that we can write

$$\delta = \sum_{k,a}\left(\delta z_{k,a}\nabla^a_k + \overline{\delta z_{k,a}}\,\bar{\nabla}^a_k\right)$$

We seek an evolution equation for $\delta z_{k,c}$ in the following way

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}\delta U_k\right)U_k^{-1} = \left(\delta\frac{\mathrm{d}}{\mathrm{d}t}U_k\right)U_k^{-1}$$

$$\Rightarrow \left\{\frac{\mathrm{d}}{\mathrm{d}t}\left[\sum_{k',c}\left(\delta z_{k',c}\nabla^c_{k'}+\overline{\delta z_{k',c}}\,\bar{\nabla}^c_{k'}\right)U_k\right]\right\}U_k^{-1} = \left[\sum_{k',a}\left(\delta z_{k',a}\nabla^a_{k'}+\overline{\delta z_{k',a}}\,\bar{\nabla}^a_{k'}\right)\left(i\sum_c T^c\bar{\nabla}^c_k\bar{S}U_k\right)\right]U_k^{-1}$$

$$\Rightarrow \left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_c \delta z_{k,c}\,i\,T^cU_k\right)\right]U_k^{-1} = i\sum_c T^c\left(\sum_a \delta z_{k,a}\bar{\nabla}^c_k\bar{S}\,i\,T^aU_k + \sum_{k',a}\overline{\delta z_{k',a}}\,\bar{\nabla}^a_{k'}\bar{\nabla}^c_k\bar{S}U_k\right)U_k^{-1}$$

$$\Rightarrow \sum_c T^c\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\delta z_{k,c}U_k\right)\right]U_k^{-1} = \sum_c T^c\left(\sum_a \delta z_{k,a}\bar{\nabla}^c_k\bar{S}\,i\,T^a + \sum_{k',a}\overline{\delta z_{k',a}}\,\bar{\nabla}^a_{k'}\bar{\nabla}^c_k\bar{S}\right)$$

$$\Rightarrow \sum_c T^c\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\delta z_{k,c}\right) + \delta z_{k,c}\left(\frac{\mathrm{d}U_k}{\mathrm{d}t}U_k^{-1}\right)\right] = i\sum_a \delta z_{k,a}\sum_b \bar{\nabla}^b_k\bar{S}\,T^bT^a + \sum_c T^c\sum_{k',a}\overline{\delta z_{k',a}}\,\bar{\nabla}^a_{k'}\bar{\nabla}^c_k\bar{S}$$

$$\Rightarrow \sum_c T^c\frac{\mathrm{d}}{\mathrm{d}t}\left(\delta z_{k,c}\right) + i\sum_a \delta z_{k,a}\sum_b T^aT^b\bar{\nabla}^b_k\bar{S} = i\sum_a \delta z_{k,a}\sum_b \bar{\nabla}^b_k\bar{S}\,T^bT^a + \sum_c T^c\sum_{k',a}\overline{\delta z_{k',a}}\,\bar{\nabla}^a_{k'}\bar{\nabla}^c_k\bar{S}$$

$$\Rightarrow \sum_c T^c\frac{\mathrm{d}}{\mathrm{d}t}\left(\delta z_{k,c}\right) = \sum_c T^c\sum_{k',a}\overline{\delta z_{k',a}}\,\bar{\nabla}^a_{k'}\bar{\nabla}^c_k\bar{S} + i\sum_a \delta z_{k,a}\sum_b \bar{\nabla}^b_k\bar{S}\,T^bT^a - i\sum_a \delta z_{k,a}\sum_b T^aT^b\bar{\nabla}^b_k\bar{S}$$

$$\Rightarrow \sum_c T^c\frac{\mathrm{d}}{\mathrm{d}t}\left(\delta z_{k,c}\right) = \sum_c T^c\sum_{k',a}\overline{\delta z_{k',a}}\,\bar{\nabla}^a_{k'}\bar{\nabla}^c_k\bar{S} - i\sum_a \delta z_{k,a}\sum_b \bar{\nabla}^b_k\bar{S}\,[T^a,T^b]$$

$$\Rightarrow \sum_c T^c\frac{\mathrm{d}}{\mathrm{d}t}\left(\delta z_{k,c}\right) = \sum_c T^c\sum_{k',a}\overline{\delta z_{k',a}}\,\bar{\nabla}^a_{k'}\bar{\nabla}^c_k\bar{S} + \sum_c T^c f^{abc}\sum_{a,b}\delta z_{k,a}\bar{\nabla}^b_k\bar{S}$$

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[26]The Hessian at a generic configuration is not symmetric because of (4.1).

so that we get

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\delta z_{k,c} \right) = \sum_{k',a} \overline{\delta z_{k',a}} \, \bar{\nabla}^a_{k'} \bar{\nabla}^c_k \bar{S} + \sum_{a,b} f^{abc} \, \delta z_{k,a} \bar{\nabla}^b_k \bar{S}$$

which is the very same as (4.4), with $\delta z_{k,c}$ being the components of some tangent space basis vector.

4.3 Morse theory and gauge symmetry

In the last section we have introduced the thimble formalism for gauge theories. We now address the problem of gauge symmetry within the framework of Morse theory. We try to be as general as possible, deferring a more detailed discussion to the study of Yang-Mills theory in Section 10. We consider a set of fields $\{U_k\}$ on a manifold $\mathcal{Y}$ over which we wish to integrate, with $\dim_{\mathbb{R}} \mathcal{Y} = n$ and a suitable complexification $\mathcal{X}$, with $\dim_{\mathbb{R}} \mathcal{X} = 2n$. Let $S : \mathcal{X} \to \mathbb{C}$ be a holomorphic function that is invariant under transformations of a gauge group $\mathcal{G}$, which is the complexification of a compact gauge group $\mathcal{H}$. We call $\mathfrak{g}$ the Lie algebra of $\mathcal{G}$ and $\mathfrak{h}$ the Lie algebra of $\mathcal{H}$, with $\dim_{\mathbb{R}} \mathfrak{h} = n_G$ and $\dim_{\mathbb{R}} \mathfrak{g} = 2n_G$. We assume that a critical point $U_\sigma \in \mathcal{X}$ of S changes non-trivially under transformations of $\mathcal{G}$, that is $U_\sigma \to U_\sigma^G \neq U_\sigma$. As a consequence, U_σ belongs to a *manifold of critical points* continuously connected by transformations $G \in \mathcal{G}$. We call such manifold $\mathcal{M}_\sigma$

$$\mathcal{M}_\sigma \equiv \left\{ U \in \mathcal{X} \, \middle| \, \exists \, G \in \mathcal{G} : U_\sigma^G = U \right\} \subset \mathcal{X}$$

which has $\dim_{\mathbb{R}} \mathcal{M}_\sigma = 2n_G$. On $\mathcal{M}_\sigma$ the action S takes on the same value $S(U_\sigma)$; thus, considering $S_R = \Re(S)$, the Hessian $H(S_R; U)$ for $U \in \mathcal{M}_\sigma$ is degenerate.[27] In particular, the Hessian of S_R is a $2n \times 2n$ real, symmetric matrix with $2n_G$ zero eigenvalues (corresponding to directions of gauge invariance of S_R), $n - n_G$ positive eigenvalues and $n - n_G$ eigenvalues which are opposite in sign. We say that $\mathcal{M}_\sigma$ is a *non degenerate critical submanifold* of $\mathcal{X}$ for $S_R : \mathcal{X} \to \mathbb{R}$ if $\mathrm{d}S_R = 0$ along $\mathcal{M}_\sigma$ and the Hessian $H(S_R; U)$ (for $U \in \mathcal{M}_\sigma$) is non degenerate on the normal bundle $\nu(\mathcal{M}_\sigma)$. The normal bundle of $\mathcal{M}_\sigma$ is subject to the decomposition

$$\nu(\mathcal{M}_\sigma) = \nu^+(\mathcal{M}_\sigma) \oplus \nu^-(\mathcal{M}_\sigma)$$

with

$$\nu^\pm(\mathcal{M}_\sigma) = \bigsqcup_{U \in \mathcal{M}_\sigma} N^\pm_U \mathcal{M}_\sigma$$

and $\dim_{\mathbb{R}} N^\pm \mathcal{M}_\sigma = n - n_G$. $N^+ \mathcal{M}_\sigma$ is the (normal) space at $U \in \mathcal{M}_\sigma$ spanned by eigenvectors of $H(S_R; U)$ with positive eigenvalues, while $N^- \mathcal{M}_\sigma$ is the normal space at U spanned by eigenvectors of $H(S_R; U)$ with negative eigenvalues. We now construct an n-cycle $\mathcal{J}_\sigma$ attached to U_σ. Morse theory [66, 34, 26] tells us[28] that such an n-cycle is constructed by considering all the SA curves (that is, those making up a *stable* thimble) attached to a *middle dimensional* manifold $\mathcal{N}_\sigma \subset \mathcal{M}_\sigma$ ($\dim_{\mathbb{R}} \mathcal{N}_\sigma = n_G$, hence the name). The most natural choice for $\mathcal{N}_\sigma$ is

$$\mathcal{N}_\sigma \equiv \left\{ U \in \mathcal{X} \, \middle| \, \exists \, H \in \mathcal{H} : U_\sigma^H = U \right\} \subset \mathcal{M}_\sigma$$

---

[27] We are generically referring to "gauge symmetry", but the reader should keep in mind that symmetries can also arise in scalar field theories; see [39] for a discussion of $O(N)$ symmetry and [36]. Moreover, we will see that factors other than symmetry may lead to a degenerate Hessian (for example, torons in pure Yang-Mills theory); this case will be worth of a detailed discussion in Section 10.

[28] Actually, things are much more involved, but, for the cases of our interest, our brief discussion suffices. See [34] for a detailed treating of symmetries and Morse theory.

$\mathcal{N}_\sigma$ is the *gauge orbit* of all those points which can be reached starting from U_σ by gauge transformations belonging to the *original* gauge group $\mathcal{H}$ (before complexification), which is a subgroup of $\mathcal{G}$. Thus the stable thimble $\mathcal{J}_\sigma$ attached to U_σ is defined by

$$\mathcal{J}_\sigma \equiv \left\{ U(0) \in \mathcal{X} \,\middle|\, \dot{U} = i\,\bar{\nabla}\bar{S}U, \lim_{t\to-\infty} U(t) \in \mathcal{N}_\sigma \right\}$$

that is the union of all the SA curves $U(t)$ starting from *anywhere* on $\mathcal{N}_\sigma$ at $t \to -\infty$. This is the so called *generalized Lefschetz thimble* and it is indeed an n-cycle, having the proper dimension $\dim_\mathbb{R} \mathcal{J}_\sigma = n - n_G + n_G = n$. All the previous statements hold analogously for $\mathcal{K}_\sigma$. More details on how one should build the thimble attached to U_σ will be given in the context of Yang-Mills theory in Section 10. We now show that the choice of $\mathcal{N}_\sigma$ as a middle dimensional cycle in $\mathcal{M}_\sigma$ is consistent with the invariance of the thimble $\mathcal{J}_\sigma$ only under transformations of the $\mathcal{H}$ subgroup of $\mathcal{G}$, even though S is invariant under transformations of the full complexified group $\mathcal{G}$. Consider an infinitesimal transformation $G \in \mathcal{G}$ such that $U \to U^G$. Recall that SA equations can be seen as an Hamilton system with Hamiltonian $S_I = \Im(S)$ after regarding the Kähler form $\Omega = \frac{i}{2} g_{i\bar{j}}\, \mathrm{d}z^i \wedge \mathrm{d}\bar{z}^j$ as a symplectic structure on $\mathcal{X}$. As a consequence, a symmetry of the thimble (*i.e.* a symmetry of the Hamilton system) must leave Ω invariant. We want to compute the change $\delta^G \Omega = \Omega^G - \Omega$ of Ω under $G \in \mathcal{G}$ infinitesimal. For the sake of simplicity, we start assuming that U consists of a collection $\{U_k\}$ of variables, each transforming in the following way: $U_k \to U_k^G = G_k U_k G_k'$ for $G_k, G_k' \in \mathcal{G}_k$. This is very close to the case of Yang-Mills theory and corresponds to taking $\mathcal{G} = \otimes_k \mathcal{G}_k$ (and $\mathcal{H} = \otimes_k \mathcal{H}_k$ as well), where $\mathfrak{g}_k$ is the Lie algebra of $\mathcal{G}_k$, the complexification of $\mathfrak{h}_k$ with $\{T^a\}$ as generators (in the fundamental representation). Consider the tangent space to $\mathcal{J}_\sigma$ at a point U; any point $U' \in \Gamma_U$ (where Γ_U is a neighbourhood of U) can be reached by an infinitesimal displacement in the Lie algebra, that is $U_k' = e^{i\mathrm{d}z_{k,a} T^a} U_k$, with $\mathrm{d}z_{k,a} \in \mathbb{C}$. We now seek which displacement $\mathrm{d}z_{k,a}^G$, when acted on U_k^G, reaches $U_k'^G$. We thus impose

$$U_k'^G = e^{i\mathrm{d}z_{k,a}^G T^a} U_k^G$$

$$\Rightarrow\ G_k U_k' G_k' = e^{i\mathrm{d}z_{k,a}^G T^a} G_k U_k G_k'$$

$$\Rightarrow\ G_k e^{i\mathrm{d}z_{k,a} T^a} U_k = e^{i\mathrm{d}z_{k,a}^G T^a} G_k U_k$$

that is

$$e^{i\mathrm{d}z_{k,a}^G T^a} = G_k e^{i\mathrm{d}z_{k,a} T^a} G_k^{-1} \tag{4.5}$$

We now make use of the following lemma (which is proved in Appendix B)

$$e^{ig_a T^a} e^{ix_b T^b} e^{-ig_a T^a} = e^{iM_{ab}x_b T^a}$$

with

$$M_{ab} = \left(e^{ig_c t^c} \right)_{ab}$$

and $(t^c)_{ab} = -if^{cab}$ are the generators of $\mathfrak{h}_k$ in the adjoint representation[29]. Applying the lemma to (4.5) means setting $G_k = e^{i\delta g_{k,a} T^a}$, with $\delta g_{k,a} \in \mathbb{C}$ in general,[30] so that

$$\mathrm{d}z_{k,a}^G = M_{ab}\mathrm{d}z_{k,b} \tag{4.6}$$

---

[29] Notice that there are no assumptions on the form of T^a, just the commutation relations of $\mathfrak{h}_k$, that is $\left[T^a, T^b \right] = i f^{abc} T^c$.

[30] When considering an SU(N) gauge theory, one should also leave open the possibility of a more general infinitesimal gauge transformation: $G_k = e^{i\delta g_{k,a} T^a} g_k$, with $g_k \in Z(\mathcal{H}_k)$, the center of $\mathcal{H}_k$. Because, by definition, g_k commutes with $e^{i\delta g_{k,a} T^a}$, it is canceled by g_k^{-1} in our application of the lemma.

After expanding to first order in δg, we get

$$\mathrm{d}z_{k,a}^G = \mathrm{d}z_{k,a} + i\delta g_{k,c} \left(t^c\right)_{ab} \mathrm{d}z_{k,b} + \mathcal{O}\left(\delta g^2\right)$$

$$\mathrm{d}\bar{z}_{k,a}^G = \mathrm{d}\bar{z}_{k,a} + i\overline{\delta g_{k,c}} \left(t^c\right)_{ab} \mathrm{d}\bar{z}_{k,b} + \mathcal{O}\left(\delta g^2\right)$$

where we used $\left(\overline{t^c}\right)_{ab} = -\left(t^c\right)_{ab}$. The Kähler form changes accordingly $\left(\text{using } \left(t^c\right)_{ab} = -\left(t^c\right)_{ba}\right)$

$$\Omega^G = \frac{i}{2}\mathrm{d}z_{k,a}^G \wedge \mathrm{d}\bar{z}_{k,a}^G = \frac{i}{2}\left[\mathrm{d}z_{k,a} + i\delta g_{k,c}\left(t^c\right)_{ab}\mathrm{d}z_{k,b}\right] \wedge \left[\mathrm{d}\bar{z}_{k,a} + i\overline{\delta g_{k,c}}\left(t^c\right)_{ab}\mathrm{d}\bar{z}_{k,b}\right]$$

$$= \frac{i}{2}\mathrm{d}z_{k,a} \wedge \mathrm{d}\bar{z}_{k,a} + \frac{i}{2}\left[i\delta g_{k,c}\left(t^c\right)_{ab}\mathrm{d}z_{k,b} \wedge \mathrm{d}\bar{z}_{k,a} + i\overline{\delta g_{k,c}}\left(t^c\right)_{ab}\mathrm{d}z_{k,a} \wedge \mathrm{d}\bar{z}_{k,b}\right]$$

$$= \Omega - \frac{1}{2}\left[-\delta g_{k,c}\left(t^c\right)_{ba}\mathrm{d}z_{k,b} \wedge \mathrm{d}\bar{z}_{k,a} + \overline{\delta g_{k,c}}\left(t^c\right)_{ab}\mathrm{d}z_{k,a} \wedge \mathrm{d}\bar{z}_{k,b}\right]$$

$$= \Omega + \frac{1}{2}\left(\delta g_{k,c} - \overline{\delta g_{k,c}}\right)\left(t^c\right)_{ab}\mathrm{d}z_{k,a} \wedge \mathrm{d}\bar{z}_{k,b}$$

so that

$$\delta^G\Omega = i\,\Im\left(\delta g_{k,c}\right)\left(t^c\right)_{ab}\mathrm{d}z_{k,a} \wedge \mathrm{d}\bar{z}_{k,b} = \Im\left(\delta g_{k,c}\right)f^{cab}\,\mathrm{d}z_{k,a} \wedge \mathrm{d}\bar{z}_{k,b}$$

We thus see that Ω is left invariant only by taking $\delta g_{k,c} \in \mathbb{R}$, that is $G_k \in \mathcal{H}_k$: the thimble is symmetric only under transformations of the $\mathcal{H}$ subgroup of $\mathcal{G}$, that is the original gauge group. This procedure, which is similar to that followed in [39], is consistent with the result discussed in [26].

5 Integration on thimbles

Having delved into the basics of Morse theory, both in the case of a scalar and a gauge field theory, the time has come to be more concrete. So far many numerical solutions have been implemented to sample configurations on thimbles [26, 60, 67, 68, 36, 61, 69, 70, 62, 71]. Here we shall discuss an approach which was introduced by us in [72] and [73, 74]. In Section 3 we showed that the expectation value of an observable $O[z]$ (where z generically represents a collection of n complexified scalar fields) can be decomposed as

$$\langle O \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}^n z \, O(z) e^{-S_R(z)} = \frac{1}{Z} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, O \, e^{-S_R} \, e^{i\,\omega}$$

with the partition function

$$Z = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}^n z \, e^{-S_R(z)} = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, e^{-S_R} \, e^{i\,\omega}$$

where we have made the change of variables $\{z_i\} \to \{\delta y_i\}$ with δy_i the infinitesimal displacements in a neighbourhood of $z \in \mathcal{J}_\sigma$ (see (3.7) and (3.8)). We can take the residual phase $e^{i\,\omega}$ into account by means of reweighting, that is writing

$$\langle O \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} Z_\sigma \, \langle\langle O \, e^{i\,\omega} \rangle\rangle_\sigma \tag{5.1}$$

with

$$Z = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-iS_I(z_\sigma)} Z_\sigma \, \langle\langle e^{i\,\omega} \rangle\rangle_\sigma \tag{5.2}$$

where we have introduced the expectation values on single thimbles

$$\langle\langle \bullet \rangle\rangle_\sigma \equiv \frac{1}{Z_\sigma} \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, \bullet \, e^{-S_R} \tag{5.3}$$

$$Z_\sigma = \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, e^{-S_R} \tag{5.4}$$

Such expectation values can be computed via Monte Carlo with e^{-S_R} as probability weight. Single thimble partition functions Z_σ cannot be evaluated explicitly; nevertheless, $\langle O \rangle$ in (5.1) may still be computed. See [73] for a sketch of this procedure. For the rest of the section, for the sake of simplicity, we shall consider only one thimble as relevant (so that an explicit calculation of Z_σ is not needed) and drop the double $\langle \rangle$ as well. Thus our goal is to compute

$$\langle O \rangle \to \frac{\langle O \, e^{i\,\omega} \rangle}{\langle e^{i\,\omega} \rangle} \tag{5.5}$$

with

$$\langle \bullet \rangle = \frac{\int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, \bullet \, e^{-S_R}}{\int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, e^{-S_R}}$$

and this last expectation value can be computed by *any* Monte Carlo which keeps field configurations on the thimble and samples them with weight e^{-S_R}. As pointed out before, reweighting the residual phase works only if it does not oscillate wildly between different field configurations on the thimble. It is expected that this *residual sign problem* be much milder than the original one. At the moment there is evidence that $e^{i\,\omega}$ varies very smoothly on the thimble [59, 60, 36, 61, 62].

5.1 Integration in terms of steepest ascent curves

Integration on the whole thimble $\mathcal{J}_\sigma$ can be thought as an integration on a single steepest ascent curve from the critical point p_σ up to infinity[31] followed by an integration over all possible SA curves starting at p_σ. Integration of *only* steepest ascent equations is desirable, as integration of steepest descent equations is problematic because of unstable directions in the vicinity of the critical point [26, 60]. Therefore, any algorithm employing only integration of SA equations is expected to be numerically robust in staying on the thimble. We follow a notation very similar to that used in [73]. One single SA curve can be identified by the "direction" $\hat{n}$ in $T_{p_\sigma}\mathcal{J}_\sigma$ along which one leaves the critical point, that is

$$\sum_{i=1}^n n_i v^{(i)}$$

With this notation we mean the set $\{n_i\}_{i=1\cdots n}$ with the normalization condition

$$\sum_{i=1}^n n_i^2 = \mathcal{R}$$

with $\mathcal{R}$ arbitrary[32] and $\{v^{(i)}\}$ the Takagi vectors of $H(S; p_\sigma)$ with (positive) Takagi values $\{\lambda_i\}$. A point z on the thimble can be singled out by giving the SA curve it lies on (identified by $\hat{n}$) and the time t at which one reaches z while integrating SA equations. Thus we have the map

$$\mathcal{J}_\sigma \ni z \leftrightarrow (\hat{n}, t) \in S_{\mathcal{R}}^{n-1} \times \mathbb{R}$$

with $S_{\mathcal{R}}^{n-1}$ the $(n-1)$-sphere of radius $\sqrt{\mathcal{R}}$. Now we employ a Faddeev-Popov-like trick [75], that is we rewrite 1 as

$$1 = \Delta_{\hat{n}}(t) \int \prod_{k=1}^n \mathrm{d}n_k\, \delta\left(|\vec{n}|^2 - \mathcal{R}\right) \int \mathrm{d}t \prod_{i=1}^n \delta\left(\delta y_i - \delta y_i(\hat{n}, t)\right) \tag{5.6}$$

where $\{\delta y_i(\hat{n}, t)\}$ are the components of the field displacement (in the spirit of (3.7)) on the local basis[33] $\{V_{\hat{n}}^{(i)}(t)\}$, parallel-transported along the SA curved identified by $\hat{n}$ until time t. The partition function can be rewritten in terms of *partial* partition functions along each possible SA curve

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[31]Strictly speaking, this is true only for purely bosonic systems. In presence of a fermionic determinant, solutions to SA equations may flow towards zeroes of the fermionic determinant in a finite amount of integration time t [40, 37, 62]. Such configurations have infinite S_R, so that "infinity" is meant with regards to the action.

[32]Different values of $\mathcal{R}$ are theoretically equivalent, but can affect the efficiency of the numerical algorithm for sampling on the thimble, so it requires some "experimental" tuning. In [73] $\mathcal{R} = 1$ was used. In [36] the authors set $\mathcal{R} = n$. In all the simulations of this work, $\mathcal{R} = 1$ was used.

[33]The basis $\{V^{(i)}\}$ does not need to be unitary: if it is not, in the integrals $\det V = e^{i\,\omega}$ must be replaced by $|\det V| e^{i\,\omega}$. We shall discuss the choice of basis later on.

$$Z = \int \prod_{i=1}^{n} \mathrm{d}\delta y_i \, e^{-S_R} = \int \prod_{i=1}^{n} \mathrm{d}\delta y_i \, e^{-S_R} \Delta_{\hat{n}}(t) \int \prod_{k=1}^{n} \mathrm{d}n_k \, \delta\left(|\vec{n}|^2 - \mathcal{R}\right) \int \mathrm{d}t \prod_{i=1}^{n} \delta\left(\delta y_i - \delta y_i(\hat{n}, t)\right)$$

$$= \int \prod_{k=1}^{n} \mathrm{d}n_k \, \delta\left(|\vec{n}|^2 - \mathcal{R}\right) \int \mathrm{d}t \int \prod_{i=1}^{n} \mathrm{d}\delta y_i \, \delta\left(\delta y_i - \delta y_i(\hat{n}, t)\right) \Delta_{\hat{n}}(t) e^{-S_R}$$

$$= \int \prod_{k=1}^{n} \mathrm{d}n_k \, \delta\left(|\vec{n}|^2 - \mathcal{R}\right) \int \mathrm{d}t \, \Delta_{\hat{n}}(t) e^{-S_R(\hat{n}, t)}$$

Thus we can rephrase the expression for the partition function as

$$Z = \int \mathcal{D}\hat{n} \, Z_{\hat{n}} \tag{5.7}$$

with the measure over $S_{\mathcal{R}}^{n-1}$

$$\mathcal{D}\hat{n} \equiv \prod_{k=1}^{n} \mathrm{d}n_k \delta\left(|\vec{n}|^2 - \mathcal{R}\right)$$

and the *partial* partition function

$$Z_{\hat{n}} = \int_{-\infty}^{+\infty} \mathrm{d}t \, \Delta_{\hat{n}}(t) \, e^{-S_R(\hat{n}, t)} \tag{5.8}$$

The integral (5.8) is one-dimensional and can be easily computed numerically while integrating SA (and PT) equations. Algorithmic issues about an efficient sampling of $\hat{n}$-space will be discussed in Section 5.3. For the moment, let us focus on finding an expression for $\Delta_{\hat{n}}(t)$. Recall our Faddeev-Popov-like trick in (5.6). In the integral, the only external variables are the $\{\delta y_i\}$ and there are $(n+1)$ integrations, which matches precisely the number of δ conditions. We linearize the δ conditions around their solutions $(\hat{n}, t)$ and solve (5.6) for $\Delta_{\hat{n}}(t)$

$$1 = \Delta_{\hat{n}}(t) \int \prod_{k=1}^{n} \mathrm{d}n'_k \, \delta\left(|\vec{n}'|^2 - \mathcal{R}\right) \int \mathrm{d}t' \prod_{i=1}^{n} \delta\left(\delta y_i - \delta y_i(\hat{n}', t')\right)$$

$$= \Delta_{\hat{n}}(t) \int \prod_{k=1}^{n} \mathrm{d}n'_i \prod_{i=1}^{n} \delta\left(n'_i - n_i\right) \int \mathrm{d}t' \, \delta\left(t' - t\right) \left| \frac{\partial\left(|\vec{n}'|^2 - \mathcal{R}, \delta y_i - \delta y_i(\hat{n}', t')\right)}{\partial\left(t', \hat{n}'\right)} \right|^{-1}$$

$$= \Delta_{\hat{n}}(t) \left| \frac{\partial\left(|\vec{n}|^2 - \mathcal{R}, \delta y_i - \delta y_i(\hat{n}, t)\right)}{\partial\left(t, \hat{n}\right)} \right|^{-1}$$

which we can write more explicitly as

$$\Delta_{\hat{n}}(t) = \left| \det \begin{pmatrix} \frac{\partial\left(|\vec{n}|^2 - \mathcal{R}\right)}{\partial t} & \frac{\partial\left(|\vec{n}|^2 - \mathcal{R}\right)}{\partial n_1} & \cdots & \frac{\partial\left(|\vec{n}|^2 - \mathcal{R}\right)}{\partial n_n} \\ \frac{\partial(\delta y_1 - \delta y_1(\hat{n},t))}{\partial t} & \frac{\partial(\delta y_1 - \delta y_1(\hat{n},t))}{\partial n_1} & \cdots & \frac{\partial(\delta y_1 - \delta y_1(\hat{n},t))}{\partial n_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial(\delta y_n - \delta y_n(\hat{n},t))}{\partial t} & \frac{\partial(\delta y_n - \delta y_n(\hat{n},t))}{\partial n_1} & \cdots & \frac{\partial(\delta y_n - \delta y_n(\hat{n},t))}{\partial n_n} \end{pmatrix} \right|$$

$$= \left| \det \begin{pmatrix} 0 & 2n_1 & \cdots & 2n_n \\ \frac{\partial \delta y_1(\hat{n},t)}{\partial t} & \frac{\partial \delta y_1(\hat{n},t)}{\partial n_1} & \cdots & \frac{\partial \delta y_1(\hat{n},t))}{\partial n_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial \delta y_n(\hat{n},t)}{\partial t} & \frac{\partial \delta y_n(\hat{n},t)}{\partial n_1} & \cdots & \frac{\partial \delta y_n(\hat{n},t)}{\partial n_n} \end{pmatrix} \right|$$

This expression for $\Delta_{\hat{n}}(t)$ needs to be manipulated in order to be expressed as a function of known quantities. Recall what was discussed in Section 3.6, in particular the second order expansion of the action around the critical point p_σ (3.5) as well as the change of variables $Z = W\eta$ with $\eta \in \mathbb{R}^n$ and $W_{ij} = v_i^{(j)}$ ($v_i^{(j)}$ being the j-th Takagi vector of $H(S; p_\sigma)$ with Takagi value $\lambda_j > 0$). This change of variables automatically keeps one on the stable thimble in the vicinity of the critical point. The action in the η variables becomes

$$S(\eta) = S(z_\sigma) + \frac{1}{2}\sum_{i=1}^{n}\lambda_i\eta_i^2 + \cdots \tag{5.9}$$

Close enough to p_σ, this second order approximation holds reasonably well for the original theory. However, we could as well consider the quadratic action (5.9) as being valid everywhere in $\mathbb{R}^n$: this is a different, *Gaussian* theory, whose thimble associated to p_σ is *flat* and everywhere spanned by $\{v^{(i)}\}$, its (constant) residual phase being $\det W = e^{i\omega_\sigma}$. SA and PT equations for the Gaussian theory take the form

$$\frac{\mathrm{d}\eta_i}{\mathrm{d}t} = \overline{\frac{\partial S}{\partial \eta_i}} = \lambda_i\eta_i$$

$$\frac{\mathrm{d}V_j^{(i)}}{\mathrm{d}t} = \sum_{k=1}^{n}\bar{V}_k^{(i)}\overline{H_{kj}(S; p_\sigma)}$$

These equations, with the initial condition

$$\eta_i(0) = n_i$$

$$V^{(i)}(0) = v^{(i)}$$

have the solution[34]

$$\eta_i(t) = n_i\,e^{\lambda_i t}$$

$$V^{(i)}(t) = v^{(i)}\,e^{\lambda_i t} \tag{5.10}$$

which implies

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[34] For the Gaussian theory $V_{\hat{n}}^{(i)}(t) = V^{(i)}(t)$: the tangent basis vectors are independent on $\hat{n}$

$$z_j(t) = z_{\sigma,j} + \sum_{k=1}^{n} W_{jk}\eta_k(t) = z_{\sigma,j} + \sum_{k=1}^{n} n_k \, e^{\lambda_k t} \, v_j^{(k)}$$

as well as

$$S(t) = S(z_\sigma) + \frac{1}{2}\sum_{i=1}^{n} \lambda_i n_i^2 \, e^{2\lambda_i t}$$

At a reference time $t_0 \ll 0$ (ideally, one would take $t_0 \to -\infty$), the Gaussian theory and the exact one (the original theory with action S) can be identified, so that (5.10) computed at $t = t_0$ yield a valid *initial condition* for SA and PT equations of the exact theory. Let us now come back to the original theory and consider an infinitesimal displacement $\delta z(\hat{n}, t)$ around a point $z \in \mathcal{J}_\sigma$ reached by flowing along the SA curve identified by $\hat{n}$ until a time t. $\delta z(\hat{n}, t)$ belongs to $T_z \mathcal{J}_\sigma$ and thus satisfies PT equations (which are *linear*) just as any $V_{\hat{n}}^{(i)}(t)$ [73, 36]; therefore $\delta z(\hat{n}, t)$ can be written as a linear combination of tangent basis vectors with *constant* coefficients $\{\delta y_i\}$, that is

$$\delta z(\hat{n}, t) = \sum_{i=1}^{n} \delta y_i \, V_{\hat{n}}^{(i)}(t)$$

The coefficients δy_i can be easily worked out for the exact theory using the expression for $z(t)$ and $V_{\hat{n}}^{(i)}(t)$ at $t \to -\infty$, which are those of the Gaussian theory. We have

$$\delta z(\hat{n}, t \to -\infty) = \delta\left(z_\sigma + \sum_{i=1}^{n} v^{(i)} \, e^{\lambda_i t} \, n_i\right) = \sum_{i=1}^{n} v^{(i)} \left(\sum_{j=1}^{n} \delta n_j \frac{\partial}{\partial n_j} + \delta t \frac{\partial}{\partial t}\right) \left(e^{\lambda_i t} \, n_i\right)$$

$$= \sum_{i=1}^{n} v^{(i)} \, e^{\lambda_i t} \, (\delta n_i + \lambda_i n_i \delta t) = \sum_{i=1}^{n} V^{(i)}(t) \, (\delta n_i + \lambda_i n_i \delta t)$$

from which it follows

$$\delta y_i = \delta n_i + \lambda_i n_i \delta t \tag{5.11}$$

In the very same way, we can easily derive a useful consistency relation for the gradient of the action, as it also belongs to the tangent space [36]. Let us write the decomposition

$$\bar{\nabla}_z \bar{S} = \sum_{i=1}^{n} g_i \, V_{\hat{n}}^{(i)}(t)$$

The coefficients g_i can be found with the aid of the Gaussian form of the action for $t \to -\infty$, that is

$$\bar{\nabla}_z \bar{S} = \overline{\nabla_z\left(S(z_\sigma) + \frac{1}{2}Z^T H(S; p_\sigma)Z\right)} = \overline{H(S; p_\sigma)Z(t)} = \overline{HW\eta(t)} = \overline{W\Lambda\eta(t)} = W\Lambda\eta(t)$$

$$= \sum_{i=1}^{n} v^{(i)} \lambda_i \eta_i(t) = \sum_{i=1}^{n} v^{(i)} \lambda_i n_i \, e^{\lambda_i t} = \sum_{i=1}^{n} V^{(i)}(t)\lambda_i n_i$$

so that $g_i = n_i \lambda_i$. Thus, during the integration of SA and PT equations, we can keep checked the norm

$$\kappa \equiv \left\| \bar{\nabla}_z \bar{S} - \sum_{i=1}^{n} n_i \lambda_i V_{\hat{n}}^{(i)}(t) \right\| \tag{5.12}$$

and make sure that it is small with respect to the scale of the system. Now we have all is needed in order to compute $\Delta_{\hat{n}}(t)$ explicitly: from (5.11) it follows

$$\Delta_{\hat{n}}(t) = \Delta_{\hat{n}} = \left| \det \begin{pmatrix} 0 & 2n_1 & \cdots & 2n_n \\ \lambda_1 n_1 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_n n_n & 0 & \cdots & 1 \end{pmatrix} \right| = 2 \sum_{i=1}^{n} \lambda_i n_i^2 \tag{5.13}$$

which turns out to be time independent. All the computations carried out so far involved displacements δy_i with respect to local tangent basis vectors $V^{(i)}$ which are solutions of PT equations at a generic time t. This basis is not unitary in general, so that, in our integrals, we have

$$\mathrm{d}^n z = \mathrm{d}^n \delta y \, \det V = \mathrm{d}^n \delta y \, |\det V| \, e^{i\omega}$$

where $e^{i\omega}$ is the same residual phase we would have ended up with if we had used a unitary basis.[35] Thus expression (5.8) for the partial partition function becomes

$$Z_{\hat{n}} = 2 \sum_{i=1}^{n} \lambda_i n_i^2 \int_{-\infty}^{+\infty} \mathrm{d}t \, e^{-S_{\mathrm{eff}}(\hat{n}, t)} \tag{5.14}$$

with

$$S_{\mathrm{eff}}(\hat{n}, t) = S_R(\hat{n}, t) - \log |\det V_{\hat{n}}(t)| \tag{5.15}$$

We have computed $\Delta_{\hat{n}}(t)$ for the exact theory; of course the Gaussian one has the same expression for $\Delta_{\hat{n}}$, but in that case we can compute $\det V_{\hat{n}}(t)$ analytically as well. Being $V_{\hat{n}}^{(i)}(t) = v^{(i)} e^{\lambda_i t}$, we have

$$\det V(t) = \det \begin{pmatrix} e^{\lambda_1 t} v^{(1)} & \cdots & e^{\lambda_n t} v^{(n)} \end{pmatrix} = \prod_{i=1}^{n} e^{\lambda_i t} \det \begin{pmatrix} v^{(1)} & \cdots & v^{(n)} \end{pmatrix} = e^{\left(\sum_{i=1}^{n} \lambda_i \right) t} \det W = e^{\Lambda t + i\omega_\sigma}$$

where $\Lambda \equiv \sum_{i=1}^{n} \lambda_i$ and $e^{i\omega_\sigma}$ is the residual phase at the critical point. Therefore the expression for $Z_{\hat{n}}$ of the Gaussian theory is

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[35]In [73] a unitary basis $\{U^{(i)}\}$ was used, yielding $\det U = e^{i\omega}$ and a time-dependent expression $\tilde{\Delta}_{\hat{n}}(t)$, which encoded the stretching of basis vectors (that is the change in volume of an infinitesimal parallelepiped generated by the $V^{(i)}$) along the SA flow). Here we have chosen to work with the non-unitary base $\{V^{(i)}\}$. Had we worked with a unitary one, say $\{U^{(i)}\}$, we would have ended up with the same residual phase $e^{i\omega}$. This can be readily seen by using QR decomposition (*e.g.* by means of Gram-Schmidt process, like in [36]) on the matrix V defined by $V_{ij} \equiv V_i^{(j)}$. QR decomposition yields $V = UE$ with U unitary, so that $\det V = \det U \det E = e^{i\omega} \det E$. Now, being all the $V^{(i)}$ linearly independent, $\det V \neq 0$ and thus there is a (unique) factorization with all the diagonal elements of the *upper triangular* matrix E real and positive. The conclusion is that $\det E > 0$, so that $|\det V| = \det E$ and the residual phase $e^{i\omega}$ of the present work is the same as the one in [73]. It is also easy to check that $\tilde{\Delta}_{\hat{n}}(t) = \Delta_{\hat{n}}(t) \det E = \Delta_{\hat{n}} |\det V|$ (where $\Delta_{\hat{n}}$ is given by (5.13)), so that the two choices of basis are perfectly equivalent.

$$Z_{\hat{n}} = 2 \sum_{i=1}^{n} \lambda_i n_i^2 \int_{-\infty}^{+\infty} \mathrm{d}t \, e^{\Lambda \, t - \frac{1}{2} \sum_{i=1}^{n} \lambda_i n_i^2 e^{2\lambda_i t}} \tag{5.16}$$

As a final note for this section, we consider the case of a gauge theory. All the previous statements apply, keeping in mind that infinitesimal displacements are in the algebra of the gauge group, that is a neighbourhood Γ_U of $U \in \mathcal{J}_\sigma$ is explored by means of $\{\mathrm{d}z_{k,a}\}$ such that $U' \in \Gamma_U$ is

$$U'_k = e^{i \, \mathrm{d}z_{k,a} T^a} U_k \tag{5.17}$$

with $\mathrm{d}z_{k,a} = \sum_i \delta y_i V_{k,a}^{(i)}$ ($\{V^{(i)}\}$ being a local basis of $T_U \mathcal{J}_\sigma$). All the integrals we are interested in are of the type

$$\int \mathcal{D}U = \int \prod_k \mathrm{d}U_k$$

$\mathrm{d}U_k$ being the invariant measure of the gauge group. As in (3.8), we want to rewrite such integrals in terms of δy, that is

$$\prod_k \mathrm{d}U_k = \sqrt{\det g} \, \mathrm{d}^n \delta y$$

with the metric g given by

$$\mathrm{d}s^2 = \sum_k \mathrm{d}s^2 \big|_k = \sum_k \left[-\mathrm{Tr}\left(U_k^{-1}\mathrm{d}U_k U_k^{-1}\mathrm{d}U_k\right)\right] = \sum_{i,j} g_{ij}\delta y_i \delta y_j$$

The invariant measure $\mathrm{d}s^2\big|_k$ of the gauge group can be computed as follows

$$\mathrm{d}s^2\big|_k = -\mathrm{Tr}\left(U_k^{-1}\mathrm{d}U_k U_k^{-1}\mathrm{d}U_k\right) = -\mathrm{Tr}\left[U_k^{-1}\left(e^{i\,\mathrm{d}z_{k,a}T^a} - \mathbb{1}\right)U_k U_k^{-1}\left(e^{i\,\mathrm{d}z_{k,b}T^b} - \mathbb{1}\right)U_k\right]$$

$$= -\mathrm{Tr}\left[\left(i\,\mathrm{d}z_{k,a}T^a + \mathcal{O}\left(\mathrm{d}z^2\right)\right)\left(i\,\mathrm{d}z_{k,b}T^b + \mathcal{O}\left(\mathrm{d}z^2\right)\right)\right] = \mathrm{Tr}\left(T^a T^b\right)\mathrm{d}z_{k,a}\mathrm{d}z_{k,b} = \frac{1}{2}\delta_{ab}\mathrm{d}z_{k,a}\mathrm{d}z_{k,b} \sim \sum_a \mathrm{d}z_{k,a}^2$$

In the last step the factor $1/2$ has been neglected, being a constant which is dependent only on the normalization of T^a (it is cancelled out in ratios of integrals anyway). It follows that

$$\mathrm{d}s^2 = \sum_{k,a}\mathrm{d}z_{k,a}^2 = \sum_{k,a}\sum_i \delta y_i V_{k,a}^{(i)}\sum_j \delta y_j V_{k,a}^{(j)} = \sum_{i,j}\left(\sum_{k,a}V_{k,a}^{(i)}V_{k,a}^{(j)}\right)\delta y_i \delta y_j$$

so that we can read out the components of the metric

$$g_{ij} = \sum_{k,a}V_{k,a}^{(i)}V_{k,a}^{(j)} = \left(V^T V\right)_{ij}$$

From this, we have the determinant

$$\sqrt{\det g} = \sqrt{\det\left(V^T V\right)} = \det V$$

which is the one we already know. It is this determinant that will give rise to the gauge group (complexified) Haar measure: in fact, the basis $\{V^{(i)}\}$ is parallel-transported under equations (4.4), which know of the non-abelian nature of the gauge group.

5.2 Semiclassical expansion around thimbles

In this section we show how a semiclassical expansion may be performed in the context of Lefschetz thimbles. Semiclassical (leading order) approximation means expanding the action S of the theory to second order around each critical point p_σ (that is classical solutions of the quantum theory) and performing Gaussian integrals analytically. We employ the same notation of the previous section. Consider the quadratic expansion of the action around the critical point p_σ in (5.9). After setting $Z = W\eta$, so that $\mathrm{d}^n z = \det W \mathrm{d}^n \eta = e^{i\,\omega_\sigma} \mathrm{d}^n \eta$, the partition function becomes

$$Z \approx \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-S(z_\sigma)} \, e^{i\,\omega_\sigma} \int_{\mathbb{R}^n} \mathrm{d}^n\eta \, e^{-\frac{1}{2}\sum_{i=1}^{n} \lambda_i \eta_i^2} = (2\pi)^{\frac{n}{2}} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, \frac{e^{-S(z_\sigma)}}{\sqrt{\det \Lambda_\sigma}} \, e^{i\,\omega_\sigma} \tag{5.18}$$

where the Gaussian integral

$$\int_{-\infty}^{+\infty} \mathrm{d}\eta_i \, e^{-\frac{1}{2}\lambda_i \eta_i^2} = \sqrt{\frac{2\pi}{\lambda_i}}$$

has been computed and it has been assumed that all λ_i are positive ($\det \Lambda_\sigma = \prod_i \lambda_i$). From the last expression for Z, it is clear that the critical point with the smallest value of S_R is dominant in the expansion. Now we want to compute the expectation value of an observable O. We expand $O(z)$ around p_σ

$$O(z) \approx O(z_\sigma) + \nabla_Z^T O Z + \frac{1}{2} Z^T H_\sigma^O Z$$

with

$$\nabla_Z^T O \equiv \left(\frac{\partial O}{\partial z_1}\Big|_{z_\sigma}, \cdots, \frac{\partial O}{\partial z_n}\Big|_{z_\sigma} \right)$$

and

$$\left(H_\sigma^O \right)_{ij} \equiv \frac{\partial^2 O}{\partial z_i \partial z_j}\Big|_{z_\sigma}$$

It is obvious that, in general, $[H(S; p_\sigma), H_\sigma^O] \neq 0$ and therefore we cannot expect W to "diagonalize" both $H(S; p_\sigma)$ and H_σ^O. The expectation value of the observable is given by

$$\langle O \rangle \approx \frac{1}{Z} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-S(z_\sigma)} \, e^{i\,\omega_\sigma} \int_{\mathbb{R}^n} \mathrm{d}^n\eta \left(O(z_\sigma) + \nabla_Z^T O W \eta + \frac{1}{2} \eta^T C_\sigma^O \eta \right) e^{-\frac{1}{2}\sum_{i=1}^{n} \lambda_i \eta_i^2}$$

with $C_\sigma^O \equiv W^T H_\sigma^O W$. The first term in the expansion of O comes out of the integral, giving the partition function itself (actually, the contribution of the thimble $\mathcal{J}_\sigma$). The second term is linear in η_i and therefore gives no contribution to the Gaussian integral. For the same reason, the third term contributes only with terms which are quadratic in η_i, that is when

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$$\eta^T C_\sigma^O \eta = \sum_{i=1}^{n} \sum_{j=1}^{n} \left(C_\sigma^O \right)_{ij} \eta_i \eta_j \rightarrow \sum_{i=1}^{n} \left(C_\sigma^O \right)_{ii} \eta_i^2$$

Therefore we need to compute only the diagonal terms of C_σ^O and, after performing the Gaussian integral

$$\int_{-\infty}^{+\infty} \mathrm{d}\eta_i \, \eta_i^2 \, e^{-\frac{1}{2}\lambda_i \eta_i^2} = \frac{1}{\lambda_i} \sqrt{\frac{2\pi}{\lambda_i}}$$

we arrive at

$$\langle O \rangle \approx \frac{1}{Z}(2\pi)^{\frac{n}{2}} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \frac{e^{-S(z_\sigma)}}{\sqrt{\det \Lambda_\sigma}} \, e^{i\,\omega_\sigma} \left(O(z_\sigma) + \frac{1}{2} \sum_{i=1}^{n} \frac{\left(C_\sigma^O \right)_{ii}}{\lambda_i} \right) \tag{5.19}$$

We can work out a more useful expression for $\left(C_\sigma^O \right)_{ii}$ in terms of Takagi vectors

$$\left(C_\sigma^O \right)_{ii} = \sum_{j=1}^{n} \sum_{k=1}^{n} \left(H_\sigma^O \right)_{jk} W_{ji} W_{ki} = \sum_{j=1}^{n} \sum_{k=1}^{n} \left(H_\sigma^O \right)_{jk} v_j^{(i)} v_k^{(i)}$$

It is nice to see that, if we take the action S itself as observable, then $H_\sigma^O \equiv H(S; p_\sigma)$ and, being $H(S; p_\sigma) v^{(i)} = \lambda_i \bar{v}^{(i)}$ and $\sum_j v_j^{(i)} \bar{v}_j^{(i')} = \delta_{ii'}$, we have

$$\left(C_\sigma^O \right)_{ii} = \sum_{j=1}^{n} v_j^{(i)} \lambda_i \bar{v}_j^{(i)} = \lambda_i$$

yielding the contribution

$$S(z_\sigma) + \frac{n}{2}$$

which is nothing but the equipartition theorem.

5.3 Numerical algorithms to sample on a thimble

We have seen how a thimble can be decomposed in terms of $\hat{n}$ and t. Now it is time to devise an algorithm to perform Monte Carlo sampling on the thimble taking advantage of this parametrization. Recall that we want to compute the expectation value of some observable O through (5.1), (5.2), (5.3), (5.4), making use of the parametrization of the partition function in terms of partial partition functions in (5.7), (5.14) and (5.15). To summarize, what we wish to compute is

$$\langle O \rangle = \frac{1}{Z} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-i\,S_I(z_\sigma)} \, Z_\sigma \left(\frac{1}{Z_\sigma} \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, O \, e^{i\,\omega} \, e^{-S_R} \right) \tag{5.20}$$

$$Z = \frac{1}{Z} \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \, e^{-i\,S_I(z_\sigma)} \, Z_\sigma \left(\frac{1}{Z_\sigma} \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y \, e^{i\,\omega} \, e^{-S_R} \right) \tag{5.21}$$

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with

$$\frac{1}{Z_\sigma} \int_{\mathcal{J}_\sigma} \mathrm{d}^n \delta y\, f\, e^{-S_R} = \frac{1}{Z_\sigma} \int \mathcal{D}\hat{n}\, f_{\hat{n}} = \int \mathcal{D}\hat{n}\, \frac{Z_{\hat{n}}}{Z_\sigma} \frac{f_{\hat{n}}}{Z_{\hat{n}}} \tag{5.22}$$

in which

$$f_{\hat{n}} = 2\sum_{i=1}^{n} \lambda_i n_i^2 \int_{-\infty}^{+\infty} \mathrm{d}t\, f(\hat{n}, t)\, e^{-S_{\mathrm{eff}}(\hat{n}, t)}$$

$$Z_{\hat{n}} = 2\sum_{i=1}^{n} \lambda_i n_i^2 \int_{-\infty}^{+\infty} \mathrm{d}t\, e^{-S_{\mathrm{eff}}(\hat{n}, t)}$$

where it is understood $Z_\sigma = \int \mathcal{D}\hat{n}\, Z_{\hat{n}}$. Let us focus on a single thimble $\mathcal{J}_\sigma$. From (5.22) we see that what we should do in principle is extract a sequence (a Markov chain) $\{\hat{n}^{(j)}\}_{j=1\cdots N}$ according to the (correctly normalized) probability $P(\hat{n}) = Z_{\hat{n}}/Z_\sigma$; then the expectation value of f (being either $O\,e^{i\,\omega}$ or $e^{i\,\omega}$) on $\mathcal{J}_\sigma$ would be simply given by

$$\lim_{N\to\infty} \frac{1}{N} \sum_{j=1}^{N} \frac{f_{\hat{n}^{(j)}}}{Z_{\hat{n}^{(j)}}}$$

As a first proposal to sample the $\hat{n}$-space, we consider the simplest one: doing no importance sampling at all. The static, crude Monte Carlo consists of a Markov chain of $\hat{n}$ which are *uniformly* distributed on $S_{\mathcal{R}}^{n-1}$.[36] Then one is able to directly compute the ratio

$$\langle O \rangle = \frac{\sum_{\sigma\in\Sigma} \mathfrak{n}_\sigma\, e^{-i\,S_I(z_\sigma)} \int \mathcal{D}\hat{n}\, \left(O\,e^{i\,\omega}\right)_{\hat{n}}}{\sum_{\sigma\in\Sigma} \mathfrak{n}_\sigma\, e^{-i\,S_I(z_\sigma)} \int \mathcal{D}\hat{n}\, \left(e^{i\,\omega}\right)_{\hat{n}}} \tag{5.23}$$

This method is expected to be rather inefficient for systems whose $Z_{\hat{n}}$ vary a lot as functions of $\hat{n}$. This is in fact the cause of the larger error bars at lower values of $\tilde{m}$ in Figure 7.3. Nevertheless, this method was used in [73] and was successful in recovering correct results for the Chiral Random Matrix model, as discussed in Section 7. From (5.23), we also see that this method enables us to automatically take into account the contribution of more than one thimble. The static, crude Monte Carlo was also used for $\mathrm{SU}(N)$ one-link models and $0+1$-dimensional QCD, where more than one thimble is relevant; see Sections 9 and 8 for details.

Let us now discuss a more sophisticated way to sample $\hat{n}$ according to the probability $P(\hat{n}) = Z_{\hat{n}}/Z_\sigma$. The problem one immediately faces is that the computation of $Z_{\hat{n}}$ for a given $\hat{n}$ needs integration of an *entire* SA curve, which requires solving SA and PT equations for a long enough time for the integral in $\mathrm{d}t$ to converge. Therefore a Von Neumann-like procedure to extract $\hat{n}$ according to $P(\hat{n})$ is unfeasible. One possible way around this is the *flat Metropolis* algorithm: given $\hat{n}^{(j)}$ at the j-th step of the Markov chain, one extracts $\hat{n}'$ *uniformly* on $S_{\mathcal{R}}^{n-1}$ and accepts it with probability

$$P_{\mathrm{acc}}\left(\hat{n}'|\hat{n}\right) = \min\left\{1, \frac{Z_{\hat{n}'}}{Z_{\hat{n}}}\right\} \tag{5.24}$$

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[36]Extracting $\hat{n} \in S_{\mathcal{R}}^{n-1}$ uniformly is easy [76]: one extracts n independent Gaussian numbers, that is $n_j \in \mathcal{N}(0, 1)$ and then normalizes the resulting vector with norm $\sqrt{\mathcal{R}}$. Extracting $\hat{n}$ uniformly on $S_{\mathcal{R}}^{n-1}$ gives a volume factor $\mathrm{Vol}(S_{\mathcal{R}}^{n-1})$ in front of each $\int \mathcal{D}\hat{n}$ (the normalized probability density being $\delta(|\vec{n}|^2 - \mathcal{R})/\mathrm{Vol}(S_{\mathcal{R}}^{n-1})$). As we are interested only in ratios, we shall omit the factor $\mathrm{Vol}(S_{\mathcal{R}}^{n-1})$ from now on.

where Z_σ has disappeared in the ratio. The drawback of this approach is that the acceptance rate can become very small in case of $Z_{\hat{n}}$ varying by orders of magnitude as a function of $\hat{n}$. A far better approach consists of *proposing* the new configuration $\hat{n}'$ according to a probability distribution which is expected to have a far greater overlap with $P(\hat{n})$ than the uniform one. The best candidate is the probability for the Gaussian theory, that is $P^{\mathcal{G}}(\hat{n}) = Z^{\mathcal{G}}_{\hat{n}}/Z^{\mathcal{G}}_\sigma$ with $Z^{\mathcal{G}}_{\hat{n}}$ given by (5.16). This distribution has far better chances of yielding a higher acceptance rate compared to a uniform extraction of $\hat{n}$. Thus we generate a Markov chain $\left\{\hat{n}^{(j)}\right\}_{j=1\cdots N}$; at the j-th step, we *propose* $\hat{n}'$ with probability $P^{\mathcal{G}}(\hat{n}')$ and *accept* it with probability

$$P_{\text{acc}}\left(\hat{n}'|\hat{n}\right) = \min\left\{1, \frac{Z_{\hat{n}'}}{Z_{\hat{n}}}\frac{Z^{\mathcal{G}}_{\hat{n}}}{Z^{\mathcal{G}}_{\hat{n}'}}\right\} \tag{5.25}$$

where $Z^{\mathcal{G}}_\sigma$ drops as well as Z_σ and $\text{Vol}(S^{n-1}_{\mathcal{R}})$. The only remaining task is to devise a procedure to extract $\hat{n}$ according to $P^{\mathcal{G}}(\hat{n})$. To this purpose, we shall discuss an *heat-bath* algorithm in $\hat{n}$ space for the Gaussian theory. Consider a given $\hat{n} \in S^{n-1}_{\mathcal{R}}$; we want to extract $\hat{n}'$ with probability $P^{\mathcal{G}}(\hat{n}') \propto Z^{\mathcal{G}}_{\hat{n}'}$. Let us pick two *random, different* components of $\hat{n}$, say (n_i, n_j) with $i \neq j$. We define C by

$$C \equiv n_i^2 + n_j^2 = \mathcal{R} - \sum_{k\neq i,j} n_k^2$$

which is fixed by the normalization $|\vec{n}| = \sqrt{\mathcal{R}}$ and the values of all $\{n_k\}_{k\neq i,j}$. We can therefore parametrize the "subspace" (n_i, n_j) by

$$n_i = \sqrt{C}\,\cos\phi$$
$$n_j = \sqrt{C}\,\sin\phi \tag{5.26}$$

with $\phi \in [0, 2\pi)$. We will now describe a procedure to extract $\phi' \in [0, 2\pi)$ such that

$$n'_k = \begin{cases} \sqrt{C}\,\cos\phi' & \text{if } k=i \\ \sqrt{C}\,\sin\phi' & \text{if } k=j \\ n_k & \text{if } k \neq i,j \end{cases} \tag{5.27}$$

is distributed according to $P^{\mathcal{G}}(\hat{n}') = P^{\mathcal{G}}(\hat{n}'(\phi')) \propto Z^{\mathcal{G}}_{\hat{n}'(\phi')}$. As the only correction for the proposal probability appearing in (5.25) is $Z^{\mathcal{G}}_{\hat{n}'(\phi')}$, we have to check that the choice of a random pair (i,j) and the parametrization (5.26) is *uniform* on $S^{n-1}_{\mathcal{R}}$. This can be readily seen by changing variables from Cartesian to polar on the $(n-1)$-sphere

$$n_1 = \sqrt{\mathcal{R}}\,\cos\phi_1$$

$$n_2 = \sqrt{\mathcal{R}}\,\sin\phi_1\,\cos\phi_2$$

$$n_3 = \sqrt{\mathcal{R}}\,\sin\phi_1\,\sin\phi_2\,\cos\phi_3$$

$$\vdots \tag{5.28}$$

$$n_{n-1} = \sqrt{\mathcal{R}}\sin\phi_1\cdots\sin\phi_{n-2}\,\cos\phi_{n-1}$$

$$n_n = \sqrt{\mathcal{R}}\sin\phi_1\cdots\sin\phi_{n-2}\,\sin\phi_{n-1}$$

with area element

$$d_{S^{n-1}} V = \sin^{n-2} \phi_1 \, \sin^{n-3} \phi_2 \cdots \sin \phi_{n-2} \, d\phi_1 d\phi_2 \cdots d\phi_{n-1} \tag{5.29}$$

For any choice of (n_i, n_j) with $i \neq j$, one can choose a system of coordinates in which n_i and n_j play the role of n_{n-1} and n_n in (5.28) respectively, with the identification

$$\sqrt{C} \quad \leftrightarrow \quad \sqrt{\mathcal{R}} \prod_{k=1}^{n-2} \sin \phi_k$$

$$\phi \quad \leftrightarrow \quad \phi_{n-1}$$

Then any choice of $\phi \in [0, 2\pi)$ is equally probable on the $(n-1)$-sphere because the area element (5.29) $d_{S^{n-1}} V \sim d\phi$ is *flat* in ϕ. Our remaining task is to show how to extract ϕ' with probability $P^{\mathcal{G}}(\hat{n}'(\phi'))$. Let us turn to (5.16) and plug in (5.27)

$$Z^{\mathcal{G}}_{\hat{n}'(\phi')} = 2 \left[\sum_{k \neq i,j} \lambda_k n_k^2 + C \left(\lambda_i \cos^2 \phi' + \lambda_j \sin^2 \phi' \right) \right] \int\limits_{-\infty}^{+\infty} dt \, e^{\Lambda t - \frac{1}{2} \left[\sum\limits_{k \neq i,j} \lambda_k n_k^2 e^{2\lambda_k t} + C \left(\lambda_i \cos^2 \phi' e^{2\lambda_i t} + \lambda_j \sin^2 \phi' e^{2\lambda_j t} \right) \right]} \tag{5.30}$$

The reader should keep in mind that this expression is dependent on $\{n_k\}_{k \neq i,j}$. Consider now the cumulative distribution function defined by

$$F^{\mathcal{G}}_{\hat{n}'}(\phi') \equiv \frac{\int\limits_0^{\phi'} d\varphi \, Z^{\mathcal{G}}_{\hat{n}'(\varphi)}}{\int\limits_0^{2\pi} d\varphi \, Z^{\mathcal{G}}_{\hat{n}'(\varphi)}}$$

By extracting $\xi \in [0, 1]$ uniformly distributed and computing $\phi' = F^{\mathcal{G}-1}_{\hat{n}'}(\xi)$[37], we have that ϕ' is distributed according to $P(\phi') \propto Z_{\hat{n}'(\phi')}$. Then we use (5.27) to get $\hat{n}'$ and all is ready to perform the Metropolis acceptance test (5.25) ($Z_{\hat{n}'(\phi')}$ is readily available once ϕ' is known). We call this procedure a heat-bath-based (HBB) Metropolis.

An interesting observation can be made out of (5.30): if (i, j) is such that $\lambda_i = \lambda_j$, then $Z^{\mathcal{G}}_{\hat{n}'(\phi')}$ is effectively independent on ϕ'; thus all that is needed is the extraction of ϕ' uniformly distributed in $[0, 2\pi)$ and the use of (5.27). Moreover, if *all* the λ_i are equal, then $Z^{\mathcal{G}}_{\hat{n}'} = Z^{\mathcal{G}}_{\hat{n}} \, \forall \hat{n}, \hat{n}'$ and this Gaussian *heat-bath-based* Metropolis does not perform any better than the flat Metropolis in (5.24). In such cases (for example one-link $SU(N)$ models and $0 + 1$-dimensional QCD) we even made use of the static, crude Monte Carlo. Another important observation is that, although in some sense trivial with respect to the actual theory, its Gaussian counterpart is still highly non-trivial when reformulated in terms of $\hat{n}$. The use of importance sampling for the Chiral Random Matrix theory described in Section 7 provided the same, correct results of the static, crude Monte Carlo with far less statistics and smaller error bars; it also made it possible to explore a region in parameter space (namely, small rescaled masses) in which the static, crude Monte Carlo was unable to reach correct estimates [77, 78]. The main problem with this kind of importance sampling is that one extracts observables according to the right distribution on a given thimble $\mathcal{J}_\sigma$, but without knowing Z_σ itself (see formulae (5.20) and (5.21)). As a consequence, taking into account more than one thimble can be tricky. For a sketch of a procedure for doing this, the reader can refer to [73].

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[37] $F^{\mathcal{G}}_{\hat{n}'}(\phi')$, being the integral of a manifestly positive function, is monotonically increasing and can be easily inverted numerically.

As a final remark, we notice that the parametrization (5.26) leaves space for other possible algorithmic solutions. For example, one could extract $\delta\phi$ uniformly distributed in $[-\varepsilon, \varepsilon]$[38] and propose $\phi' = \phi + \delta\phi$ (modulo 2π), accepting $\hat{n}'$ with probability (5.24). By tuning ε, one could look for a reasonable compromise between acceptance rate and correlations: small values of ε will yield an $\hat{n}'$ which is highly correlated to $\hat{n}$, whilst large values of ε will be likely to kill the acceptance rate if $Z_{\hat{n}}$ is highly dependent on $\hat{n}$. Numerical results for the application of this last prescription to the Chiral Random Matrix model, as well as results for the HBB Metropolis algorithm, are presented in Section 7.

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[38]Such choice of interval ensures that the proposal be symmetric.

6   Zero-dimensional ϕ^4 model

After studying Morse theory in general and laying out an algorithm to perform integration on thimbles, let us go back to the simple case of a one-dimensional integral. This model will be a useful tool to familiarize with the basics of Morse theory and at the same time to discuss the relevance of more than one critical point within the thimble decomposition. We consider the zero-dimensional ϕ^4 model, whose only degree of freedom consists of a real field ϕ. The partition function is

$$Z(\sigma, \lambda) = \int\limits_{-\infty}^{+\infty} \mathrm{d}\phi \, e^{-S(\phi)} \tag{6.1}$$

$$S(\phi) = \frac{1}{2}\sigma\phi^2 + \frac{1}{4}\lambda\phi^4 \tag{6.2}$$

with $\lambda \in \mathbb{R}^+$ and $\sigma = \sigma_R + i\,\sigma_I \in \mathbb{C}$. The sign problem is due to σ_I, which plays the role of a "chemical potential". This model was first introduced about thirty years ago in [79] as a toy model for one of the first tests of complex Langevin [80]. The model, although seemingly simple, proved to be quite hard for complex Langevin; in particular, for some values of the parameters σ and λ, it was difficult to keep simulations under control. Another problem the complex Langevin faced was the divergence of the expectation value of high-order momenta, that is $\langle \phi^n \rangle$ with $n \geq 6$. This behaviour was later shown to be due to a power-law decay of the equilibrium probability distribution for the (complexified) field, solution to the associated Fokker-Planck equation [81, 82, 83, 84]. Recently, this model has also been studied within the framework of Morse theory in [85, 73] (and also in [86], though in a slightly different representation). Despite being so simple, this toy model proves to be quite valuable for understanding the relevance of more than one thimble depending on the value of a parameter in the action (in this case σ_R). Being the model one-dimensional, it is easier and more transparent to work in terms of the two real components (x, y) of the (complexified) field $\phi = x + i\,y$ and of the eigenvectors of $H(S_R; p_\sigma)$ instead of referring to the Takagi vectors of $H(S; p_\sigma)$. From (6.2) we have

$$S_R(x, y) = \frac{1}{2}\left[\sigma_R(x^2 - y^2) - 2\sigma_I xy\right] + \frac{1}{4}\lambda\left(x^4 + y^4 - 6x^2 y^2\right)$$

$$S_I(x, y) = \frac{1}{2}\left[\sigma_I(x^2 - y^2) + 2\sigma_R xy\right] + \lambda xy(x^2 - y^2)$$

In order to find the critical points, we impose

$$\frac{\mathrm{d}S(\phi)}{\mathrm{d}\phi} = \sigma\phi + \lambda\phi^3 = \phi(\sigma + \lambda\phi^2) = 0 \tag{6.3}$$

so that there are three critical points: the *classical vacuum* $\phi_0 = 0$ and two *Higgs vacua*[39]

$$\phi_\pm = \pm i\,\sqrt{\frac{\sigma}{\lambda}} = x_\pm \pm i\,y_\pm$$

The drift is given by

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[39]To get a flavour of the physical meaning of these critical points, it is useful to consider the action (6.2) on the original domain of integration only (that is $\phi \in \mathbb{R}$). We have already stated that the complex nature of S comes from the "chemical potential" σ_I. Now let us consider the zero-dimensional ϕ^4 theory at zero density, so that $S(\phi) = \frac{1}{2}\sigma_R\phi^2 + \frac{1}{4}\lambda\phi^4$. The critical points are given by $\phi(\sigma_R + \lambda\phi^2) = 0$. For $\sigma_R > 0$ there is just one critical point $\phi_0 = 0$, which is a *minimum* of the action. On the contrary, for $\sigma_R < 0$, there are three critical points: $\phi_0 = 0$, which is now a *maximum* of the action, and $\phi_\pm = \pm\sqrt{-\sigma_R/\lambda}$, which are *minima* of the action. Therefore the sign of σ_R parametrizes a *spontaneous symmetry breaking* (SSB). From these considerations, we can foresee that the sign of σ_R will play a crucial role in the thimble analysis of the ϕ^4 model.

$$\frac{\partial S_R(x,y)}{\partial x} = \sigma_R x - \sigma_I y + \lambda x^3 - 3\lambda x y^2$$

$$\frac{\partial S_R(x,y)}{\partial y} = -\sigma_R y - \sigma_I x + \lambda y^3 - 3\lambda x^2 y$$

while the Hessian is

$$H(S_R; x, y) = \begin{pmatrix} \sigma_R + 3\lambda(x^2 - y^2) & -\sigma_I - 6\lambda xy \\ -\sigma_I - 6\lambda xy & -\sigma_R - 3\lambda(x^2 - y^2) \end{pmatrix} \tag{6.4}$$

It is now useful to rewrite the defining relation for $\phi_\pm$, that is

$$\phi_\pm^2 = (x_\pm + i\, y_\pm)^2 = (x_\pm^2 - y_\pm^2) + 2i\, x_\pm y_\pm = -\frac{\sigma}{\lambda} = -\frac{\sigma_R}{\lambda} + i\left(-\frac{\sigma_I}{\lambda}\right)$$

implying that

$$x_\pm^2 - y_\pm^2 = -\frac{\sigma_R}{\lambda}$$

$$x_\pm y_\pm = -\frac{\sigma_I}{2\lambda} \tag{6.5}$$

These relations are useful to evaluate S_I at the critical points

$$S_I(\phi_0) = S_I(0,0) = 0$$

$$S_I(\phi_\pm) = S_I(x_\pm, y_\pm) = \frac{1}{2}\left[\sigma_I\left(-\frac{\sigma_R}{\lambda}\right) + 2\sigma_R\left(-\frac{\sigma_I}{2\lambda}\right)\right] + \lambda\left(-\frac{\sigma_I}{2\lambda}\right)\left(-\frac{\sigma_R}{\lambda}\right) = -\frac{\sigma_R \sigma_I}{2\lambda}$$

We immediately notice that $S_I(\phi_+) = S_I(\phi_-) = S_I(\phi_0)$ whenever $\sigma_R = 0$ or $\sigma_I = 0$ (in this work we always take $\sigma_I > 0$), so that the imaginary axis in the complex σ-plane is a candidate for a Stokes line (so that a Stokes phenomenon may occur at $\sigma_R = 0$ - see Section 3.5). We will later see that this is indeed the case. The Hessian at ϕ_0 is

$$H(S_R; \phi_0) = \begin{pmatrix} \sigma_R & -\sigma_I \\ -\sigma_I & -\sigma_R \end{pmatrix}$$

with eigenvalues $\lambda_0^{(\pm)} = \pm\sqrt{\sigma_R^2 + \sigma_I^2} = \pm|\sigma|$ and eigenvectors, respectively

$$v_0^{(\pm)} = \frac{1}{\sqrt{2\left(1 + \frac{\sigma_R^2}{\sigma_I^2} \pm |\sigma| \frac{\sigma_R}{\sigma_I^2}\right)}} \begin{pmatrix} -\frac{-\sigma_R \pm |\sigma|}{\sigma_I} \\ 1 \end{pmatrix}$$

where the upper $\pm$ marks the stable/unstable direction at ϕ_0. Plugging (6.5) into (6.4) gives the Hessian at $\phi_\pm$

$$H(S_R; \phi_\pm) = 2\begin{pmatrix} -\sigma_R & \sigma_I \\ \sigma_I & \sigma_R \end{pmatrix}$$

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with eigenvalues $\lambda_{\pm}^{(\pm)} = \pm 2 |\sigma|$ and eigenvectors

$$v_{\pm}^{(\pm)} = \frac{1}{\sqrt{2 \left(1 + \frac{\sigma_R^2}{\sigma_I^2} \mp |\sigma| \frac{\sigma_R}{\sigma_I^2}\right)}} \begin{pmatrix} -\frac{-\sigma_R \mp |\sigma|}{\sigma_I} \\ 1 \end{pmatrix}$$

Notice that ϕ_+ and ϕ_- share the same tangent space, which is orthogonal to the respective stable/unstable tangent space of ϕ_0.

Now we have all the ingredients we need in order to perform the thimble analysis of the model. We are interested in the partition function (6.1), with $Z(\sigma, \lambda)$ a (complex) *continuous* function of σ and λ, which will guide us while searching for the correct set of $\mathfrak{n}_\sigma$ in going through the Stokes phenomenon (see Section 3.5 for details). The integral in (6.1) is convergent thanks to $\lambda \in \mathbb{R}^+$. For $\sigma_R > 0$, we can evaluate Z in closed form

$$Z(\sigma, \lambda) = \sqrt{\frac{4\xi}{\sigma}} \, e^\xi \, K_{-\frac{1}{4}}(\xi)$$

with $\xi \equiv \frac{\sigma^2}{8\lambda}$ and $K_\nu(\xi)$ the modified Bessel function of the second kind. The thimble decomposition provides an *analytical continuation* for negative values of σ_R (see [34] for a thorough discussion on Morse theory and analytical continuation of the Airy function). We also look for the correlators of the field

$$\langle \phi^{2n} \rangle = \frac{1}{Z} \int\limits_{-\infty}^{+\infty} \mathrm{d}\phi \, \phi^{2n} \, e^{-\frac{1}{2}\sigma\phi^2 - \frac{1}{4}\lambda\phi^4} = \frac{(-2)^n}{Z(\sigma, \lambda)} \frac{\partial^n}{\partial\sigma^n} Z(\sigma, \lambda) \tag{6.6}$$

where all odd correlators vanish as $S(\phi)$ is even in ϕ. On Lefschetz thimbles, all these integrals are convergent, so that $n > 2$ shall not pose any problem in this approach. In order to compute the decomposition

$$Z = \mathfrak{n}_0 \int\limits_{\mathcal{J}_0} \mathrm{d}\phi \, e^{-S(\phi)} + \mathfrak{n}_1 \int\limits_{\mathcal{J}_1} \mathrm{d}\phi \, e^{-S(\phi)} + \mathfrak{n}_2 \int\limits_{\mathcal{J}_2} \mathrm{d}\phi \, e^{-S(\phi)} \tag{6.7}$$

we have to start at each critical point, make an infinitesimal displacement along the stable direction and then start to integrate the SA equations for a sufficiently long time so that integrals converge. Notice that, in one dimension, to get the whole thimble $\mathcal{J}_\sigma$ attached to a critical point p_σ, one has to consider the two possible directions at p_σ given by $\pm v_\sigma^{(+)}$ where $v_\sigma^{(+)}$ is the stable eigenvector of $H(S_R; p_\sigma)$. In the notation of Section 5.3 this corresponds to $n = \pm\sqrt{\mathcal{R}}$ (as long as one is aware of this double possible choice of sign, there is no need for the $(\hat{n}, t)$ notation in one dimension, being the thimble simply parametrized by the SA flow time t). In Figure 6.2 all the stable and unstable thimbles are plotted for both positive and negative σ_R. In Figure 6.2a (referring to $\sigma_R > 0$), we see that the unstable thimbles $\mathcal{K}_\pm$ attached to the Higgs vacua $\phi_\pm$ do not intersect the original domain of integration (the real axis), so that $\mathfrak{n}_+ = \mathfrak{n}_- = 0$. In this region of the complex σ-plane, only $\mathcal{J}_0$ is relevant for the decomposition (6.7). Correct results are indeed obtained for $\mathfrak{n} = (\mathfrak{n}_0, \mathfrak{n}_+, \mathfrak{n}_-) = (1, 0, 0)$. The case $\sigma_R < 0$, illustrated in Figure 6.2b, is quite different. When going from $\sigma_R \sim 0^+$ to $\sigma_R \sim 0^-$, the thimble $\mathcal{J}_0$ undergoes a radical change of shape, so that integrals along $\mathcal{J}_0$ feature a sudden jump. In order to keep the integrals (such as (6.1) or (6.6)) *continuous* in σ, the jump in $\int_{\mathcal{J}_0}$ must be compensated by a jump in the coefficients $\{\mathfrak{n}_\sigma\}$. In fact, correct results at $\sigma_R < 0$ are recovered by taking $\mathfrak{n} = (-1, 1, 1)$.[40] Actually, it is not surprising that $\mathfrak{n}_\pm \neq 0$ for $\sigma_R < 0$: in Figure 6.2b we see that the unstable thimbles $\mathcal{K}_\pm$ do intersect the real axis, thus indicating a contribution to (6.7) from $\mathcal{J}_\pm$. This is a manifestation of the aforementioned Stokes phenomenon. In this case the Stokes curve in the complex σ-plane is the imaginary axis. In Figure 6.1 we see the structure of the thimbles at purely imaginary σ. The thimble $\mathcal{J}_0$ is ill-defined, in the sense that, by integrating the SA equation starting close to ϕ_0, one flows into $\phi_\pm$ at $t \to +\infty$. The two green segments forming $\mathcal{J}_0$ coincide with half of the unstable thimbles attached

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[40]The actual sign of each $\mathfrak{n}_\sigma$ depends on the choice of orientation for $\mathcal{J}_\sigma$.

to the Higgs vacua, that is $\mathcal{K}_+$ and $\mathcal{K}_-$. When such phenomenon occurs, the decomposition in (6.7) does not hold, as $\mathcal{J}_0$ does not connect regions of convergence at infinity.[41] As already mentioned, this is not a problem, as the coefficients $\mathfrak{n}_\sigma$ for $\sigma_R \to 0^-$ can be figured out by imposing continuity in, say Z or $\langle \phi^n \rangle$ while knowing the $\mathfrak{n}_\sigma$ for $\sigma_R \to 0^+$. The zero-dimensional ϕ^4 model was used as a benchmark for different algorithms devised to do importance sampling on Lefschetz thimbles [85]. In particular, successful results were obtained by using the Metropolis-like algorithm introduced in [67], which proved to be of great use even in the case where more than one thimble were relevant, showing no sign of instabilities in the computation of high-order momenta.
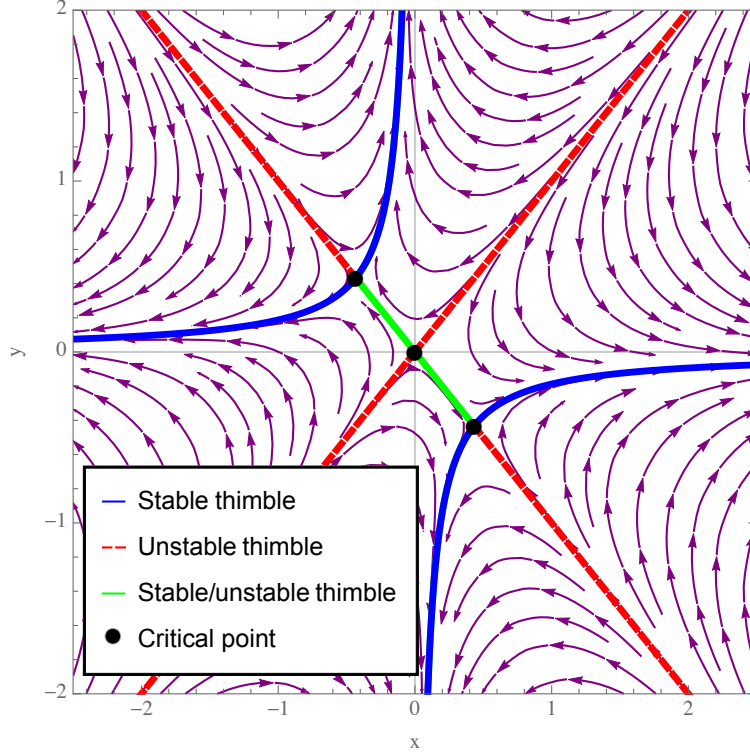
Figure 6.1: The figure shows the Stokes phenomenon appearing in the zero-dimensional ϕ^4 model at $\sigma = 0.75\,i$ and $\lambda = 2$. Stable and unstable thimbles associated to the three critical points are plotted. The ill-defined thimble $\mathcal{J}_0$ is depicted in green.

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[41]To be more precise, thimbles do not necessarily connect regions in which the fields tend to infinity. In order to ensure convergence of the integrals, the thimble has to connect regions in which $S_R \to +\infty$ (in the present case, this fails precisely at $\sigma_R = 0$, as $\mathcal{J}_0$ flows into $\phi_\pm$, where S_R is finite). In fermionic systems [40, 62, 37, 86] there are thimbles connecting configurations which are finite (in field space), but on which S_R is infinite.
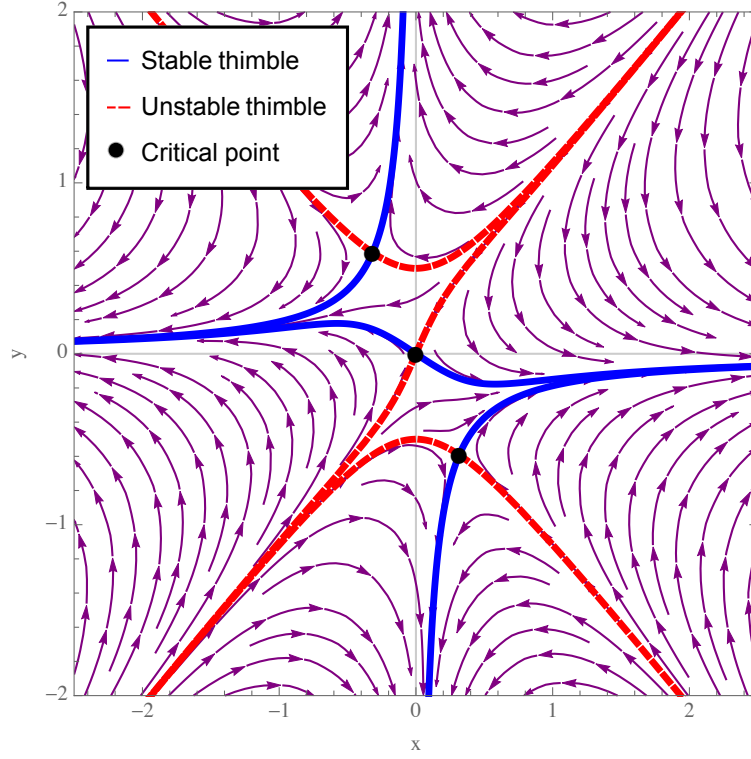
(a) Stable and unstable thimbles for $\sigma = 0.5 + 0.75\,i$ and $\lambda = 2$.
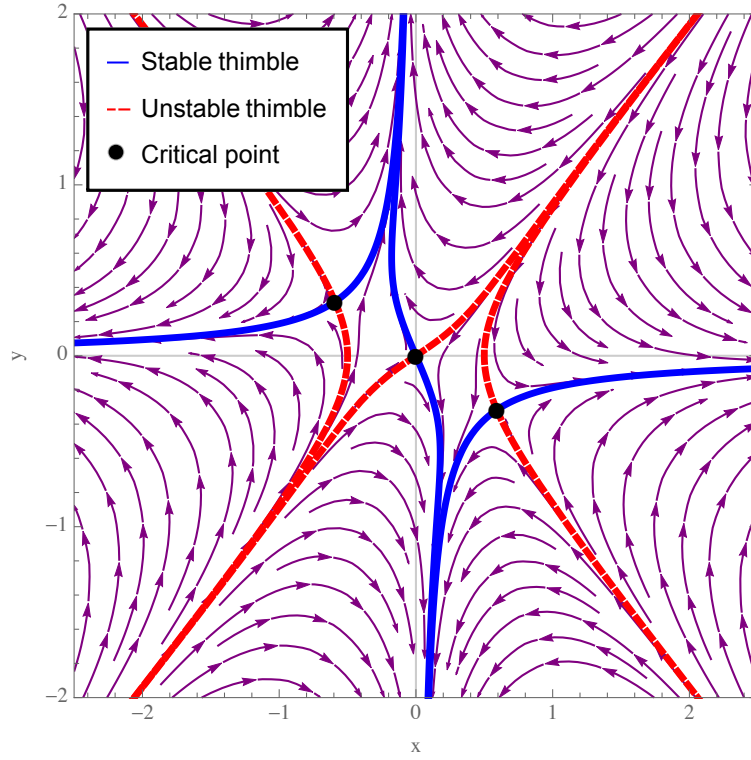
(b) Stable and unstable thimbles for $\sigma = -0.5 + 0.75\,i$ and $\lambda = 2$.

Figure 6.2: In the two figures, stable (in blue, solid lines) as well and unstable (in red, dashed lines) thimbles associated to ϕ_0 and $\phi_\pm$ are plotted. The vector field is $\nabla S_R(x, y)$, making it clear that thimbles single out directions of steepest ascent/descent. The first picture is taken at $\sigma_R > 0$, while the second depicts the case $\sigma_R < 0$.

7 Chiral Random Matrix theory

In this section we put all the machinery introduced in Section 5 at work for a multi-dimensional model. In particular, we study a *Chiral Random Matrix* (CRM) model. This model was first introduced thanks to the many features it has in common with QCD [87, 88, 89]: they have the same flavour symmetries and explicit symmetry breaking and they share the presence of the determinant of a Dirac operator (which is the source of a sign problem for both theories). In the *microscopic limit* (which we shall describe more in detail later) both theories are related to *chiral perturbation theory* at leading order in the ε domain as a low-energy theory. This made it possible to gain some insights into QCD by studying the matrix model, which is treatable analytically. In this work we shall not go into detail studying the physics of the CRM model; instead, we shall tackle it with the thimble formalism and treat it as a valuable setting to test the approach in a case which is much more involved than zero-dimensional models. Our interest in this particular model lies in the fact that complex Langevin was used to tackle its sign problem [90, 91], giving correct results in a particular formulation [91], while converging to wrong results in another [90]. We shall consider the original formulation of the model, which was a failure for complex Langevin and use the same notation as [90].

7.1 General setup

The partition function for the CRM model for N_f quark flavours of degenerate mass m is

$$Z_N = \int \mathrm{d}\Phi \mathrm{d}\Psi \, e^{-N \operatorname{Tr}\left(\Phi^\dagger \Phi + \Psi^\dagger \Psi\right)} \det^{N_f} \left(D(\mu) + m\right)$$

The degrees of freedom of the model are the two $N \times N$ *complex* matrices $\Phi = a + i\,b$ and $\Psi = \alpha + i\,\beta$, so that the total number of degrees of freedom is $n = 4N^2$. The integration measure is $\mathrm{d}\Phi \mathrm{d}\Psi = \mathrm{d}a \, \mathrm{d}b \, \mathrm{d}\alpha \, \mathrm{d}\beta$. The chemical potential enters the Dirac operator

$$D(\mu) + m = \begin{pmatrix} m & i \, \cosh \mu \, \Phi + \sinh \mu \, \Psi \\ i \, \cosh \mu \, \Phi^\dagger + \sinh \mu \, \Psi^\dagger & m \end{pmatrix} \tag{7.1}$$

The aforementioned microscopic limit consists in taking $N \to \infty$ while keeping $\tilde{m} = Nm$ and $\tilde{\mu} = \sqrt{N}\mu$ constant. In the present work we shall keep $\tilde{\mu} = 2$ fixed and $N_f = 2$ fixed as well (to be consistent with [90]), while studying the behaviour of the *chiral condensate* $\Sigma \equiv \frac{1}{N}\langle \bar{\eta}\eta \rangle = \frac{1}{N}\frac{\partial}{\partial m}\log Z$ at different values of $\tilde{m}$. We will also consider increasing values of N starting from $N = 1$. The sign problem comes from the chemical potential in (7.1) and can be a severe one, especially at lower values of $\tilde{m}$. To see this, we define a *phase-quenched* partition function

$$Z_N^{\mathrm{pq}} = \int \mathrm{d}\Phi \mathrm{d}\Psi \, e^{-N \operatorname{Tr}\left(\Phi^\dagger \Phi + \Psi^\dagger \Psi\right)} \left| \det^{N_f} \left(D(\mu) + m\right) \right|$$

from which we can compute a phase-quenched chiral condensate. We recall the analytical form of the expectation value of the chiral condensate in the full theory and in the phase-quenched one [89, 92], that is, being $x \equiv -Nm^2$,

$$\Sigma = 2m \, \frac{L_N^0(x)L_{N-1}^2(x) - L_{N+1}^0(x)L_{N-2}^2(x)}{L_N^0(x)L_N^1(x) - L_{N+1}^0(x)L_{N-1}^1(x)}$$

$$\Sigma^{\mathrm{pq}} = 4m \, \frac{\sum\limits_{k=0}^{N} \left(\cosh(2\mu)\right)^{-2k} L_k^0(x)L_{k-1}^1(x)}{\sum\limits_{k=0}^{N} \left(\cosh(2\mu)\right)^{-2k} \left(L_k^0(x)\right)^2}$$

where $L_i^j(x)$ are generalized Laguerre polynomials.[42] The chiral condensate is real: in all subsequent plots, we will show only the real part of the condensate, having verified the imaginary part to be zero within errors. By comparing phase-quenched results with exact ones (Figure 7.1), we can see in which region of parameter space the phase of the determinant of the Dirac operator plays a crucial role: at low (rescaled) masses, the sign problem is expected to be harder. This is indeed the case and complex Langevin happened to converge to incorrect results in this region [90].
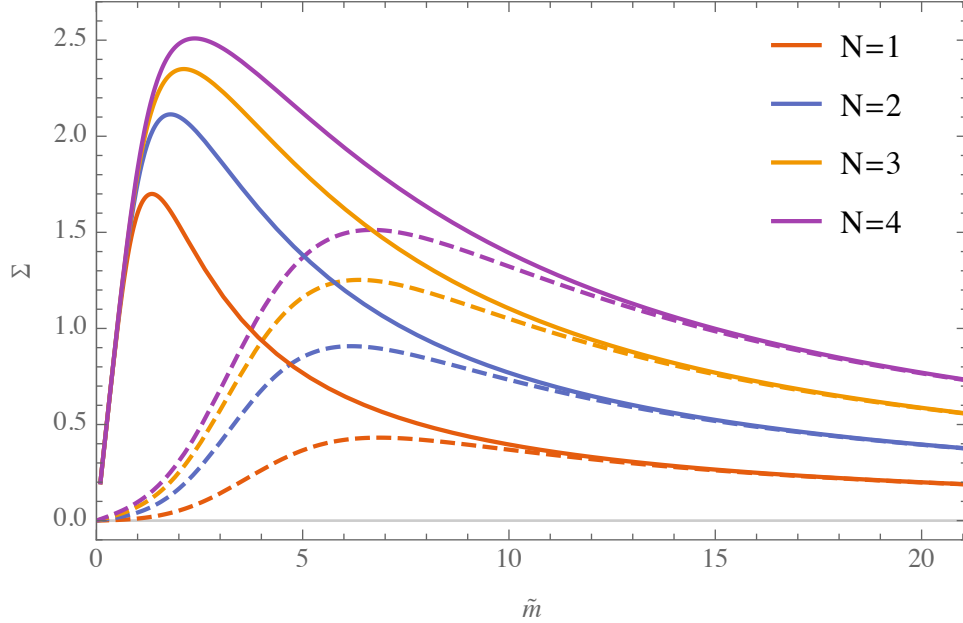
Figure 7.1: The chiral condensate for the full theory is depicted in solid lines for different values of N as a function of $\tilde{m}$. The chiral condensate for the phase-quenched theory is depicted in dashed lines. We can see that, at low masses, the two become more and more apart, which comes with a stronger sign problem.

We now complexify the entries of the 4 matrix fields a, b, α, β and put the determinant of the Dirac operator in the *effective* action[43] (using $\log \det A = \text{Tr} \log A$)

$$S(a, b, \alpha, \beta) = N \sum_{i=1}^{N} \sum_{j=1}^{N} \left(a_{ij}^2 + b_{ij}^2 + \alpha_{ij}^2 + \beta_{ij}^2 \right) - N_f \text{Tr} \log \left(m^2 \, \mathbb{1}_{N \times N} - XY \right) \tag{7.2}$$

with the (complex) $N \times N$ matrices X and Y defined by

$$X_{ij} \equiv i \cosh \mu \left(a_{ij} + i b_{ij} \right) + \sinh \mu \left(\alpha_{ij} + i \beta_{ij} \right)$$

$$Y_{ij} \equiv i \cosh \mu \left(a_{ji} - i b_{ji} \right) + \sinh \mu \left(\alpha_{ji} - i \beta_{ji} \right)$$

After defining the inverse of the Dirac operator

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[42] It is understood that $L_i^j(x) \equiv 0$ when $i < 0$.

[43] In [90] it was argued that the origin of problems with complex Langevin simulations of the model could lie in $\det \left(m^2 \, \mathbb{1}_{N \times N} - XY \right)$, whose logarithm appears in the effective action (7.2), crossing the negative real axis (for further discussions about complex Langevin with logarithms in the action, refer to [93, 94]). In the thimble approach, this cannot happen for the following reason: integration of SA equation gives a *smooth* flow along which $S_I = \Im(S)$ is conserved. If the argument of the logarithm crossed the negative real axis, then there would be a *discontinuous* jump of magnitude $2\pi N_f$ in S_I. In order for the flow to keep S_I constant, this jump would have to be compensated for by an opposite jump in the Gaussian (quadratic) part of the action; but the Gaussian part of the action is a smooth polynomial in the fields, which are *continuous* functions of the flow time and thus cannot have jumps. As expected, none of this jumps were found in our thimble simulations of the CRM model.

$$G \equiv \left(m^2 \, \mathbb{1}_{N \times N} - XY \right)^{-1}$$

we see that the chiral condensate can be computed by

$$\Sigma = \frac{1}{N} \frac{\partial}{\partial m} \log Z = \frac{1}{N} \frac{1}{Z} \frac{\partial}{\partial m} \int \mathrm{d}a \, \mathrm{d}b \, \mathrm{d}\alpha \, \mathrm{d}\beta \, e^{-S(a,b,\alpha,\beta)}$$

$$= \frac{N_f}{N} \frac{1}{Z} \int \mathrm{d}a \, \mathrm{d}b \, \mathrm{d}\alpha \, \mathrm{d}\beta \left[\frac{\partial}{\partial m} \mathrm{Tr} \, \log \left(m^2 \, \mathbb{1}_{N \times N} - XY \right) \right] e^{-S(a,b,\alpha,\beta)}$$

$$= \frac{N_f}{N} \frac{1}{Z} \int \mathrm{d}a \, \mathrm{d}b \, \mathrm{d}\alpha \, \mathrm{d}\beta \, \mathrm{Tr} \left[\left(m^2 \, \mathbb{1}_{N \times N} - XY \right)^{-1} 2m \right] e^{-S(a,b,\alpha,\beta)} = \frac{2mN_f}{N} \langle \mathrm{Tr} \, G \rangle$$

Keeping in mind the complexification of a, b, α, β, we compute the drifts, whose conjugates we need in order to integrate SA equations

$$\frac{\partial S}{\partial a_{mn}} = 2N a_{mn} + i N_f \cosh \mu \left(R_{mn} + T_{mn} \right)$$

$$\frac{\partial S}{\partial b_{mn}} = 2N b_{mn} - N_f \cosh \mu \left(R_{mn} - T_{mn} \right)$$

(7.3)

$$\frac{\partial S}{\partial \alpha_{mn}} = 2N \alpha_{mn} + N_f \sinh \mu \left(R_{mn} + T_{mn} \right)$$

$$\frac{\partial S}{\partial \beta_{mn}} = 2N \beta_{mn} + i N_f \sinh \mu \left(R_{mn} - T_{mn} \right)$$

where

$$R_{mn} \equiv \sum_{k=1}^{N} G_{km} Y_{nk}$$

$$T_{mn} \equiv \sum_{k=1}^{N} G_{mk} X_{kn}$$

From these equations, we immediately see that the *classical vacuum* $a = b = \alpha = \beta = 0$ is a critical point, being all the derivatives zero. Thus we shall consider the thimble associated to it, which we label $\mathcal{J}_0$[44] and perform integration over it. One question now arises: is there any other (non-trivial) critical point which is relevant for the thimble decomposition? In particular, we are interested in the "thermodynamic" limit $N \to \infty$: does $\mathcal{J}_0$ become the only relevant thimble in this limit? These issues will be discussed later on. The formulas for the Hessian are quite lengthy: they can be found in Appendix C. Here we just recall one remarkable result of the computation of the Hessian at the classical vacuum. The Hessian features only two different Takagi values (λ_+ and λ_-), so that $T_0 \mathcal{J}_0$ consists of two $2N^2$-dimensional subspaces with complete Takagi value degeneracy. Moreover, at large (rescaled) quark masses $\tilde{m}$, the two Takagi values become less and less apart, so that in the large-mass limit, not only the theory becomes Gaussian (which can be seen from (7.2) by direct inspection), but it also becomes completely isotropic (see Figure 7.2). This is expected to make simulations at high $\tilde{m}$ quite easy. This, as we shall see, is indeed recovered in the simulations.

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[44] $\mathcal{J}_0$, as expected, is a manifold of *real* dimension $4N^2$ which can be thought as embedded in $\mathbb{R}^{8N^2}$.
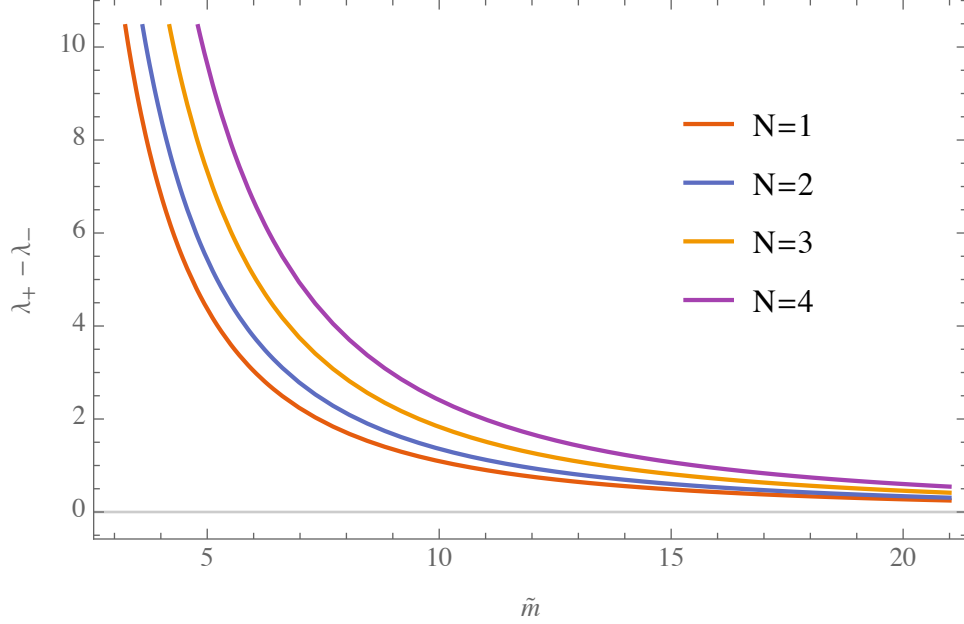
Figure 7.2: The picture shows how $\lambda_+ - \lambda_-$ changes as a function of $\tilde{m}$ for various values of N. We see that the two Takagi values become closer at large masses. Thus we expect numerical simulations to be quite easy in this region.

7.2 Numerical results

In Figure 7.3 we show the results of our numerical simulations of the CRM model (we computed the expectation value of the chiral condensate - see formula (5.5)). We have integrated only on $\mathcal{J}_0$ and employed the static, crude Monte Carlo method described in Section 5.3. Actually, the static, crude Monte Carlo proved to be pretty inefficient for this model, especially in the low mass region at high N. As mentioned before, in this region, the Takagi values of the Hessian at the critical point get more and more apart from each other, so that tiny differences in the choice of $\hat{n}$ may lead to $Z_{\hat{n}}$ varying by orders of magnitude. For this reason, the error bars are bigger in the low mass region, especially at high N, where the algorithm has to sample a larger space. Furthermore, in the low mass region, we have that the action departs more and more from its Gaussian counterpart[45], so that the curvature of the thimble becomes more relevant. In Figure 7.4 we plot the *residual-phase-quenched* results from the same simulations, that is we have neglected $e^{i\omega}$ in (5.5). It is clear that in those regions in which the curvature of the thimble is greater, the residual phase must be taken into account to recover correct results; this is more evident at lower values of N. The residual phase, though not negligible, could well be taken into account by reweighting and posed no residual sign problem at all. We also applied to the CRM model the HBB Metropolis algorithm discussed in Section 5.3. This was successful and correct results could be achieved with far less statistics (and smaller error bars) than using the static, crude Monte Carlo. It also made it possible to compute Σ at some masses which had been unfeasible with the static, crude Monte Carlo [78]. See Figure 7.5 and Table 7.1 for a comparison of results between the two algorithmic solutions. Remarkably, we were able to get correct results by integrating only on $\mathcal{J}_0$, even at low values of N. As we shall see in Section 7.3, this could have been predicted thanks to the structure of critical points for this model.

7.3 Other critical points

As already stated, correct results have been obtained (in the region of parameter space that was examined) by integrating only over $\mathcal{J}_0$, even at small N. This result is somehow surprising, therefore we return to the issue of the existence of other critical points. We initially searched for other critical points numerically [73]: the critical point condition $\nabla S = 0$ was solved via the Newton-Raphson method, checking the results against

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[45]This can be readily seen in (7.2) by noting that, at high $m^2 = (\tilde{m}/N)^2$, the logarithm approaches a constant.
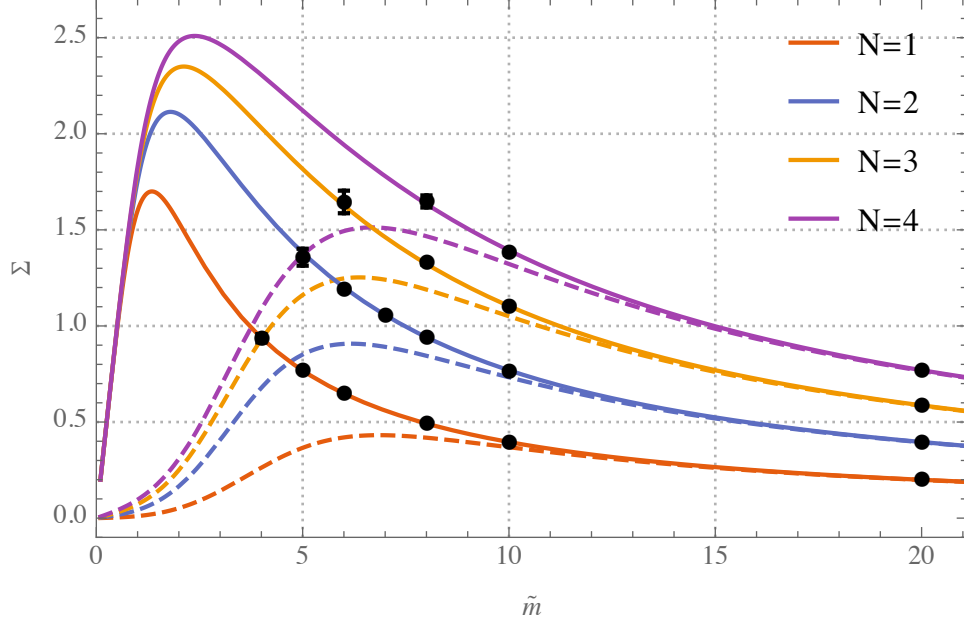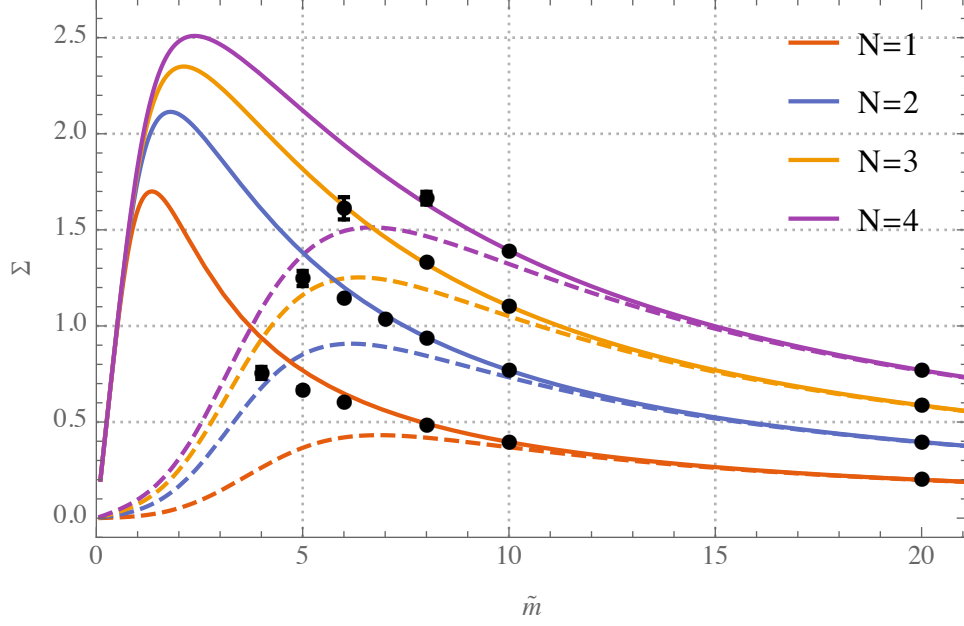
Figure 7.3: We show the results of our numerical simulations of the CRM model on $\mathcal{J}_0$ with the static, crude Monte Carlo. Solid lines depict exact results, while dashed lines depict phase-quenched results. The black points represent numerical results. Larger error bars are encountered in the low mass region, especially at larger N.

a minimization of $\|\nabla S\|^2$ with the Nelder-Mead symplex method. A few classes of critical points p_σ were found (all outside the original domain of integration, which is $a, b, \alpha, \beta \in \mathbb{R}^{N \times N}$), but all of them had $S_R(p_\sigma)$ less than its absolute minimum on the original domain of integration; so, by the argument in Section 3.4, they are irrelevant in the thimble decomposition. Actually, much insight can be gained analytically about other critical points, and this is precisely the aim of this section. Recall that critical points are configurations on which every component of the drift is zero, that is all the derivatives appearing in (7.3) are 0. In matrix form, this reads

$$
\begin{aligned}
-2Na &= +iN_f \cosh \mu (R + T) \\
-2Nb &= -N_f \cosh \mu (R - T) \\
-2N\alpha &= N_f \sinh \mu (R + T) \\
-2N\beta &= iN_f \sinh \mu (R - T)
\end{aligned}
\tag{7.4}
$$

By combining the first equation with the third and the second with the fourth, we get

$$
\begin{aligned}
\alpha &= -i \tanh \mu \, a \\
\beta &= -i \tanh \mu \, b
\end{aligned}
\tag{7.5}
$$

These are relations that have to be satisfied by *any* critical point. By employing (7.5), we can reduce the action to an expression which is dependent only on a and b. To do this, we compute

Figure 7.4: We show the residual-phase-quenched results of our numerical simulations of the CRM model on $\mathcal{J}_0$ with the static, crude Monte Carlo. Solid lines depict exact results, while dashed lines depict phase-quenched results. The black points represent numerical results obtained by completely neglecting the residual phase. The results which are more departing from the exact ones are those at low masses and low values of N.

$$X = i \cosh \mu (a + ib) + \sinh \mu (\alpha + i\beta) = i(\cosh \mu - \sinh \mu \tanh \mu)(a + ib) = \frac{i}{\cosh \mu}(a + ib)$$

$$Y = i \cosh \mu (a - ib)^T + \sinh \mu (\alpha - i\beta)^T = i(\cosh \mu - \sinh \mu \tanh \mu)(a - ib)^T = \frac{i}{\cosh \mu}(a - ib)^T$$

so that

$$G^{-1} = m^2 \mathbb{1} - XY = m^2 \mathbb{1} + \frac{1}{\cosh^2 \mu} M$$

having defined $M \equiv (a + ib)(a - ib)^{T}$.[46] Consider now the Gaussian part of the action: for the trace part, we have

$$a_{ij}^2 + b_{ij}^2 + \alpha_{ij}^2 + \beta_{ij}^2 = a_{ij}^2 + b_{ij}^2 - \tanh^2 \mu \, a_{ij}^2 - \tanh^2 \mu \, b_{ij}^2 = \left(1 - \tanh^2 \mu\right) \left(a_{ij}^2 + b_{ij}^2\right)$$

from which it follows

$$\sum_{i=1}^{N} \sum_{j=1}^{N} \left(a_{ij}^2 + b_{ij}^2 + \alpha_{ij}^2 + \beta_{ij}^2\right) = \frac{1}{\cosh^2 \mu} \operatorname{Tr} M$$

Thus the action (7.2) at a critical point becomes

---

[46]It is important to realize that $M \neq M^{\dagger}$ for *complex* a and b.

N	$\tilde{m}$	Σ_{exact}	$\langle\Sigma\rangle_{\text{static MC}}$	$\langle\Sigma\rangle_{\text{HBB Metropolis}}$	# of $\hat{n}$ (static)	# of $\hat{n}$ (Metropolis)
4	7	1.7794	-	1.7918(97)	-	216720
4	8	1.6340	1.6480(310)	1.6266(72)	122567	99969
2	5	1.3817	1.3580(440)	1.3870(82)	792360	336726
				1.4020(130)		277596
1	4	0.9379	0.9359(220)	0.9360(280)	285930	67787

Table 7.1: Comparison of simulation results for the chiral condensate: data from the static, crude Monte Carlo and from the HBB Metropolis algorithm. The number of $\hat{n}$ in the Markov chain (that is the number of SA curves that have been integrated) is also displayed. Static, crude Monte Carlo data for $N = 4$, $\tilde{m} = 7$ was not stable enough to provide a definite result. The second line at $N = 2$, $\tilde{m} = 5$ refers to the Metropolis algorithm discussed at the end of Section 5.3.

$$S_0(a,b) = \frac{N}{\cosh^2\mu}\operatorname{Tr} M - N_f \log\det\left(m^2\,\mathbb{1} + \frac{1}{\cosh^2\mu}M\right) = N\operatorname{Tr}\left(G^{-1}\right) - N_f\log\det\left(G^{-1}\right) - N^2 m^2 \quad (7.6)$$

We immediately notice that the value of the action at any critical point is determined only by the spectrum of G (or, equivalently, the spectrum of M). Thus a classification of critical points boils down to the classification of the eigenvalues of M (or of G). We use the first two equations in (7.4) to get

$$a + ib = -i\frac{N_f}{N}\cosh\mu\, T$$

$$a - ib = -i\frac{N_f}{N}\cosh\mu\, R$$

and we also have

$$T = GX = \frac{i}{\cosh\mu}G(a+ib)$$

$$R = (YG)^T = \frac{i}{\cosh\mu}\left((a-ib)^T G\right)^T = \frac{i}{\cosh\mu}G^T(a-ib)$$

which leads to

$$a + ib = \frac{N_f}{N}G(a+ib)$$
$$\qquad\qquad\qquad\qquad\qquad\qquad (7.7)$$
$$a - ib = \frac{N_f}{N}G^T(a-ib)$$

By multiplying the first with the transpose of the second, we get

(a) $N = 4$, $\tilde{m} = 7$. (b) $N = 4$, $\tilde{m} = 8$. (c) $N = 2$, $\tilde{m} = 5$. (d) $N = 1$, $\tilde{m} = 4$.
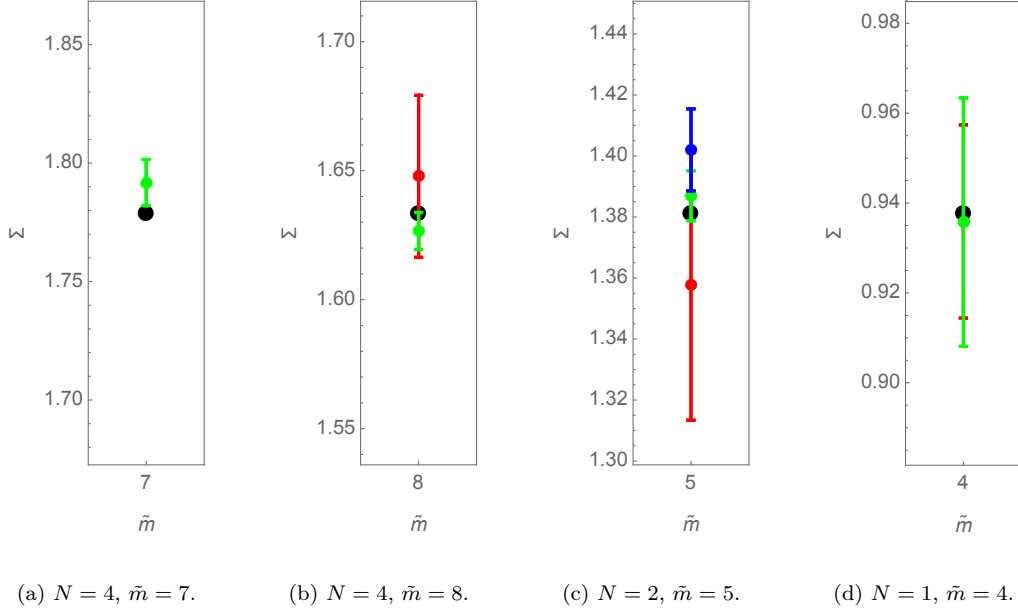
Figure 7.5: We compare results for the CRM model using the static, crude Monte Carlo and the HBB Metropolis algorithm of Section 5.3. Black dots represent analytical results for the chiral condensate. Red bars depict estimates obtained with the static, crude Monte Carlo (same data of Figure 7.3). Green bars represent results of the HBB Metropolis algorithm. The blue bar at $N = 2$, $\tilde{m} = 5$ depicts an estimate obtained using the Metropolis algorithm discussed at the very end of Section 5.3 (with $\varepsilon = 0.15$).

$$M = \left(\frac{N_f}{N}\right)^2 GMG$$

$$\Rightarrow G^{-1}MG^{-1} = \left(\frac{N_f}{N}\right)^2 M$$

$$\Rightarrow \left(m^2 \mathbb{1} + \frac{1}{\cosh^2 \mu} M\right) M \left(m^2 \mathbb{1} + \frac{1}{\cosh^2 \mu} M\right) = \left(\frac{N_f}{N}\right)^2 M$$

$$\Rightarrow m^4 M + \frac{2m^2}{\cosh^2 \mu} M^2 + \frac{1}{\cosh^4 \mu} M^3 - \left(\frac{N_f}{N}\right)^2 M = 0$$

$$\Rightarrow M \left[M^2 + 2m^2 \cosh^2 \mu \, M + \cosh^4 \mu \left(m^4 - \left(\frac{N_f}{N}\right)^2\right)\right] = 0$$

It is known from linear algebra [95] that any polynomial $P(M)$ such that $P(M) = 0$ must be a (polynomial) multiple of μ_M, the *minimal polynomial* of M, whose zeros are the eigenvalues of M. As a consequence, the eigenvalues of M we seek are solutions to

$$\lambda \left[\lambda^2 + 2m^2 \cosh^2 \mu \, \lambda + \cosh^4 \mu \left(m^4 - \left(\frac{N_f}{N}\right)^2\right)\right] = 0$$

which gives either $\lambda = 0$ or $\lambda = \cosh^2 \mu \left(\frac{N_f}{N} - m^2\right)$. Equivalently, for G^{-1}, we have either $\lambda = m^2$ or

$\lambda = \frac{N_f}{N}$. [47] We can consider two possible scenarios, depending on the determinant of M: if $\det M \neq 0$, then $\det(a + ib) \neq 0$ and $\det(a - ib) \neq 0$ as well, so that we can multiply each equation in (7.7) by the inverse of the first member, which gives

$$G = \frac{N}{N_f} \mathbb{1} \qquad \Leftrightarrow \qquad M = \cosh^2 \mu \left(\frac{N_f}{N} - m^2 \right) \mathbb{1}$$

So that this critical point is actually a *manifold* defined by

$$(a + ib)(a - ib)^T = \cosh^2 \mu \left(\frac{N_f}{N} - m^2 \right) \mathbb{1}$$

with action (using (7.6))

$$S_0 = N N_f \left[1 - \log \left(\frac{N_f}{N} \right) \right] - N^2 m^2$$

However, this does not cover the whole set of possible critical points. If $\det M = 0$, we can label the critical points by the degeneracy r of the zero eigenvalue of M. Let us set $r = N - \text{rank}(M)$, then the characteristic polynomial $\chi_{G^{-1}}$ of G^{-1} is

$$\chi_{G^{-1}}(\lambda) = \left(\lambda - m^2 \right)^r \left(\lambda - \frac{N_f}{N} \right)^{N-r}$$

so that $\text{Tr}(G^{-1}) = r m^2 + (N - r)\frac{N_f}{N}$ and $\log \det(G^{-1}) = r \log m^2 + (N - r) \log \left(\frac{N_f}{N} \right)$. By plugging this into (7.6), we get an expression for the action computed at any critical point labelled by r

$$S_0^{(r)} = N \left[r m^2 + (N - r)\frac{N_f}{N} \right] - N_f \left[r \log m^2 + (N - r) \log \left(\frac{N_f}{N} \right) \right] - N^2 m^2$$

$$= (N - r) N_f \left[1 - \log \left(\frac{N_f}{N} \right) \right] + r \left(N m^2 - N_f \log m^2 \right) - N^2 m^2 \tag{7.8}$$

in which we immediately notice that putting $r = 0$ recovers the case $\det M \neq 0$. The action $S_0^{(r)}$ is manifestly real. There are N different classes of critical points, as $r = 0 \cdots N - 1$ (the case $r = N$ corresponds to the classical vacuum, having action $S_0^{(N)} = -N N_f \log m^2$). It is worth noting that all these critical points lie outside of the original domain of integration, consisting of *real* a, b, α, β; this is due to (7.5), which forces *e.g.* α and β to be imaginary if a and b are real. It is easy to check from (7.8) that $S_0^{(r)}$ is lower than any value S_R can assume on the original domain of integration in all the region of parameter space we have explored. Therefore, as already stated, by the argument of Section 3.4, all these critical points are expected not to contribute to the thimble decomposition; so, it does not come as a surprise that correct results could be achieved by integrating only on $\mathcal{J}_0$.

---

[47] We ignore $-\frac{N_f}{N}$, being its logarithm ill-defined.

8 SU(N) one-link models

In Section 4 we have discussed thimble decomposition for gauge theories from a general point of view. Now we consider the simplest examples of "gauge" theories: SU(N) one-link models. These models, although somehow "artificial" and lacking a real (local) gauge symmetry, provide an excellent environment to test thimble integration in the formalism which is suitable for gauge theories. Moreover, as we shall see, these models involve multiple thimbles, all necessary to reconstruct the expected results.

An SU(N) one-link model consists of a single matrix $U \in$ SU(N) in the *fundamental* representation. The sign problem is introduced by hand by means of a *complex* coupling $\beta \in \mathbb{C}$. Thus complexification means taking $U \in$ SL($N, \mathbb{C}$). The action is

$$S(U) = -\frac{\beta}{N} \operatorname{Tr} U$$

and the partition function is[48]

$$Z(\beta) = \int\limits_{\mathrm{SU}(N)} \mathrm{d}U \, e^{\frac{\beta}{N}\operatorname{Tr} U} = \sum_{n=0}^{\infty} \frac{2! \cdots (N-1)!}{n! \cdots (n+N-1)!} \left(\frac{\beta}{N}\right)^{Nn}$$

As an observable, we take $\operatorname{Tr} U$, that is

$$\langle \operatorname{Tr} U \rangle = \frac{1}{Z} \int\limits_{\mathrm{SU}(N)} \mathrm{d}U \, \operatorname{Tr} U \, e^{\frac{\beta}{N}\operatorname{Tr} U} = N \frac{\partial}{\partial \beta} \ln Z(\beta)$$

In order to write SA equations, we need the gradient, that is

$$\nabla^a S(U) = -\frac{i\beta}{N} \operatorname{Tr}\left(T^a U\right)$$

while, for PT equations, we need the Hessian

$$\nabla^b \nabla^a S(U) = \frac{\beta}{N} \operatorname{Tr}\left(T^b T^a U\right)$$

In general, for SU(N), there are N critical points $\{U_k\}_{k=0 \cdots N-1}$, given by $U_k = e^{2\pi i k/N} \mathbb{1}$, that is all the elements of $Z(N)$, the center of SU(N). As all these critical points belong to SU(N) (the original domain of integration), we expect that $\mathfrak{n}_k \neq 0$ for all k. For the hessian at the critical points, after expressing $\beta = |\beta| e^{i\varphi}$, we have

$$\nabla^a \nabla^b S(U)\big|_{U_k} = \frac{|\beta|}{2N} e^{i(\varphi + 2\pi k/N)} \delta^{ab}$$

which follows from the choice of normalization $\operatorname{Tr}(T^a T^b) = \frac{1}{2}\delta^{ab}$ for the generators of $\mathfrak{su}(N)$ in the fundamental representation. We immediately see that the $N^2 - 1$ Takagi values are all equal and $\lambda = \frac{|\beta|}{2N}$ for each critical point. The corresponding Takagi vectors at U_k are $v_j^{(i)} = e^{-i(\varphi + 2\pi k/N)/2} \delta_{ij}$. It is immediate to check that such vectors satisfy Takagi's factorization theorem

$$v_a^{(i)} \nabla^a \nabla^b S(U)\big|_{U_k} v_b^{(j)} = \lambda \, \delta^{ij}$$

and are orthonormal.

---

[48] For a thorough analytical computation of $Z(\beta)$ at generic N, see [96] and references therein.

8.1 SU(2)

As a first example of one-link model[49] we will consider the case $N = 2$. Analytical computation of the partition function yields

$$Z(\beta) = \frac{2I_1(\beta)}{\beta}$$

where I_1 is the modified Bessel function of the first kind and the observable

$$\langle \mathrm{Tr}\, U \rangle = 2 \left(\frac{I_1'(\beta)}{I_1(\beta)} - \frac{1}{\beta} \right)$$

The are two critical points: $U = \mathbb{1}$ and $U = -\mathbb{1}$. This model can be reformulated in terms of the only eigenvalue of U, that is $e^{i\phi}$ (with ϕ that gets complexified in taking $\mathfrak{su}(2) \to \mathfrak{sl}(2, \mathbb{C})$); then the action becomes $S(\phi) = -\beta \cos \phi$ and the model effectively becomes one-dimensional

$$Z(\beta) = \int\limits_{\mathrm{SU}(2)} \mathrm{d}U\, e^{\frac{\beta}{2}\mathrm{Tr}\, U} = \frac{1}{\pi} \int\limits_{-\pi}^{+\pi} \mathrm{d}\phi\, \sin^2\phi\, e^{\beta \cos \phi}$$

where $\frac{1}{\pi} \sin^2 \phi$ is the (normalized) reduced Haar measure of SU(2). This formulation has been employed in [97]. Because of the effectively one-dimensional nature of the model, it is to be expected that any choice of $\hat{n}$ within the framework of Section 5.1 is irrelevant for the measure of $\langle \mathrm{Tr}\, U \rangle = 2\langle \cos \phi \rangle$ and there is effectively only *one* steepest ascent curve for each critical point. We can see this explicitly in the following way: first note that $\mathrm{Tr}\, U = \mathrm{Tr}(GUG^{-1})$ for any matrix G[50] (in particular, for $G \in \mathrm{SU}(2)$). Then all we have to show is that a different choice $\hat{n}'$ with respect to a reference $\hat{n}$ can be traded for an appropriate gauge transformation G on the initial condition for SA equation integration.[51] Consider an initial condition $U(\hat{n}, t_0)$ at a reference time $t_0 \to -\infty$ in a neighbourhood of U_k and $U(\hat{n}', t_0)$ with $|\hat{n}| = |\hat{n}'| = \sqrt{\mathcal{R}}$. We seek $G = e^{ig_a T^a} \in \mathrm{SU}(2)$ such that

$$G\, U(\hat{n}, t_0)\, G^{-1} = U(\hat{n}', t_0)$$

Using the lemma in Appendix B and the fact that, being $U_k \in Z(2)$, U_k commutes with every element of SU(2), we have

$$e^{ig_a T^a}\, e^{i \sum\limits_{j=1}^{3} n_j e^{\lambda t_0} v_a^{(j)} T^a}\, U_k\, e^{-ig_a T^a} = e^{i \sum\limits_{j=1}^{3} n_j' e^{\lambda t_0} v_a^{(j)} T^a}\, U_k$$

$$\Rightarrow\ e^{ig_a T^a}\, e^{i \sum\limits_{j=1}^{3} n_j e^{\lambda t_0} v_a^{(j)} T^a}\, e^{-ig_a T^a}\, U_k = e^{i \sum\limits_{j=1}^{3} n_j' e^{\lambda t_0} v_a^{(j)} T^a}\, U_k$$

$$\Rightarrow\ e^{i \sum\limits_{j=1}^{3} n_j e^{\lambda t_0} M_{ab} v_b^{(j)} T^a} = e^{i \sum\limits_{j=1}^{3} n_j' e^{\lambda t_0} v_a^{(j)} T^a}$$

$$\Rightarrow\ \sum\limits_{j=1}^{3} n_j' v_a^{(j)} = \sum\limits_{j=1}^{3} n_j \left(M_{ab} v_b^{(j)} \right)$$

---

[49] Actually, the simplest one-link model one can study is the (abelian) U(1) model. We shall not consider this, as its solution by means of thimble integration has already been discussed in [67].

[50] This is the "global gauge symmetry" exhibited by one-link models.

[51] What one should actually show is that all the t-integrals one computes when starting at $U(\hat{n}, t_0)$ are the same as those computed starting from $GU(\hat{n}, t_0)G^{-1}$. While this is manifest for the action, there is also the basis determinant $\det V$. Invariance of this determinant can be easily shown by an argument which is given in Section 10.2 in the more general context of Yang-Mills theory.

which, using $v_a^{(j)} = e^{-i(\varphi + \pi k)/2} \delta_{ja}$, becomes

$$n'_a = M_{ab} n_b = \left(e^{ig_c t^c} \right)_{ab} n_b$$

where $\{t_a\}$ are the generators of $\mathfrak{su}(2)$ in the adjoint representation, which are also generators of $\mathfrak{so}(3)$ in the fundamental representation. The consequence is that M_{ab} is just a rotation in the 3-dimensional n-space, which is norm-preserving. Another way of viewing this is that different choices of $\hat{n} \in S^2_{\mathcal{R}}$ are equivalent to gauge transformations on the field $U(t_0)$. The conclusion is that one *single* SA curve is enough to reconstruct the expectation value $\langle \text{Tr} \, U \rangle$. This is indeed recovered numerically.

8.2 SU(3)

The case of SU(3) is more involved, being effectively multi-dimensional. The partition function is

$$Z(\beta) = 2 \sum_{n=0}^{\infty} \frac{1}{n!(n+1)!(n+2)!} \left(\frac{\beta}{3} \right)^{3n}$$

and the observable

$$\langle \text{Tr} \, U \rangle = \frac{6}{Z} \sum_{n=1}^{\infty} \frac{1}{(n-1)!(n+1)!(n+2)!} \left(\frac{\beta}{3} \right)^{3n-1}$$

The action takes on different values at the critical points (labelled by $k = 0, 1, 2$):

$$S(U_k) = -\frac{\beta}{3} \text{Tr} \, U_k = -\beta e^{2\pi i k/3}$$

and therefore it is to be expected that the relevance of the three thimbles $\{\mathcal{J}_k\}$ is affected by the value of $\beta = |\beta| e^{i\varphi}$. By considering the *semiclassical* decomposition (see formula (5.18))

$$Z \approx Z_0 + Z_1 + Z_2$$

We can give a (semiclassical) estimate for the relative weight of $\mathcal{J}_1$ and $\mathcal{J}_2$ with respect to $\mathcal{J}_0$ in the thimble decomposition. We introduce the quantity r_0^k with k either 1 or 2

$$r_0^k \equiv \frac{|Z_k|}{|Z_0|} = e^{-(S_R(U_k) - S_R(U_0))} = e^{|\beta|(\cos(\varphi + 2\pi k/3) - \cos\varphi)} = e^{-2|\beta| \sin(\pi k/3) \sin(\varphi + \pi k/3)}$$

where the factors $\sqrt{\det \Lambda_k}$ disappear due to λ being the same for all critical points. In Figure 8.1 r_0^k is depicted as a function of φ. We see that, at the semiclassical level, $\mathcal{J}_1$ is almost irrelevant in the range of φ we have studied. This estimate is actually true for the exact theory as well: irrelevance of $\mathcal{J}_1$ is indeed recovered in numerical simulations of the model. Figure 8.1 also predicts $\mathcal{J}_2$ to become more and more important at higher values of φ (eventually, at purely imaginary β, it becomes the dominant thimble). In Figure 8.2 we show numerical results which take into account only $\mathcal{J}_0$ in the decomposition: discrepancies arise at higher values of φ. By taking into account $\mathcal{J}_2$ as well, we recover correct results for any value of $\varphi \in \left[0, \frac{\pi}{2}\right]$ (at fixed $|\beta| = 5$), as showed in Figure 8.3. All the simulations were performed using the static, crude Monte Carlo described in Section 5.3.
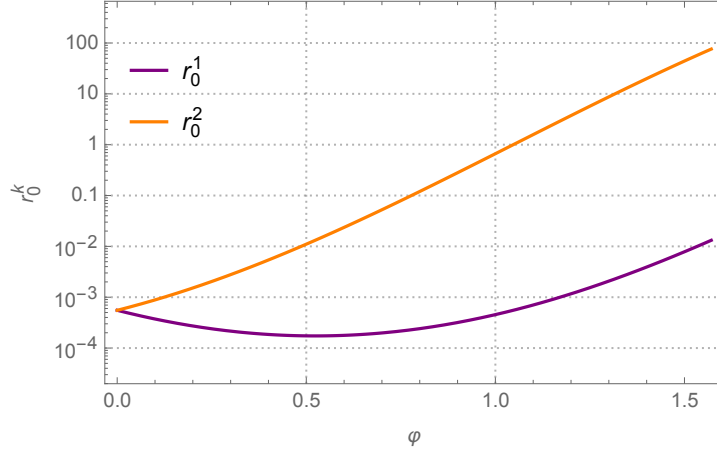
Figure 8.1: Semiclassical estimate for the relative weight of $\mathcal{J}_1$ and $\mathcal{J}_2$ with respect to $\mathcal{J}_0$ as a function of φ at $|\beta| = 5$.
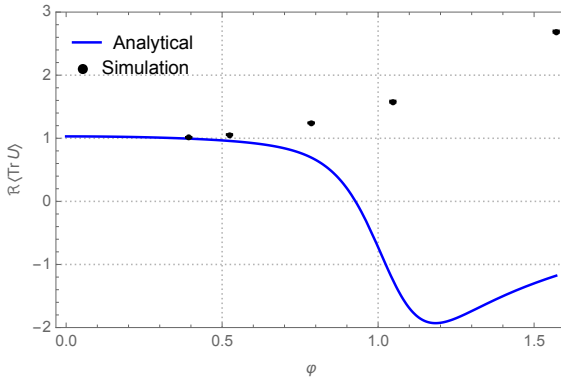
(a) Expectation value of $\operatorname{Tr} U$: real part.
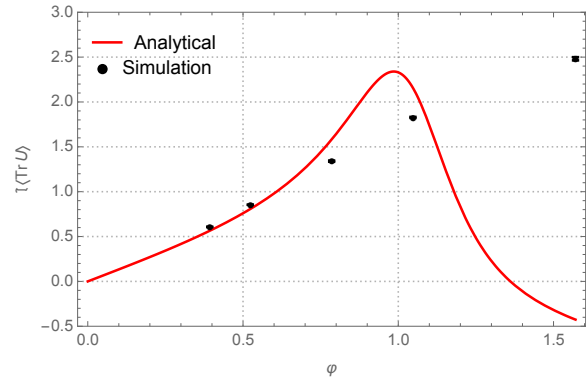
(b) Expectation value of $\operatorname{Tr} U$: imaginary part.

Figure 8.2: Thimble simulations of the one-link SU(3) model at $\beta = 5\,e^{i\varphi}$ integrating only on $\mathcal{J}_0$. Numerical results for $\operatorname{Tr} U$ as a function of φ are displayed.
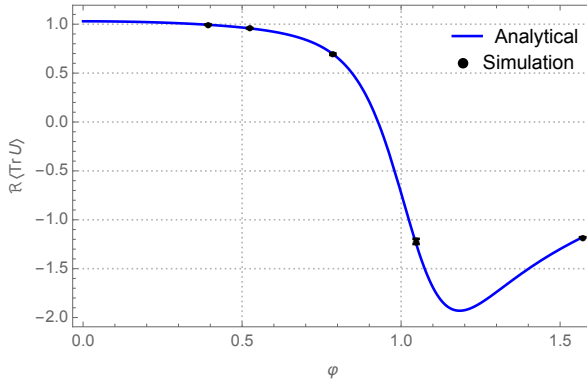
(a) Expectation value of $\operatorname{Tr} U$: real part.
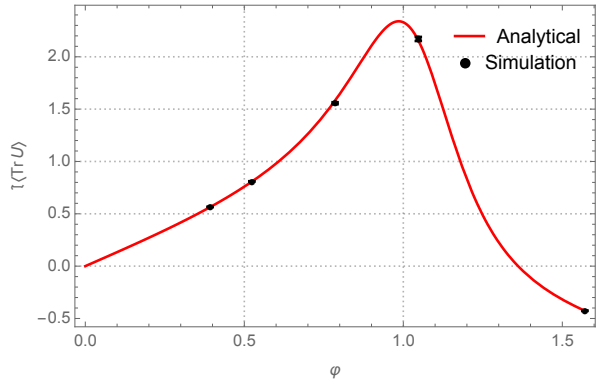
(b) Expectation value of $\operatorname{Tr} U$: imaginary part.

Figure 8.3: Thimble simulations of the one-link SU(3) model at $\beta = 5\,e^{i\varphi}$. Numerical results for $\operatorname{Tr} U$ as a function of φ are displayed.

9 QCD in 0+1 dimensions

In this section we shall study Quantum Chromodynamics on the lattice in $0 + 1$ dimensions. Despite being much simpler than its 4-dimensional counterpart, this model provides an excellent setting to test the thimble formalism in the case of gauge theories. Moreover, the sign problem in QCD is due to the presence of a (quark) chemical potential, which is far more interesting to study than one-link models, in which the sign problem is introduced by hand with a complex coupling. For $0 + 1$ QCD, analytical results are readily available [98, 99, 100, 101]; the sign problem has also been solved by means of the so called *subset method* [101]. We shall now focus on $N_c = 3$ lattice QCD with *staggered* fermions on a one-dimensional lattice with (even) N_t sites in the temporal direction. The lattice extent is related to the temperature by $aN_t = 1/T$, where a is the lattice spacing. The partition function of the theory for N_f degenerate quark flavours of mass m is

$$Z_{N_f} = \int \prod_{i=1}^{N_t} \mathrm{d}U_i \det{}^{N_f}(aD)$$

where no Yang-Mills action is present due to the absence of a "plaquette" in one dimension only[52] and D is the lattice staggered Dirac operator

$$(aD)_{ii'} = am\delta_{ii'} + \frac{1}{2}\left(e^{a\mu}U_i\tilde{\delta}_{i',i+1} - e^{-a\mu}U_{i-1}^\dagger\tilde{\delta}_{i',i-1}\right)$$

where $\tilde{\delta}_{ii'}$ is the anti-periodic Kronecker delta, *i.e.*

$$aD = \begin{pmatrix} am & e^{a\mu}U_1/2 & 0 & \cdots & 0 & e^{-a\mu}U_{N_t}^\dagger/2 \\ -e^{-a\mu}U_1^\dagger/2 & am & e^{a\mu}U_2/2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & am & e^{a\mu}U_{N_t-1}/2 \\ -e^{a\mu}U_{N_t}/2 & 0 & 0 & \cdots & -e^{-a\mu}U_{N_t-1}^\dagger/2 & am \end{pmatrix}$$

All the links $\{U_i\}$ except one can be set to $\mathbb{1}$ by an appropriate gauge transformation: the only remaining link is simply the Polyakov loop $U \equiv U_{N_t}$, making the model effectively similar to one-link SU(3). Now we have

$$\det(aD) = \det \begin{pmatrix} am & e^{a\mu}/2 & 0 & \cdots & 0 & e^{-a\mu}U^\dagger/2 \\ -e^{-a\mu}/2 & am & e^{a\mu}/2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & am & e^{a\mu}/2 \\ -e^{a\mu}U/2 & 0 & 0 & \cdots & -e^{-a\mu}/2 & am \end{pmatrix}$$

We make use of the following formula [37, 102]

---

[52] Even in the continuum, $F_{\mu\nu}^a$ is antisymmetric, so that, if there is only a temporal direction, $F_{00}^a = 0$ is the only term.

$$
\det
\begin{pmatrix}
a_1 & b_1 & 0 & \cdots & 0 & c_0 \\
c_1 & a_2 & b_2 & \cdots & 0 & 0 \\
0 & c_2 & a_3 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & a_{L-1} & b_{L-1} \\
b_L & 0 & 0 & \cdots & c_{L-1} & a_L
\end{pmatrix}
$$

$$
= -\,(b_L \cdots b_1 + c_{L-1} \cdots c_0) + \mathrm{Tr}\left[\begin{pmatrix} a_L & -b_{L-1}c_{L-1} \\ 1 & 0 \end{pmatrix} \cdots \begin{pmatrix} a_2 & -b_1 c_1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a_1 & -b_L c_0 \\ 1 & 0 \end{pmatrix} \right]
$$

In our case $L = N_t$ and the entries are 3×3 matrices, in particular

$$
a_j = am\,\mathbb{1} \qquad j = 1 \cdots N_t
$$

$$
b_j = \begin{cases} e^{a\mu}/2\,\mathbb{1} & j = 1 \cdots N_t - 1 \\ -e^{a\mu}\,U/2 & j = N_t \end{cases}
$$

$$
c_j = \begin{cases} -e^{-a\mu}/2\,\mathbb{1} & j = 1 \cdots N_t - 1 \\ e^{-a\mu}\,U^\dagger/2 & j = 0 \end{cases}
$$

so that

$$
\det(aD) = \det_{3\times3}\left\{ -\left[\left(\frac{e^{a\mu}}{2}\right)^{N_t-1}\left(-\frac{e^{a\mu}U}{2}\right) + \left(-\frac{e^{-a\mu}}{2}\right)^{N_t-1}\left(\frac{e^{-a\mu}U^\dagger}{2}\right)\right] + \mathrm{Tr}\left[\begin{pmatrix} am & 1/4 \\ 1 & 0 \end{pmatrix}^{N_t-1}\begin{pmatrix} am & 1/4 \\ 1 & 0 \end{pmatrix}\right]\right\}
$$

$$
= \det_{3\times3}\left\{ \frac{1}{2^{N_t}}\left(e^{aN_t\mu}U + e^{-aN_t\mu}U^\dagger\right) + \mathrm{Tr}\left[\begin{pmatrix} am & 1/4 \\ 1 & 0 \end{pmatrix}^{N_t}\right]\right\}
$$

$$
= \det_{3\times3}\left\{ \frac{1}{2^{N_t}}\left(e^{\mu/T}U + e^{-\mu/T}U^\dagger\right) + \left(\frac{am + \sqrt{(am)^2 + 1}}{2}\right)^{N_t} + \left(\frac{am - \sqrt{(am)^2 + 1}}{2}\right)^{N_t}\right\}
$$

$$
= \frac{1}{2^{3N_t}}\det_{3\times3}\left\{ e^{\mu/T}U + e^{-\mu/T}U^\dagger + \left(am + \sqrt{(am)^2 + 1}\right)^{N_t} + \left(am - \sqrt{(am)^2 + 1}\right)^{N_t}\right\}
$$

$$
= \frac{1}{2^{3N_t}}\det_{3\times3}\left\{ e^{\mu/T}U + e^{-\mu/T}U^\dagger + e^{N_t \sinh^{-1}(am)} + (-1)^{N_t}e^{N_t \sinh^{-1}(-am)}\right\}
$$

$$
= \frac{1}{2^{3N_t}}\det_{3\times3}\left\{ e^{\mu/T}U + e^{-\mu/T}U^\dagger + e^{\sinh^{-1}(am)/(aT)} + e^{-\sinh^{-1}(am)/(aT)}\right\}
$$

$$
= \frac{1}{2^{3N_t}}\det_{3\times3}\left(A\,\mathbb{1}_{3\times3} + e^{\mu/T}U + e^{-\mu/T}U^\dagger\right)
$$

with $A = 2\cosh(\mu_c/T)$ and $a\mu_c = \sinh^{-1}(am)$. We will set $a = 1$ in all the following calculations. The partition function we have to compute is (the coefficient in front of the integral can be neglected)

$$
Z_{N_f} = \int\limits_{\mathrm{SU}(3)} dU\, \det^{N_f}\left(A\,\mathbb{1}_{3\times3} + e^{\mu/T}U + e^{-\mu/T}U^\dagger\right) \tag{9.1}
$$

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9.1 Analytical computation of the partition function

Now we make use of the relation $6 \det M = (\operatorname{Tr} M)^3 - 3 \operatorname{Tr} M \operatorname{Tr} M^2 + 2 \operatorname{Tr} M^3$, which holds for a generic 3×3 matrix and we also apply it to the matrix $U \in \mathrm{SU}(3)$, which gives $(\operatorname{Tr} U)^3 - 3 \operatorname{Tr} U \operatorname{Tr} U^2 + 2 \operatorname{Tr} U^3 = 6$; by making use of $\operatorname{Tr} U^2 = (\operatorname{Tr} U)^2 - 2 \operatorname{Tr} U^\dagger$ for $U \in \mathrm{SU}(3)$ as well, the integrand in (9.1) becomes

$$
\Big[\big((A^2 - 2)\operatorname{Tr} U + (\operatorname{Tr} U^\dagger)^2 \big) e^{\mu/T} + \big((A^2 - 2)\operatorname{Tr} U^\dagger + (\operatorname{Tr} U)^2 \big) e^{-\mu/T}
$$

$$
A \operatorname{Tr} U^\dagger e^{2\mu/T} + A \operatorname{Tr} U e^{-2\mu/T} + e^{3\mu/T} + e^{-3\mu/T} + A^3 - 3A + A \operatorname{Tr} U \operatorname{Tr} U^\dagger \Big]^{N_f}
$$

When this expression is expanded for a given value of N_f, the generic term of the resulting sum is proportional to $(\operatorname{Tr} U)^a (\operatorname{Tr} U^\dagger)^b$ and

$$
\int \mathrm{d}U \, (\operatorname{Tr} U)^a (\operatorname{Tr} U^\dagger)^b = \int \mathrm{d}U \, \chi_{\mathcal{R}}(U)
$$

with $\chi_{\mathcal{R}}(U)$ the character of U in the representation $\mathcal{R}$ defined by the group direct product of the fundamental and anti-fundamental representations of $\mathrm{SU}(3)$

$$
\mathcal{R} = \overset{a}{\bigotimes} \mathbf{3} \otimes \overset{b}{\bigotimes} \bar{\mathbf{3}} = \bigoplus_i n_i \mathcal{R}_i
$$

The second equality states the decomposition of $\mathcal{R}$ into a direct sum of irreducible representations $\{\mathcal{R}_i\}$, whose multiplicities are $\{n_i\}$. The group integral now selects only the *trivial* representation $\mathbf{1}$, being

$$
\int \mathrm{d}U \, \chi_{\mathcal{R}}(U) = \delta_{\mathcal{R}, \mathbf{1}}
$$

and therefore

$$
\int \mathrm{d}U \, (\operatorname{Tr} U)^a (\operatorname{Tr} U^\dagger)^b = \sum_i n_i \int \mathrm{d}U \, \chi_{\mathcal{R}_i}(U) = n_{\mathbf{1}}
$$

For example, we have

$$
\mathbf{3} \otimes \bar{\mathbf{3}} = \mathbf{8} \oplus \mathbf{1} \ \Rightarrow \ \int \mathrm{d}U \, \operatorname{Tr} U \operatorname{Tr} U^\dagger = 1
$$

and it turns out that $n_{\mathbf{1}} \neq 0$ only if $((a - b) \mod 3) = 0$. For all the irreducible representation decompositions involved, the *Mathematica* package *LieART* [103] was used.[53] The computation of $\langle \operatorname{Tr} U \rangle$ and

---

[53] There is another method which can be used to carry out the previous calculations: the eigenvalue representation of the Polyakov loop. We can diagonalize U with a unitary matrix S with $U = S \Lambda S^\dagger$ and $\Lambda = \operatorname{diag}\left(e^{i\varphi_1}, e^{i\varphi_2}, e^{-i\varphi_1 - i\varphi_2} \right)$, $\varphi_1, \varphi_2 \in [0, 2\pi]$. Using the (normalized) Haar measure of this parametrization, we can write

$$
\mathrm{d}U = \frac{8}{3\pi^2} \sin^2\left(\frac{\varphi_1 - \varphi_2}{2} \right) \sin^2\left(\frac{2\varphi_1 + \varphi_2}{2} \right) \sin^2\left(\frac{\varphi_1 + 2\varphi_2}{2} \right) \mathrm{d}\varphi_1 \mathrm{d}\varphi_2
$$

And the Dirac determinant is

$$
\det D = \prod_{k=1}^{3} \left(A \mathbb{1}_{3 \times 3} + e^{\mu/T + i\varphi_k} + e^{-\mu/T - i\varphi_k} \right)
$$

where it is understood $\varphi_3 = -\varphi_1 - \varphi_2$. The integrals are now easy to compute for any value of N_f.

$\langle \mathrm{Tr}\, U^\dagger \rangle$ can be carried out in the very same way. Appendix D gathers analytical results for the computation of Z and $\langle \mathrm{Tr}\, U \rangle$ for different values of N_f.

9.2 Simulating the theory

For numerical simulations, we turn the quark determinant into an effective action

$$Z_{N_f} = \int_{\mathrm{SU}(3)} \mathrm{d}U\, e^{-S(U)}$$

with

$$S(U) = -N_f \mathrm{Tr}\log M(U)$$

and $M(U) = A\,\mathbb{1}_{3\times 3} + e^{\mu/T}U + e^{-\mu/T}U^{-1}$.

There are three main observables we are interested in. The first is the chiral condensate

$$\Sigma \equiv T\frac{\partial}{\partial m}\log Z = T\left\langle N_f \mathrm{Tr}\left(M^{-1}\frac{\partial M}{\partial m}\right)\right\rangle = N_f\sqrt{\frac{A^2-4}{m^2+1}}\left\langle \mathrm{Tr}\left(M^{-1}\right)\right\rangle$$

while the other two are the Polyakov loop $\langle \mathrm{Tr}\, U \rangle$ and the anti-Polyakov loop $\langle \mathrm{Tr}\, U^\dagger \rangle = \langle \mathrm{Tr}\, U \rangle_{\mu\to-\mu}$. The latter two can be related to the quark number density $n \equiv T\frac{\partial}{\partial \mu}\log Z$ by a relation which takes quite different forms for different values of N_f [101]. The drift of the action is given by

$$\nabla^a S(U) = -i\,N_f \mathrm{Tr}\left[M^{-1}(U)\left(e^{\mu/T}T^a U - e^{-\mu/T}U^{-1}T^a\right)\right]$$

while the Hessian is

$$\nabla^b\nabla^a S(U) = N_f \mathrm{Tr}\Bigg[M^{-1}(U)\big[\big(e^{\mu/T}T^a T^b U + e^{-\mu/T}U^{-1}T^b T^a\big)$$

$$- \big(e^{\mu/T}T^b U - e^{-\mu/T}U^{-1}T^b\big)M^{-1}(U)\big(e^{\mu/T}T^a U - e^{-\mu/T}U^{-1}T^a\big)\big]\Bigg]$$

There are three critical points $\{U_k = e^{2\pi ik/3}\mathbb{1}\}$ with $k = 0,1,2$. After defining

$$B_k \equiv 2\left[\cosh\left(\frac{\mu_c}{T}\right) + \cosh\left(\frac{\mu}{T} + \frac{2\pi ik}{3}\right)\right]$$

we have $S(U_k) = -3N_f\log B_k$ and $\nabla^b\nabla^a S(U)\big|_{U_k} = \lambda_k e^{i\,\varphi_k}\delta^{ab}$, with

$$\lambda_k e^{i\,\varphi_k} \equiv N_f\left[B_k^{-1}\left(\cosh\left(\frac{\mu}{T} + \frac{2\pi ik}{3}\right) - 2B_k^{-1}\sinh^2\left(\frac{\mu}{T} + \frac{2\pi ik}{3}\right)\right)\right]$$

The only Takagi value is thus λ_k, while the 8 Takagi vectors are given by $v_j^{[k](i)} = e^{-i\,\varphi_k/2}\delta_{ij}$.

We will now show that the action of 0+1 QCD fulfills a reflection symmetry described in [42] and discussed in detail in Appendix E: $\overline{S(A)} = S(-\bar{A})$ with $U = e^{iA}$. This ensures the *reality* of the partition function (and

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of the expectation value of the Polyakov loop as well). This symmetry of the theory is manifestly fulfilled by the decomposition in thimbles [42] and holds at every order in perturbation theory as well, so we shall recover it in the semiclassical expansion. Consider the QCD partition function

$$Z_{N_f}(\mu) = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \mathcal{D}U \, e^{-N_f \bar{\psi} D(U,\mu)\psi} = \int \mathcal{D}U \det^{N_f}(D(U,\mu))$$

The action (whose only component, in our case, is the Dirac determinant) is invariant under charge conjugation $\mathcal{C}$ defined by [28]

$$\mathcal{C} \begin{cases} \psi \to C^{-1}\bar{\psi}^T \\ \bar{\psi} \to -\psi^T C \\ U_{\hat{\nu}}(n) \to \bar{U}_{\hat{\nu}}(n) \quad \left(A_{\hat{\nu}}(n) \to -A_{\hat{\nu}}^T(n) = -\bar{A}\right) \\ \mu \to -\mu \end{cases}$$

with the matrix C satisfying $C\gamma_\mu C^{-1} = -\gamma_\mu^T$.[54] Thus, we can employ charge conjugation to substitute $\det D(U,\mu) \to \det D(\bar{U},-\mu)$ leaving the action invariant. We also recall the generalization of γ_5-hermiticity at finite chemical potential [29, 28]

$$\det D(U,-\mu) = \overline{\det D(U,\mu)}$$

This implies that

$$\overline{S(A)} \sim \overline{\det D(U,\mu)} \stackrel{\gamma_5\text{-herm.}}{=} \det D(U,-\mu) \stackrel{\mathcal{C}\text{-inv.}}{=} \det D(\bar{U},\mu) \sim S(-\bar{A})$$

We have shown that the aforementioned reflection symmetry is fulfilled and thus we expect thimbles to appear in conjugate pairs. This is indeed the case: consider the three critical points $\{U_k\}$. $U_0 = \mathbb{1}$ is real and therefore self-conjugate; the consequence of this is that computations on the associated thimble yield real results. As for the other two critical points, being $e^{4\pi i/3} = e^{-2\pi i/3}$, we immediately see that $U_2 = \overline{U_1}$. This implies that U_1 and U_2 form a conjugate pair of critical points and results of integration on U_2 should be the complex conjugate of those on U_1, yielding an overall real contribution to the partition function (and also to the expectation value of observables). This is recovered in numerical simulations. As a final remark, we state that these results hold not only for the partition function, but also for the Polyakov loop (it is obvious, since $\overline{\mathrm{Tr}\,U} = \mathrm{Tr}\,\bar{U}$) and anti-Polyakov loop.[55]

9.3 Semiclassical expansion

In this section we will compute semiclassical expansions around thimbles in $0+1$ QCD. Consider the semiclassical expression for the thimble decomposition of the partition function which is given in (5.18). In our case, we have $\det \Lambda_k = \lambda_k^8$ and $e^{i\omega_k} = \left(e^{-i\varphi_k/2}\right)^8$, so that

$$Z \approx (2\pi)^4 \sum_{k=0,1,2} \mathfrak{n}_k \, e^{3N_f \log B_k} \lambda_k^{-4} \, e^{-4i\varphi_k}$$

The expectation value of the Polyakov loop can be computed in the following way, starting from expression (5.19)

---

[54] A caveat is in order as for notation $\bar{U}$: this is not to be intended as in Section 4.1, but as the ordinary complex conjugate.
[55] The chiral condensate and the quark number density automatically respect this symmetry, being derivatives of the partition function.

$$\langle \operatorname{Tr} U \rangle \approx \frac{1}{Z} (2\pi)^4 \sum_{k=0,1,2} \mathfrak{n}_k \, e^{3N_f \log B_k} \lambda_k^{-4} \, e^{-4i\,\varphi_k} \left(\operatorname{Tr} U_k + \frac{1}{2} \frac{1}{\lambda_k} \sum_{i=1}^{8} \left(C_k^{\operatorname{Tr} U} \right)_{ii} \right)$$

where

$$\left(C_k^{\operatorname{Tr} U} \right)_{ii} = \sum_{j=1}^{8} \sum_{l=1}^{8} \left(H_k^{\operatorname{Tr} U} \right)_{jl} v_j^{(i)} v_l^{(i)} = e^{-i\,\varphi_k} \left(H_k^{\operatorname{Tr} U} \right)_{ii} = e^{-i\,\varphi_k} \nabla^i \nabla^i \operatorname{Tr} U \big|_{U_k}$$

$$= -e^{-i\,\varphi_k} e^{2\pi i k/3} \operatorname{Tr} \left(T^i T^i \, \mathbb{1} \right) = -\frac{1}{2} e^{-i\,\varphi_k} e^{2\pi i k/3}$$

Being $\operatorname{Tr} U_k = e^{2\pi i k/3} \operatorname{Tr} \mathbb{1} = 3 \, e^{2\pi i k/3}$, it follows that

$$\operatorname{Tr} U_k + \frac{1}{2} \frac{1}{\lambda_k} \sum_{i=1}^{8} \left(C_k^{\operatorname{Tr} U} \right)_{ii} = e^{2\pi i k/3} \left(3 - \frac{2}{\lambda_k} e^{-i\,\varphi_k} \right)$$

and finally

$$\langle \operatorname{Tr} U \rangle \approx \frac{1}{Z} (2\pi)^4 \sum_{k=0,1,2} \mathfrak{n}_k \, e^{3N_f \log B_k} \lambda_k^{-4} \, e^{-4i\,\varphi_k + 2\pi i k/3} \left(3 - \frac{2}{\lambda_k} e^{-i\,\varphi_k} \right)$$

From the previous considerations on the reflection symmetry featured by $0 + 1$ QCD, we can see that reality of Z and $\langle \operatorname{Tr} U \rangle$ is achieved by setting $\mathfrak{n}_1 = \mathfrak{n}_2$. This is so since the contribution of $\mathcal{J}_2$ to Z and $\langle \operatorname{Tr} U \rangle$ is the complex conjugate of the contribution of $\mathcal{J}_1$. This is manifest in the semiclassical expansion thanks to $S(U_2) = \overline{S(U_1)}$, $B_2 = \bar{B}_1$, $\lambda_2 = \lambda_1$, $e^{i\,\varphi_2} = \overline{e^{i\,\varphi_1}} = e^{-i\,\varphi_1}$, all following from $e^{4\pi i/3} = e^{-2\pi i/3} = \overline{e^{2\pi i/3}}$. Thus we can rephrase Z as

$$Z \approx Z_0 + Z_1 + Z_2$$

with $Z_0 \in \mathbb{R}$ and $Z_2 = \bar{Z}_1$ (so that $|Z_1| = |Z_2|$). The semiclassical expansion on thimbles also provides an easy way to compute an estimate for the relevance of $\mathcal{J}_{1,2}$ with respect to $\mathcal{J}_0$ in the computation of $e.g.$ the partition function. We define the relative weight $r_0^{1,2}$

$$r_0^{1,2} \equiv \frac{|Z_{1,2}|}{|Z_0|} = \frac{\left| e^{3N_f \log B_{1,2}} \right| \lambda_{1,2}^{-4}}{\left| e^{3N_f \log B_0} \right| \lambda_0^{-4}} = \left(\frac{\lambda_{1,2}}{\lambda_0} \right)^{-4} \left| \frac{B_{1,2}}{B_0} \right|^{3N_f} \tag{9.2}$$

and study it at different values of $\frac{\mu}{T}$ and m. This, as we shall see, provides a reliable estimate which can be compared with the results of numerical simulations. We note that, being $B_0 = A + 2\cosh(\mu/T) \in \mathbb{R}$ and $B_1 = A - \cosh(\mu/T) + i\sqrt{3}\sinh(\mu/T)$

$$|B_{1,2}|^2 = A^2 + \cosh^2\left(\frac{\mu}{T} \right) - 2A\cosh\left(\frac{\mu}{T} \right) + 3\sinh^2\left(\frac{\mu}{T} \right)$$

$$= A^2 + 4\cosh^2\left(\frac{\mu}{T} \right) - 2A\cosh\left(\frac{\mu}{T} \right) - 3 < A^2 + 4\cosh^2\left(\frac{\mu}{T} \right) + 4A\cosh\left(\frac{\mu}{T} \right) = |B_0|^2$$

so that

$$r_0^{1,2} \xrightarrow[N_f \to \infty]{} 0$$

for any value of $\frac{\mu}{T}$ and m (the ratio $\lambda_{1,2}/\lambda_0$ is independent on N_f). As a consequence, we expect that integrating only over $\mathcal{J}_0$ will give more accurate results at high number of quark flavours.[56]

9.4 Numerical results

Numerical results of thimble simulations for the chiral condensate and the Polyakov loop are displayed in Figures 9.1 to 9.7. As all the three critical points belong to the original domain of integration (SU(3)), we expect all of them to be relevant in the thimble decomposition. However, a deeper insight with regards to their actual weight in such decomposition can be gained from the semiclassical arguments of the previous section. Figures from 9.8 to 9.11 depict $r_0^{1,2}$ (defined in (9.2)) as a function of $\frac{\mu}{T}$ and m; by studying this quantity one can predict for which values of the parameters $(\frac{\mu}{T}, m)$ integration only over $\mathcal{J}_0$ is expected to capture substantially correct results. In Figures 9.12 and 9.13 numerical results obtained by integrating only on $\mathcal{J}_0$ are shown for $m = 1$, $N_f = 2$ and $m = 0.1$, $N_f = 6$ respectively. In the regions in which Figures 9.8b and 9.10b predict $\mathcal{J}_1$ and $\mathcal{J}_2$ to be relevant, results computed by taking only $\mathcal{J}_0$ into account are clearly wrong, while taking into account $\mathcal{J}_1$ and $\mathcal{J}_2$ as well provides correct results, as shown in Figures 9.2c, 9.2d and 9.6a, 9.6b. In this model, all Takagi values are equal, so that the HBB Metropolis algorithm of Section 5.3 is inapplicable. Therefore one could either use the static, crude Monte Carlo or the Metropolis algorithm at the end of Section 5.3. All the numerical results presented here were obtained with the static, crude Monte Carlo. As a consequence of the total degeneracy of the Hessian eigenvalues, we expect the dependence of $Z_{\hat{n}}$ on $\hat{n}$ be due to purely non-Gaussian effects. The reader will notice that Figures 9.1 to 9.7 do not show simulation results beyond certain values of μ/T which are dependent on m and N_f. At higher values of N_f, all μ/T were simulated to a success. This is consistent with the observation that semiclassical estimates (which rely on the isotropy of the Hessian spectrum) become exact in the limit $N_f \to \infty$, thus rendering the model easier to simulate at high N_f. The regions of parameters which are difficult to simulate (namely, high μ/T) are those which make integration of SA and PT equations difficult.[57] This difficulty is due to the "curvature" of the thimble becoming increasingly higher, which requires more care in carrying out numerical integrations.[58] It turns out that these problems are much more severe for $\mathcal{J}_1$ and $\mathcal{J}_2$ than they are for $\mathcal{J}_0$. This is a problem which is specific to this model and a solution to it is currently under investigation. This technical difficulty in integrating on $\mathcal{J}_1$ and $\mathcal{J}_2$ is the reason why for low values of N_f we could not simulate the model in the high μ/T region, especially at lower masses. This is again in accordance with semiclassical estimates of Figures 9.8 to 9.11, which predicts $\mathcal{J}_1$ and $\mathcal{J}_2$ to be more relevant in those regions of parameters. Anyway, the aforementioned reflection symmetry helps in knowing what to expect from simulations on $\mathcal{J}_1$ and $\mathcal{J}_2$. All in all, despite some serious technical problems still to be solved, a quite clear scenario for thimble-regularized $0 + 1$ QCD at finite density emerges.

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[56]This is of course a semiclassical estimate. The reliability of this prediction will be checked against numerical simulations.

[57]For example, at high μ/T, it was difficult to keep the consistency check (5.12) under control using the Euler integration scheme.

[58]This problem is related to the chaoticity of the system. In fact, the factor $\det V$ appearing in our integrals is closely related to the Lyapunov spectrum of the system. This is so, as $|\det V|$ measures the stretch of an infinitesimal parallelepiped spanned by $\{V_{\hat{n}}^{(i)}(t)\}$ from the critical point to the point $U(t)$ along the steepest ascent curve.

(a) Chiral condensate at $T = 0.5$, $N_f = 1$, $m = 0.1$.

(b) Polyakov loop at $T = 0.5$, $N_f = 1$, $m = 0.1$.

(c) Chiral condensate at $T = 0.5$, $N_f = 1$, $m = 1$.

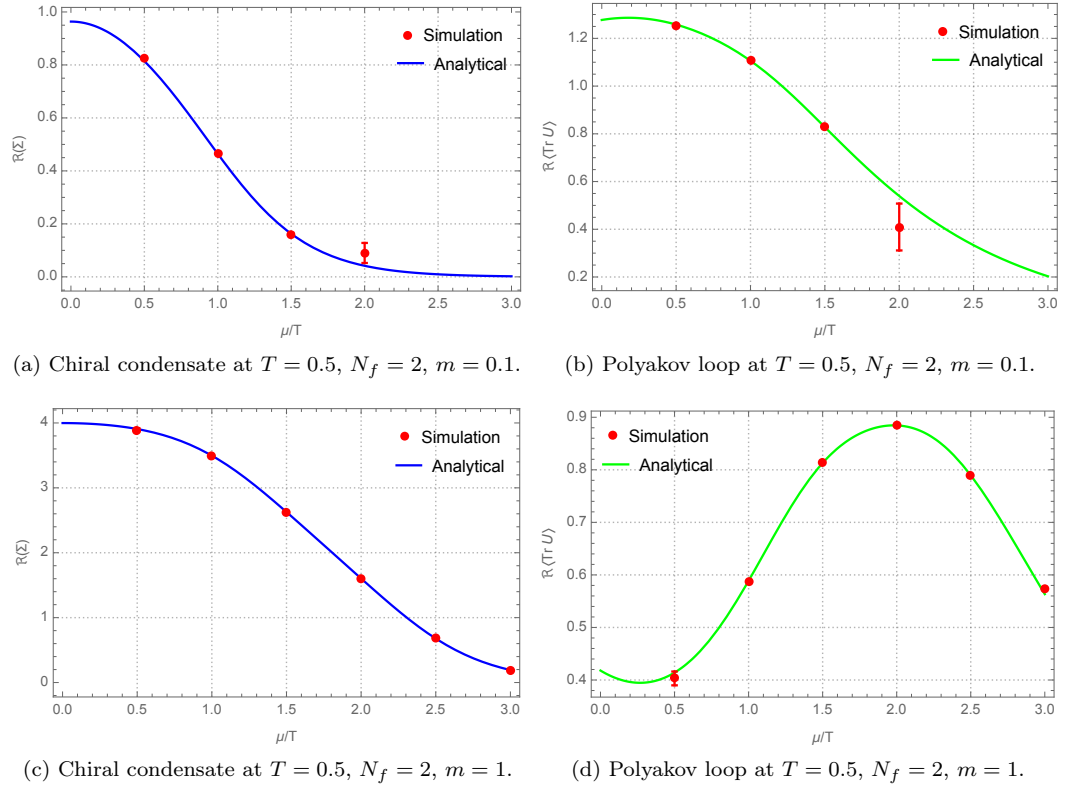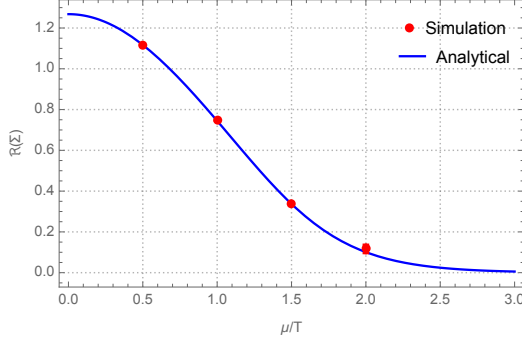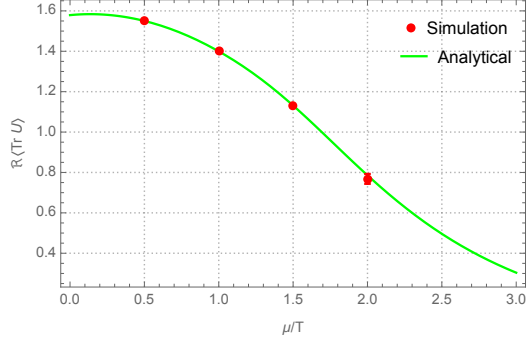(d) Polyakov loop at $T = 0.5$, $N_f = 1$, $m = 1$.
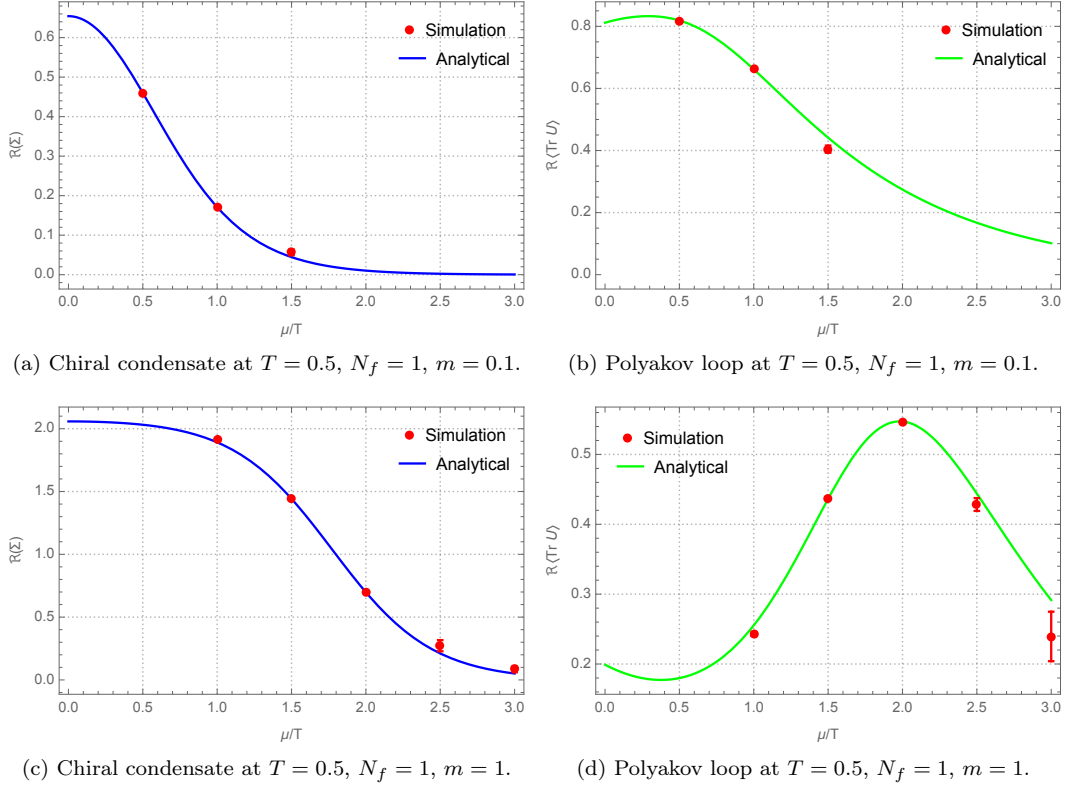
Figure 9.1: Chiral condensate and Polyakov loop expectation value for 0+1 QCD at $N_f = 1$. Other parameters are $T = 0.5$ and $m = 0.1, 1$.
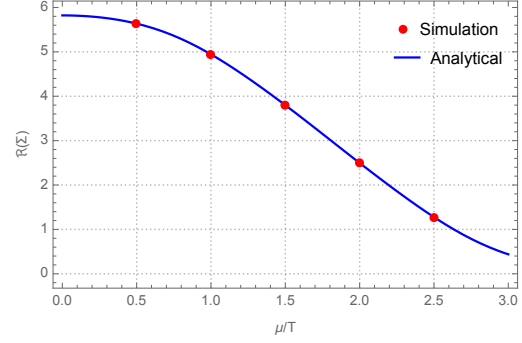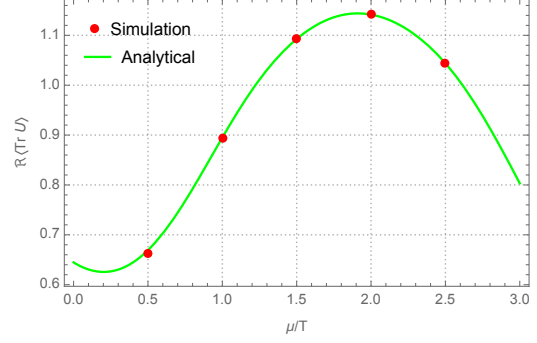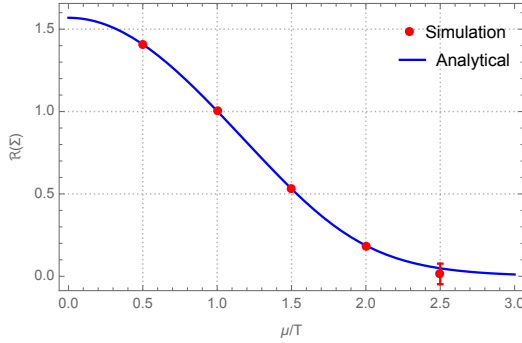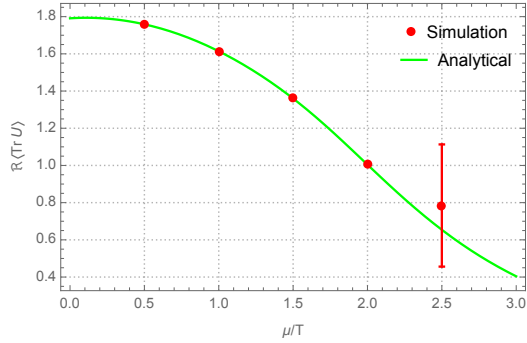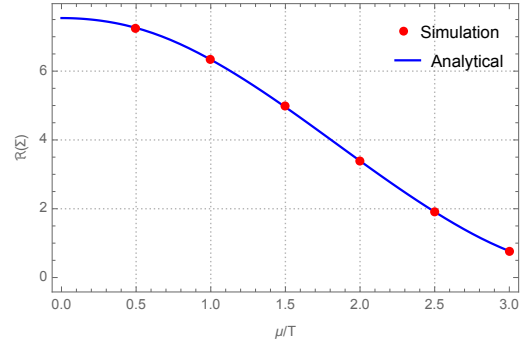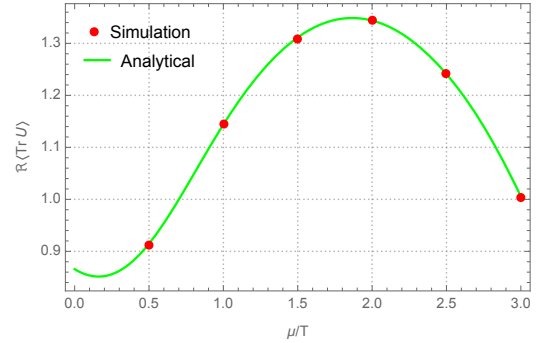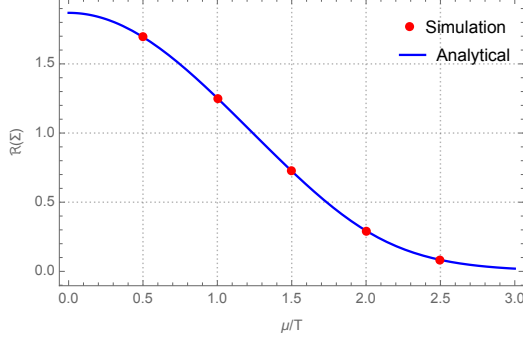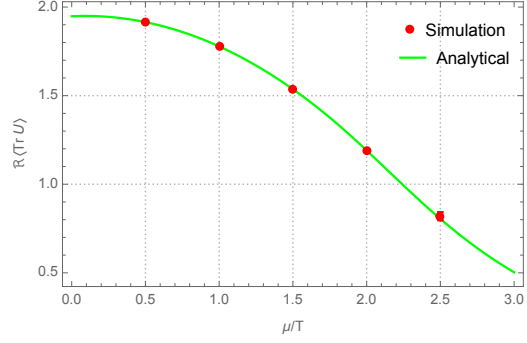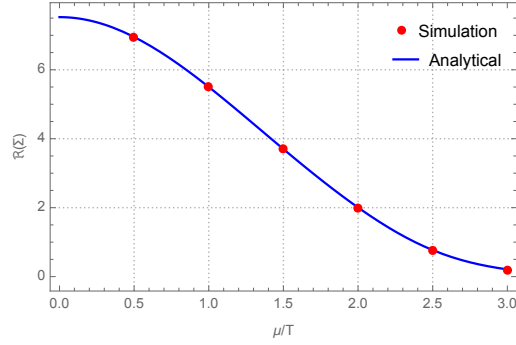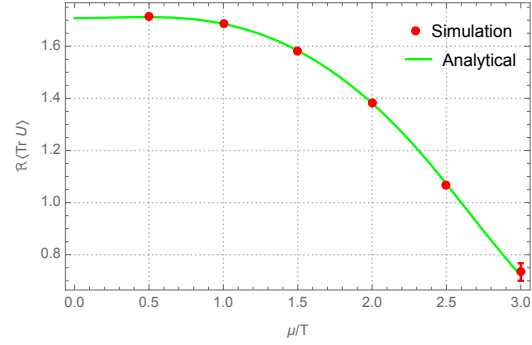

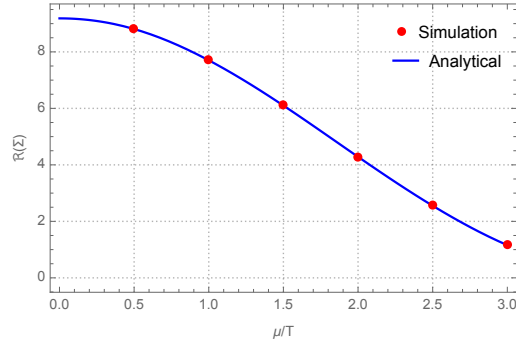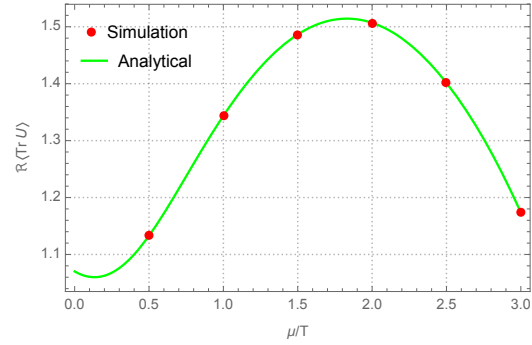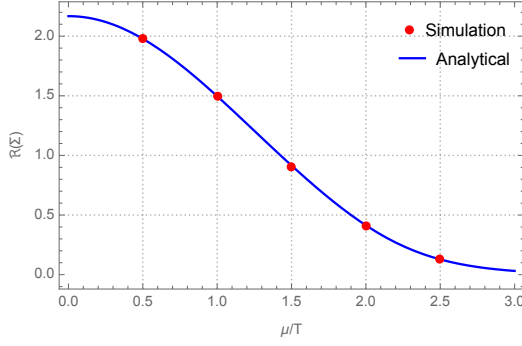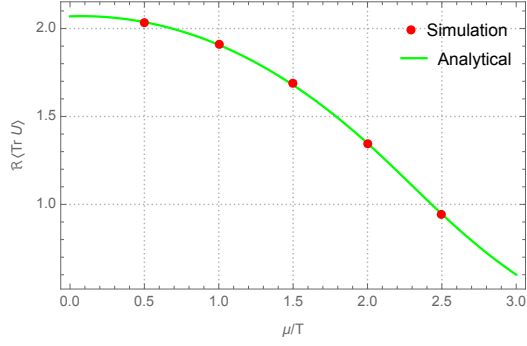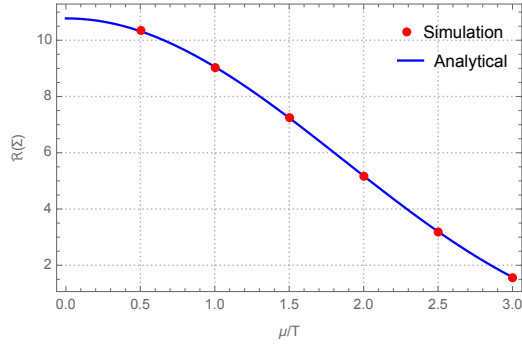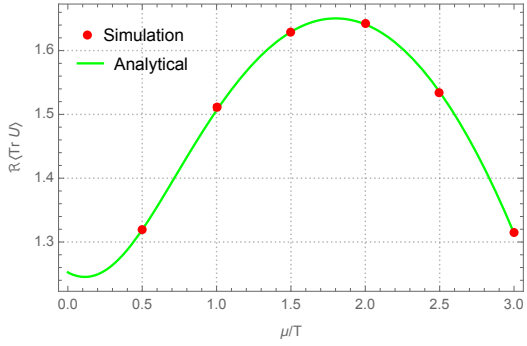(a) Chiral condensate at $T = 0.5$, $N_f = 2$, $m = 0.1$.

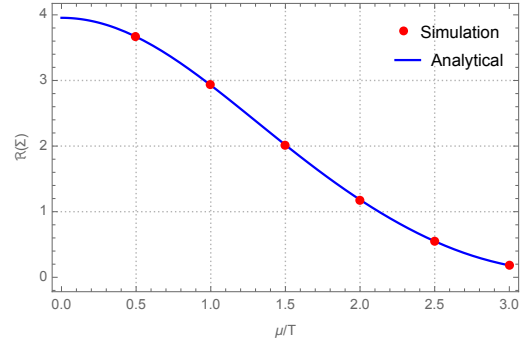(b) Polyakov loop at $T = 0.5$, $N_f = 2$, $m = 0.1$.

(c) Chiral condensate at $T = 0.5$, $N_f = 2$, $m = 1$.

(d) Polyakov loop at $T = 0.5$, $N_f = 2$, $m = 1$.

Figure 9.2: Chiral condensate and Polyakov loop expectation value for 0+1 QCD at $N_f = 2$. Other parameters are $T = 0.5$ and $m = 0.1, 1$.

(a) Chiral condensate at $T = 0.5$, $N_f = 3$, $m = 0.1$.

(b) Polyakov loop at $T = 0.5$, $N_f = 3$, $m = 0.1$.

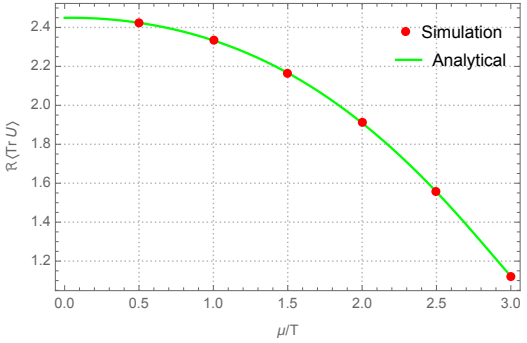(c) Chiral condensate at $T = 0.5$, $N_f = 3$, $m = 1$.

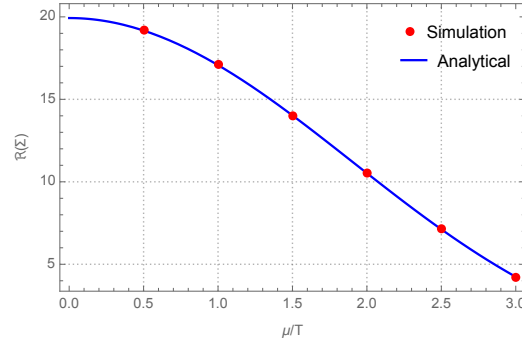(d) Polyakov loop at $T = 0.5$, $N_f = 3$, $m = 1$.

Figure 9.3: Chiral condensate and Polyakov loop expectation value for 0+1 QCD at $N_f = 3$. Other parameters are $T = 0.5$ and $m = 0.1, 1$.

(a) Chiral condensate at $T = 0.5$, $N_f = 4$, $m = 0.1$.

(b) Polyakov loop at $T = 0.5$, $N_f = 4$, $m = 0.1$.

(c) Chiral condensate at $T = 0.5$, $N_f = 4$, $m = 1$.

(d) Polyakov loop at $T = 0.5$, $N_f = 4$, $m = 1$.

Figure 9.4: Chiral condensate and Polyakov loop expectation value for 0+1 QCD at $N_f = 4$. Other parameters are $T = 0.5$ and $m = 0.1, 1$.
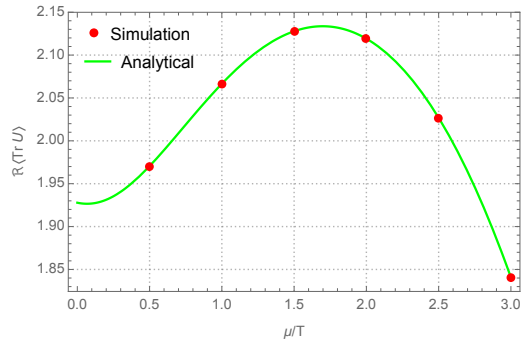
(a) Chiral condensate at $T = 0.5$, $N_f = 5$, $m = 0.1$.

(b) Polyakov loop at $T = 0.5$, $N_f = 5$, $m = 0.1$.

(c) Chiral condensate at $T = 0.5$, $N_f = 5$, $m = 0.5$.

(d) Polyakov loop at $T = 0.5$, $N_f = 5$, $m = 0.5$.

(e) Chiral condensate at $T = 0.5$, $N_f = 5$, $m = 1$.

(f) Polyakov loop at $T = 0.5$, $N_f = 5$, $m = 1$.

Figure 9.5: Chiral condensate and Polyakov loop expectation value for 0+1 QCD at $N_f = 5$. Other parameters are $T = 0.5$ and $m = 0.1, 0.5, 1$.
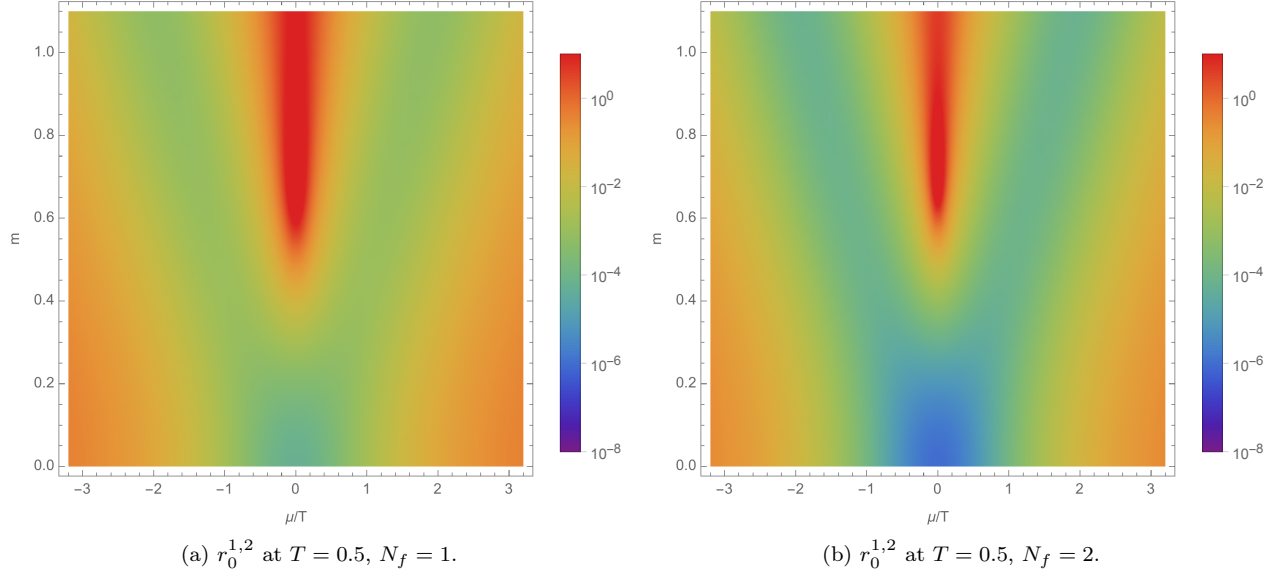
(a) Chiral condensate at $T = 0.5$, $N_f = 6$, $m = 0.1$.

(b) Polyakov loop at $T = 0.5$, $N_f = 6$, $m = 0.1$.

(c) Chiral condensate at $T = 0.5$, $N_f = 6$, $m = 1$.

(d) Polyakov loop at $T = 0.5$, $N_f = 6$, $m = 1$.

Figure 9.6: Chiral condensate and Polyakov loop expectation value for 0+1 QCD at $N_f = 6$. Other parameters are $T = 0.5$ and $m = 0.1, 1$.

(a) Chiral condensate at $T = 0.5$, $N_f = 12$, $m = 0.1$.

(b) Polyakov loop at $T = 0.5$, $N_f = 12$, $m = 0.1$.

(c) Chiral condensate at $T = 0.5$, $N_f = 12$, $m = 1$.

(d) Polyakov loop at $T = 0.5$, $N_f = 12$, $m = 1$.

Figure 9.7: Chiral condensate and Polyakov loop expectation value for 0+1 QCD at $N_f = 12$. Other parameters are $T = 0.5$ and $m = 0.1, 1$.

(a) $r_0^{1,2}$ at $T = 0.5$, $N_f = 1$.
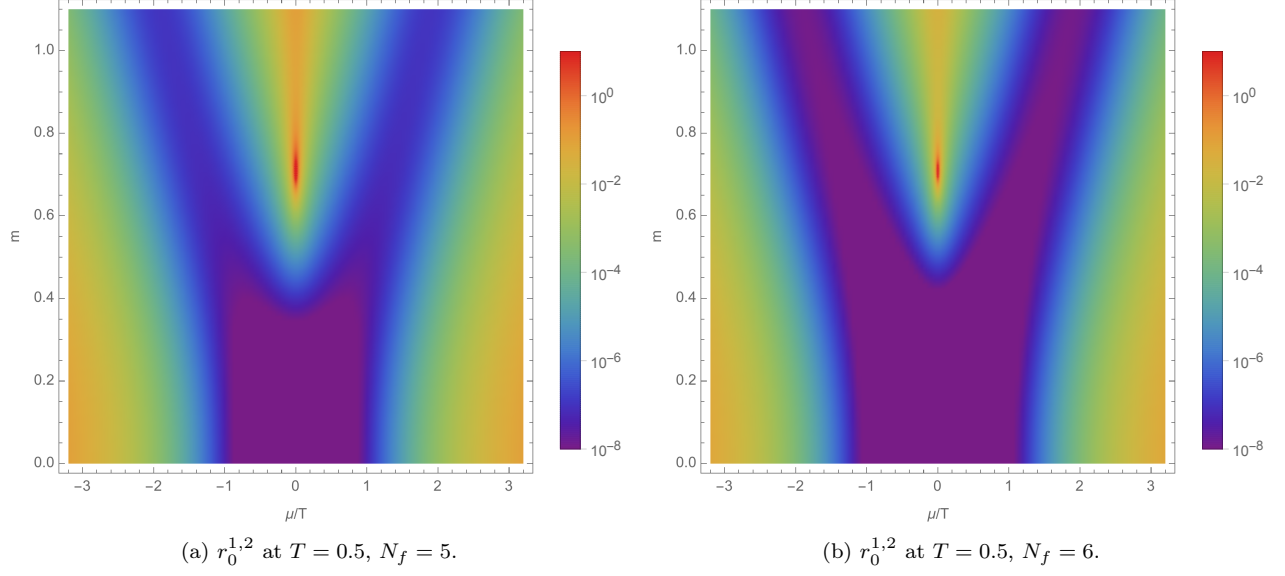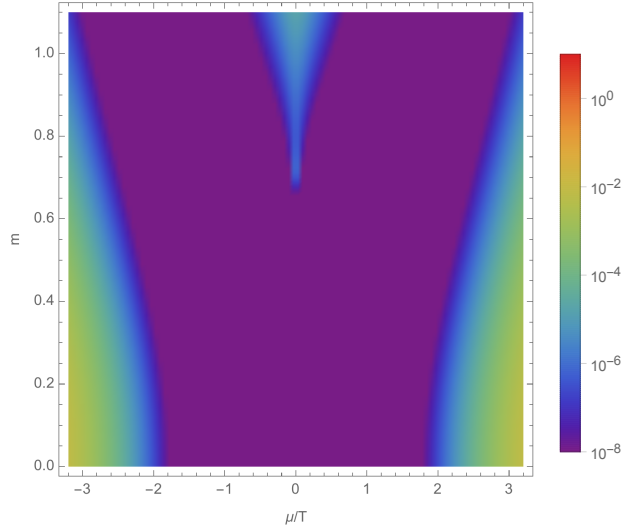
(b) $r_0^{1,2}$ at $T = 0.5$, $N_f = 2$.

Figure 9.8: The plots represent $r_0^{1,2}$ for 0+1 QCD at $T = 0.5$ and $N_f = 1, 2$ as a function of μ/T and m.

(a) $r_0^{1,2}$ at $T = 0.5$, $N_f = 3$.

(b) $r_0^{1,2}$ at $T = 0.5$, $N_f = 4$.
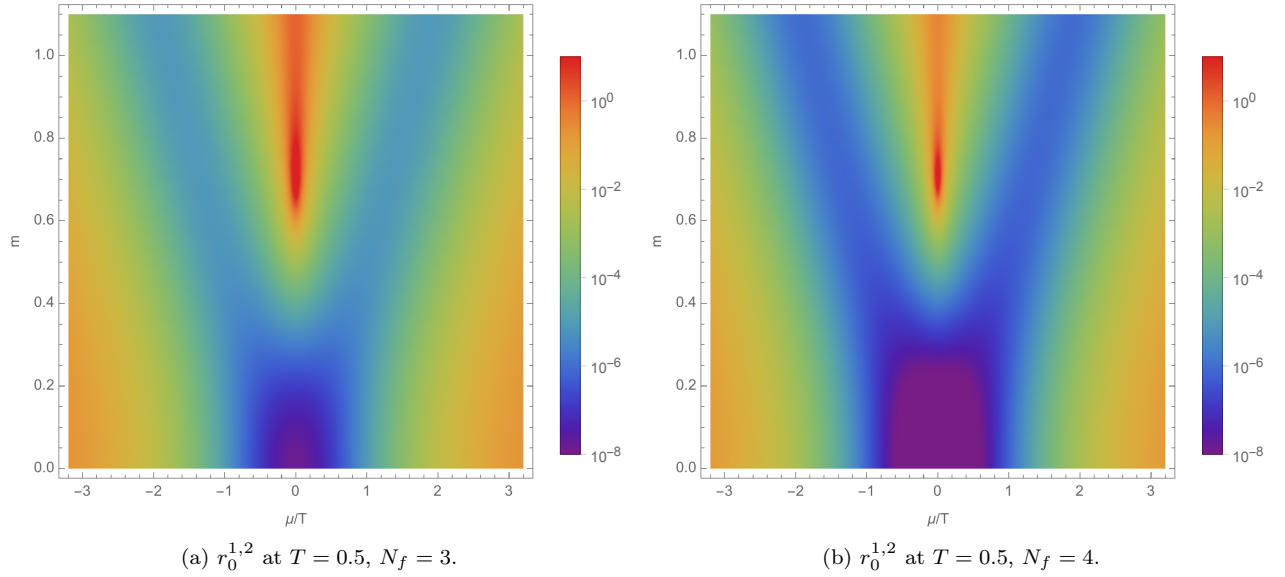
Figure 9.9: The plots represent $r_0^{1,2}$ for 0+1 QCD at $T = 0.5$ and $N_f = 3, 4$ as a function of μ/T and m.

(a) $r_0^{1,2}$ at $T = 0.5$, $N_f = 5$.

(b) $r_0^{1,2}$ at $T = 0.5$, $N_f = 6$.

Figure 9.10: The plots represent $r_0^{1,2}$ for 0+1 QCD at $T = 0.5$ and $N_f = 5, 6$ as a function of μ/T and m.
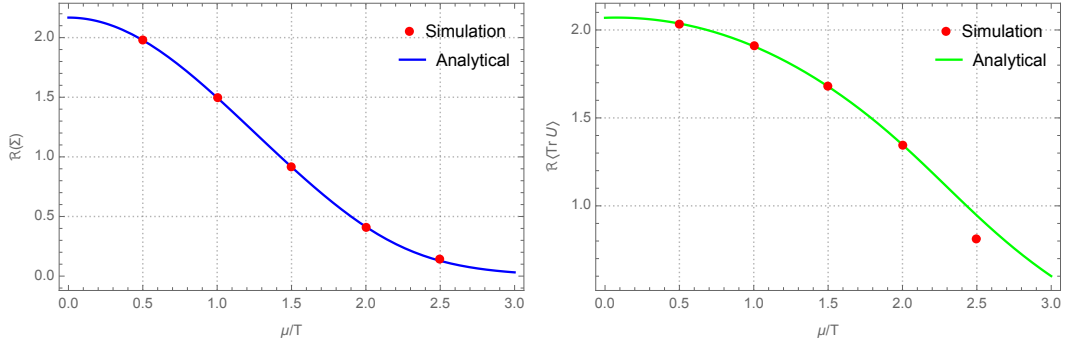

Figure 9.11: The plot represents $r_0^{1,2}$ for 0+1 QCD at $T = 0.5$ and $N_f = 12$ as a function of μ/T and m.
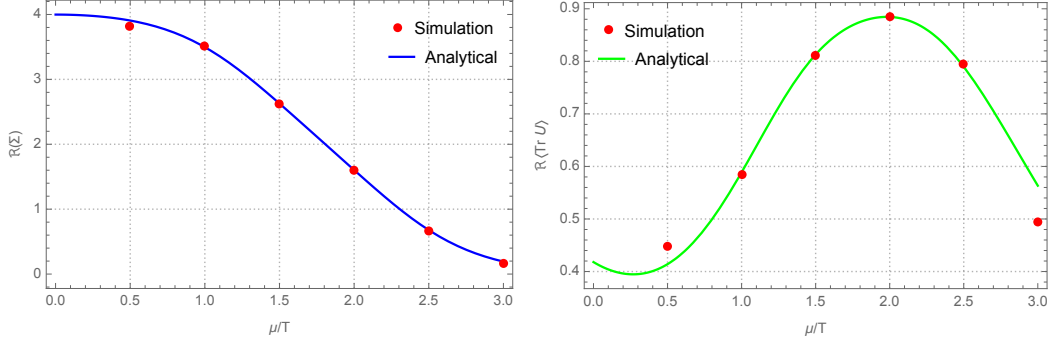
(a) Chiral condensate at $T = 0.5$, $N_f = 2$, $m = 1$ (integrating only on $\mathcal{J}_0$).

(b) Polyakov loop at $T = 0.5$, $N_f = 2$, $m = 1$ (integrating only on $\mathcal{J}_0$).

Figure 9.12: Chiral condensate and Polyakov loop expectation value for 0+1 QCD at $N_f = 2$. Other parameters are $T = 0.5$ and $m = 1$. These results are obtained by integrating only over $\mathcal{J}_0$.

(a) Chiral condensate at $T = 0.5$, $N_f = 6$, $m = 0.1$ (integrating only on $\mathcal{J}_0$).

(b) Polyakov loop at $T = 0.5$, $N_f = 6$, $m = 0.1$ (integrating only on $\mathcal{J}_0$).

Figure 9.13: Chiral condensate and Polyakov loop expectation value for 0+1 QCD at $N_f = 6$. Other parameters are $T = 0.5$ and $m = 0.1$. These results are obtained by integrating only over $\mathcal{J}_0$.

10 Complex SU(N) Yang-Mills theory in 2 dimensions

After studying the models of the previous sections, the time has come to tackle a real gauge theory with the thimble approach. In this section we study the (compact) lattice $SU(N)$ Yang-Mills theory in 2 dimensions with *complex* coupling as a source of sign problem. Even though we will not perform numerical computations, many issues concerning this model will be discussed in detail. In particular, we will describe the general structure of the theory, the problem of constructing a vacuum configuration which is suitable for thimble regularization in presence of periodic boundary conditions and the issue of performing integration on a gauge-symmetric thimble. After these discussions, all will be ready to perform actual simulations of the model; moreover, many of the issues described in this section also apply to more realistic models (such as QCD in 4 dimensions or Yang-Mills in presence of a θ-term). For Yang-Mills theory in 2 dimensions, analytical results are available: see Appendix F for the computation of the partition function.

Consider the $SU(N)$ Wilson action on a lattice Λ with *periodic boundary conditions* [29, 28, 104, 105]. Recall the (inverse) coupling $\beta \in \mathbb{C}$; in order to complexify the fields (the gauge links for each spacetime direction at each point of the lattice), we make the substitution $U^\dagger \to U^{-1}$. The action is

$$S[U] = \beta \sum_{m \in \Lambda} \sum_{\hat\rho < \hat\nu} \left[1 - \frac{1}{2N} \mathrm{Tr} \left(U_{\hat\rho\hat\nu}(m) + U_{\hat\rho\hat\nu}^{-1}(m) \right) \right] \tag{10.1}$$

with

$$U_{\hat\rho\hat\nu}(m) \equiv U_{\hat\rho}(m) U_{\hat\nu}(m + \hat\rho) U_{\hat\rho}^{-1}(m + \hat\nu) U_{\hat\nu}^{-1}(m)$$

the elementary *plaquette* attached to the point m lying in the $\hat\rho\hat\nu$-plane. β is related to the (bare) coupling constant g_0 by

$$\beta = \frac{2N}{g_0^2}$$

The Wilson action (10.1) is manifestly holomorphic, as it depends only on U and not on $\bar{U} \equiv \left(U^\dagger \right)^{-1}$. From the definition of Lie derivative, it follows that

$$\nabla^a U = i\, T^a U$$

$$\nabla^a U^{-1} = -i\, U^{-1} T^a$$

In order to compute $\nabla^a_{n,\hat\mu} S[U]$, let us consider only those terms in the action involving $U_{\hat\mu}(n)$

$$\nabla^a_{n,\hat{\mu}} S[U] = -\frac{\beta}{2N} \sum_{\hat{\nu} \neq \hat{\mu}} \operatorname{Tr} \nabla^a_{n,\hat{\mu}} \left(\vphantom{\Bigg|} \right.$$ $$\left. \vphantom{\Bigg|} \right)$$

$$= -\frac{\beta}{2N} \sum_{\hat{\nu} \neq \hat{\mu}} \operatorname{Tr} \nabla^a_{n,\hat{\mu}} \left[U_{\hat{\mu}}(n) \left(\vphantom{\Bigg|} \text{ } + \text{ } \right) + \left(\text{ } + \text{ } \right) U_{\hat{\mu}}^{-1} \right]$$

$$= -\frac{i\beta}{2N} \sum_{\hat{\nu} \neq \hat{\mu}} \operatorname{Tr} \left\{ T^a \left[U_{\hat{\mu}\hat{\nu}}(n) + \mathcal{U}_{\hat{\mu}\hat{\nu}}(n) - U_{\hat{\mu}\hat{\nu}}^{-1}(n) - \mathcal{U}_{\hat{\mu}\hat{\nu}}^{-1}(n) \right] \right\}$$

with

$$U_{\hat{\mu}\hat{\nu}}(n) \equiv U_{\hat{\mu}}(n) U_{\hat{\nu}}(n + \hat{\mu}) U_{\hat{\mu}}^{-1}(n + \hat{\nu}) U_{\hat{\nu}}^{-1}(n)$$

$$\mathcal{U}_{\hat{\mu}\hat{\nu}}(n) \equiv U_{\hat{\mu}}(n) U_{\hat{\nu}}^{-1}(n + \hat{\mu} - \hat{\nu}) U_{\hat{\mu}}^{-1}(n - \hat{\nu}) U_{\hat{\nu}}(n - \hat{\nu})$$

The computation of the Hessian is more involved. Making use of

$$\sum_{\hat{\nu} \neq \hat{\mu}} = \sum_{\hat{\nu}} \left(1 - \delta_{\hat{\nu},\hat{\mu}} \right)$$

we have

$$\nabla^b_{m,\hat{\rho}}\nabla^a_{n,\hat{\mu}}S[U]$$

$$=-\frac{i\,\beta}{2N}\sum_{\hat{\nu}}(1-\delta_{\hat{\nu},\hat{\mu}})\mathrm{Tr}\Big\{T^a\Big[(i\,T^bU_{\hat{\mu}}(n))U_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n)\delta_{n,m}\delta_{\hat{\mu},\hat{\rho}}+U_{\hat{\mu}}(n)(i\,T^bU_{\hat{\nu}}(n+\hat{\mu}))U_{\hat{\mu}}^{-1}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n)\delta_{n+\hat{\mu},m}\delta_{\hat{\nu},\hat{\rho}}$$

$$+U_{\hat{\mu}}(n)U_{\hat{\nu}}(n+\hat{\mu})(-i\,U_{\hat{\mu}}^{-1}(n+\hat{\nu})T^b)U_{\hat{\nu}}^{-1}(n)\delta_{n+\hat{\nu},m}\delta_{\hat{\mu},\hat{\rho}}+U_{\hat{\mu}}(n)U_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})(-i\,U_{\hat{\nu}}^{-1}(n)T^b)\delta_{n,m}\delta_{\hat{\nu},\hat{\rho}}$$

$$+(i\,T^bU_{\hat{\mu}}(n))U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})U_{\hat{\nu}}(n-\hat{\nu})\delta_{n,m}\delta_{\hat{\mu},\hat{\rho}}+U_{\hat{\mu}}(n)(-i\,U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})T^b)U_{\hat{\mu}}^{-1}(n-\hat{\nu})U_{\hat{\nu}}(n-\hat{\nu})\delta_{n+\hat{\mu}-\hat{\nu},m}\delta_{\hat{\nu},\hat{\rho}}$$

$$+U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})(-i\,U_{\hat{\mu}}^{-1}(n-\hat{\nu})T^b)U_{\hat{\nu}}(n-\hat{\nu})\delta_{n-\hat{\nu},m}\delta_{\hat{\mu},\hat{\rho}}+U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})(i\,T^bU_{\hat{\nu}}(n-\hat{\nu}))\delta_{n-\hat{\nu},m}\delta_{\hat{\nu},\hat{\rho}}$$

$$-(i\,T^bU_{\hat{\nu}}(n))U_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n)\delta_{n,m}\delta_{\hat{\nu},\hat{\rho}}-U_{\hat{\nu}}(n)(i\,T^bU_{\hat{\mu}}(n+\hat{\nu}))U_{\hat{\nu}}^{-1}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n)\delta_{n+\hat{\nu},m}\delta_{\hat{\mu},\hat{\rho}}$$

$$-U_{\hat{\nu}}(n)U_{\hat{\mu}}(n+\hat{\nu})(-i\,U_{\hat{\nu}}^{-1}(n+\hat{\mu})T^b)U_{\hat{\mu}}^{-1}(n)\delta_{n+\hat{\mu},m}\delta_{\hat{\nu},\hat{\rho}}-U_{\hat{\nu}}(n)U_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})(-i\,U_{\hat{\mu}}^{-1}(n)T^b)\delta_{n,m}\delta_{\hat{\mu},\hat{\rho}}$$

$$-(-i\,U_{\hat{\nu}}^{-1}(n-\hat{\nu})T^b)U_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\delta_{n-\hat{\nu},m}\delta_{\hat{\nu},\hat{\rho}}-U_{\hat{\nu}}^{-1}(n-\hat{\nu})(i\,T^bU_{\hat{\mu}}(n-\hat{\nu}))U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\delta_{n-\hat{\nu},m}\delta_{\hat{\mu},\hat{\rho}}$$

$$-U_{\hat{\nu}}^{-1}(n-\hat{\nu})U_{\hat{\mu}}(n-\hat{\nu})(i\,T^bU_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu}))U_{\hat{\mu}}^{-1}(n)\delta_{n+\hat{\mu}-\hat{\nu},m}\delta_{\hat{\nu},\hat{\rho}}-U_{\hat{\nu}}^{-1}(n-\hat{\nu})U_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})(-i\,U_{\hat{\mu}}^{-1}(n)T^b)\delta_{n,m}\delta_{\hat{\mu},\hat{\rho}}\Big]\Big\}$$

$$=\frac{\beta}{2N}\sum_{\hat{\nu}}(1-\delta_{\hat{\nu},\hat{\mu}})\Big\{\delta_{\hat{\mu},\hat{\rho}}\Big[\delta_{n,m}\mathrm{Tr}\Big[T^aT^b\left(U_{\hat{\mu}\hat{\nu}}(n)+\mathcal{U}_{\hat{\mu}\hat{\nu}}(n)\right)+T^bT^a\left(U_{\hat{\mu}\hat{\nu}}^{-1}(n)+\mathcal{U}_{\hat{\mu}\hat{\nu}}^{-1}(n)\right)\Big]$$

$$-\delta_{n+\hat{\nu},m}\mathrm{Tr}\Big[T^a\left(U_{\hat{\mu}}(n)U_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})T^bU_{\hat{\nu}}^{-1}(n)+U_{\hat{\nu}}(n)T^bU_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n)\right)\Big]$$

$$-\delta_{n-\hat{\nu},m}\mathrm{Tr}\Big[T^a\left(U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})T^bU_{\hat{\nu}}(n-\hat{\nu})+U_{\hat{\nu}}^{-1}(n-\hat{\nu})T^bU_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\right)\Big]\Big]$$

$$+\delta_{\hat{\nu},\hat{\rho}}\Big[-\delta_{n,m}\mathrm{Tr}\Big[T^aT^bU_{\hat{\mu}\hat{\nu}}^{-1}(n)+T^bT^aU_{\hat{\mu}\hat{\nu}}(n)\Big]$$

$$+\delta_{n+\hat{\mu},m}\mathrm{Tr}\Big[T^a\left(U_{\hat{\mu}}(n)T^bU_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n)+U_{\hat{\nu}}(n)U_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})T^bU_{\hat{\mu}}^{-1}(n)\right)\Big]$$

$$+\delta_{n-\hat{\nu},m}\mathrm{Tr}\Big[T^a\left(U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})T^bU_{\hat{\nu}}(n-\hat{\nu})+U_{\hat{\nu}}^{-1}(n-\hat{\nu})T^bU_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\right)\Big]$$

$$-\delta_{n+\hat{\mu}-\hat{\nu},m}\mathrm{Tr}\Big[T^a\left(U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})T^bU_{\hat{\mu}}^{-1}(n-\hat{\nu})U_{\hat{\nu}}(n-\hat{\nu})+U_{\hat{\nu}}^{-1}(n-\hat{\nu})U_{\hat{\mu}}(n-\hat{\nu})T^bU_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\right)\Big]\Big]\Big\}$$

This formula is needed in order to solve parallel transport equations for the tangent space basis. Actually, for computer simulations, it is more convenient to work with a matrix notation: computations for the drift and the Hessian in matrix form are available in Appendix G.

10.1   Vacuum structure

The first step in the thimble approach is to choose a critical point of the action. For Yang-Mills theory, the most natural choice is the classical vacuum $U_{\mathbb{1}}\equiv\{U_{\hat{\mu}}(n)=\mathbb{1}\}$ (that is $A_{\hat{\mu}}(n)=0$ in the algebra). Let us compute the Hessian at the critical point $U_{\mathbb{1}}$

$$\nabla^b_{m,\hat\rho}\nabla^a_{n,\hat\mu}S[U]\big|_{U_\mathbb{1}} = \frac{\beta}{2N}\sum_{\hat\nu}(1-\delta_{\hat\nu,\hat\mu})\Big\{\delta_{\hat\mu,\hat\rho}\big[\delta_{n,m}\mathrm{Tr}\left[2T^aT^b+2T^bT^a\right]$$

$$-\delta_{n+\hat\nu,m}\mathrm{Tr}\left[T^a\left(T^b+T^b\right)\right]-\delta_{n-\hat\nu,m}\mathrm{Tr}\left[T^a\left(T^b+T^b\right)\right]\big]+\delta_{\hat\nu,\hat\rho}\big[-\delta_{n,m}\mathrm{Tr}\left[T^aT^b+T^bT^a\right]$$

$$+\delta_{n+\hat\mu,m}\mathrm{Tr}\left[T^a\left(T^b+T^b\right)\right]+\delta_{n-\hat\nu,m}\mathrm{Tr}\left[T^a\left(T^b+T^b\right)\right]-\delta_{n+\hat\mu-\hat\nu,m}\mathrm{Tr}\left[T^a\left(T^b+T^b\right)\right]\big]\Big\}$$

$$=\frac{\beta}{2N}\sum_{\hat\nu}(1-\delta_{\hat\nu,\hat\mu})\left\{\delta_{\hat\mu,\hat\rho}\left[2\delta_{n,m}-\delta_{n+\hat\nu,m}-\delta_{n-\hat\nu,m}\right]+\delta_{\hat\nu,\hat\rho}\left[-\delta_{n,m}+\delta_{n+\hat\mu,m}+\delta_{n-\hat\nu,m}-\delta_{n+\hat\mu-\hat\nu,m}\right]\right\}\delta^{ab}$$

$$=\frac{\beta}{2N}\delta^{ab}\Big\{\sum_{\hat\nu}\delta_{\hat\mu,\hat\rho}\left[2\delta_{n,m}-\delta_{n+\hat\nu,m}-\delta_{n-\hat\nu,m}\right]+\sum_{\hat\nu}\delta_{\hat\nu,\hat\rho}\left[-\delta_{n,m}+\delta_{n+\hat\mu,m}+\delta_{n-\hat\nu,m}-\delta_{n+\hat\mu-\hat\nu,m}\right]$$

$$-\sum_{\hat\nu}\delta_{\hat\nu,\hat\mu}\delta_{\hat\mu,\hat\rho}\left[2\delta_{n,m}-\delta_{n+\hat\nu,m}-\delta_{n-\hat\nu,m}\right]-\sum_{\hat\nu}\delta_{\hat\nu,\hat\mu}\delta_{\hat\nu,\hat\rho}\left[-\delta_{n,m}+\delta_{n+\hat\mu,m}+\delta_{n-\hat\nu,m}-\delta_{n+\hat\mu-\hat\nu,m}\right]\Big\}$$

$$=\frac{\beta}{2N}\delta^{ab}\Big\{2d\,\delta_{n,m}\delta_{\hat\mu,\hat\rho}-\delta_{\hat\mu,\hat\rho}\sum_{\hat\nu}\left(\delta_{n+\hat\nu,m}+\delta_{n-\hat\nu,m}\right)-\delta_{n,m}+\delta_{n+\hat\mu,m}+\delta_{n-\hat\rho,m}-\delta_{n+\hat\mu-\hat\rho,m}$$

$$-2\delta_{\hat\mu,\hat\rho}\delta_{n,m}+\delta_{\hat\mu,\hat\rho}\delta_{n+\hat\mu,m}+\delta_{\hat\mu,\hat\rho}\delta_{n-\hat\mu,m}+\delta_{\hat\mu,\hat\rho}\delta_{n,m}-\delta_{\hat\mu,\hat\rho}\delta_{n+\hat\mu,m}-\delta_{\hat\mu,\hat\rho}\delta_{n-\hat\mu,m}+\delta_{\hat\mu,\hat\rho}\delta_{n,m}\Big\}$$

$$=\frac{\beta}{2N}\delta^{ab}\left[2d\,\delta_{n,m}\delta_{\hat\mu,\hat\rho}-\delta_{n,m}+\delta_{n+\hat\mu,m}+\delta_{n-\hat\rho,m}-\delta_{n+\hat\mu-\hat\rho,m}-\delta_{\hat\mu,\hat\rho}\sum_{\hat\nu}\left(\delta_{n+\hat\nu,m}+\delta_{n-\hat\nu,m}\right)\right]$$

$$(10.2)$$

where we have used $\mathrm{Tr}\left(T^aT^b\right)=\frac{1}{2}\delta^{ab}$ and d is the number of spacetime dimensions. Notice that the last expression is symmetric under $(n,\hat\mu,a)\leftrightarrow(m,\hat\rho,b)$, as it should be. As we have discussed in Section 4.3, gauge degrees of freedom show up as zero-modes of the Hessian at any critical point. Consider the Hessian at $U_\mathbb{1}$ computed above: it easy to check that vectors defined by

$$V^a_{\hat\mu}(n)=\Lambda^a(n+\hat\mu)-\Lambda^a(n)$$

(where $\Lambda(n)$ is a generic function of the lattice point) are eigenvectors of the Hessian (10.2) with eigenvalue 0. These are precisely the discretized version of infinitesimal gauge transformations $\delta A^a_\mu(x)=\partial_\mu\Lambda^a(x)$ at $A_\mu(x)=0$. The number of these zero-modes equals the number of elements in a basis over which to decompose all possible functions $\Lambda^a(n)$ one can have on a lattice of volume V respecting periodic boundary conditions. This can be easily viewed in Fourier space, that is, using plane waves as a function basis: the number of different plane waves is the number of momenta that are allowed in a periodic lattice, $V(N^2-1)$. However, the momentum $k=0$ should be discarded, as it corresponds to a constant function Λ^a, which gives a null eigenvector (constant gauge transformations leave $U_\mathbb{1}$ unchanged). The conclusion is that the number of gauge-originated zero-modes of the Hessian (10.2) is $(V-1)(N^2-1)$. Later on we will argue that gauge-originated zero-modes pose no problems, as far as only computation of gauge-invariant observables is concerned. However, there is another subtlety with regards to this Hessian. Any vector of the form $V^a_{\hat\mu}$ (that is, constant in spacetime) is an eigenvector with eigenvalue 0. These $d(N^2-1)$ zero-modes are due to *torons*, that is a non-trivial zero-action manifold for the pure gauge action.[59] [106, 107, 108, 109, 110]. Torons pose a serious problem, as they cannot be simply ignored, due to the action (as well as observables) not being invariant under changes of such degrees of freedom.[60] One should note, however, that they are expected to become less and less relevant when going to larger lattice volumes. One possible way out for the toron problem at finite V is to introduce *twisted boundary conditions* [111, 108, 112], that is every time a link crosses the lattice boundaries, it transforms with an appropriate set of *twist matrices*

---

[59]Toronic modes disappear when fermions are introduced in the theory.

[60]For the case of Wilson action around $U_\mathbb{1}$, the $d(N^2-1)$ zero-modes are directions along which the action varies by terms of order >2 [109, 110].

$$U_{\hat{\nu}}(n + L_{\hat{\mu}}\hat{\mu}) = \Omega_{\hat{\mu}} U_{\hat{\nu}}(n) \Omega_{\hat{\mu}}^{\dagger}$$

where $L_{\hat{\mu}}$ is the lattice size along the $\hat{\mu}$-th direction and the (constant) twist matrices $\Omega_{\hat{\mu}} \in \mathrm{SU}(N)$ obey the twist algebra

$$\Omega_{\hat{\nu}}\Omega_{\hat{\mu}} = e^{2\pi i \eta_{\mu\nu}/N} \Omega_{\hat{\mu}}\Omega_{\hat{\nu}}$$

with $\eta_{\mu\nu}$ the (antisymmetric) twist tensor, which has integer components. The gauge group is given by all fields $G(n) \in \mathrm{SU}(N)$ satisfying

$$G(n + L_{\hat{\mu}}\hat{\mu}) = \Omega_{\hat{\mu}} G(n) \Omega_{\hat{\mu}}^{\dagger}$$

It can be shown [111] that this formulation is equivalent to keeping the usual periodic boundary conditions, while substituting the *twisted action* in place of the Wilson one

$$S^{(\mathrm{t})}[U] = \sum_P f_P^{(\mathrm{t})}(U_P)$$

with the action density at each plaquette P [112]

$$f_P^{(\mathrm{t})}(U_P) = \begin{cases} f_P\left(z_{\hat{\mu}\hat{\nu}} U_P\right) & P \in R_{\hat{\mu}\hat{\nu}} \\ f_P\left(U_P\right) & P \notin R_{\hat{\mu}\hat{\nu}} \end{cases}$$

where $f_P(U_P)$ is the ordinary Wilson action density

$$f(U_P) = \beta \left[1 - \frac{1}{2N} \mathrm{Tr}\left(U_P + U_P^{-1}\right)\right]$$

and $z_{\hat{\mu}\hat{\nu}} = z_{\hat{\nu}\hat{\mu}}^{-1} = \bar{z}_{\hat{\nu}\hat{\mu}}$ is

$$z_{\hat{\mu}\hat{\nu}} = e^{2\pi i n_{\hat{\mu}\hat{\nu}}/N} \in Z(N)$$

in which $n_{\hat{\mu}\hat{\nu}}$ is the anti symmetric twist tensor given by a collection of $d(d-1)/2$ integers and $Z(N)$ is the center of $\mathrm{SU}(N)$. $R_{\hat{\mu}\hat{\nu}}$ consists of a particular set of plaquettes (one for each $\hat{\mu}\hat{\nu}$-torus). From now on we will specialize to the case $d = 2$, in which there is only one such plaquette, which we shall name P_0. In 2 dimensions the twist is determined by a single integer $k = 1 \cdots N - 1$, that is $z = e^{2\pi i k/N}$ and it is present only at P_0. Now we shall address the problem of torons by explicitly constructing all the configurations which have $S = 0$, that is global minima of the (twisted) action. We will follow [112]. The first step is to build the so called *gauge tree*, that is we fix the axial gauge and gauge-transform as many links as possible to $\mathbb{1}$. Figure 10.1a highlights such links. What we have done so far is feasible for any generic lattice configuration. Now we notice that (for real β) $S \geq 0$ and $S = 0$ if and only if $f_P^{(\mathrm{t})} = 0$ for every plaquette and thus we try to look for the most general lattice configuration featuring this: in Figure 10.1b we highlight in bold the links that must be set to $\mathbb{1}$ in order to ensure that the action density reaches its minimum. In general, the remaining links need not to be set to $\mathbb{1}$, but any *constant* value (one for each direction) suffices. This gives rise to two *ladders* of constant $U_{\hat{\mu}}(n) = G_{\hat{\mu}}$ and we call them $L_{\hat{\mu}}$ and $L_{\hat{\nu}}$ (in Figure 10.1b they are depicted with dotted lines). Now the only plaquette whose action density is not automatically 0 is P_0. It is immediate to see that $f_P^{(\mathrm{t})}(P_0) = 0$ can be achieved through the twisted commutation relation

$$G_{\hat{\nu}} G_{\hat{\mu}} = z_{\hat{\mu}\hat{\nu}} \, G_{\hat{\mu}} G_{\hat{\nu}}$$

It is this relation that compensates the $z_{\hat{\mu}\hat{\nu}}$ in the twisted action, giving 0. For this reason such configurations are often referred to as *twist eaters*. It is thus obvious that, apart from the usual (local) gauge freedom, one has the ability to choose any set of d matrices $G_{\hat{\mu}} \in \mathrm{SU}(N)$ respecting the twisted commutation relation to form a zero-action configuration. In fact, it can be shown that, calling $\mathcal{N}_0$ the zero-action configuration manifold, it is diffeomorphic to $\otimes^{V-1}\mathrm{SU}(N) \otimes \mathcal{M}_0(z_{\hat{\mu}\hat{\nu}})$, where $\mathcal{M}_0(z_{\hat{\mu}\hat{\nu}})$ is the (twist-dependent) manifold defined by

$$\mathcal{M}_0(z_{\hat{\mu}\hat{\nu}}) = \left\{(G_1, \cdots, G_d) \,\middle|\, G_{\hat{\mu}} \in \mathrm{SU}(N), G_{\hat{\nu}}G_{\hat{\mu}} = z_{\hat{\mu}\hat{\nu}}\, G_{\hat{\mu}}G_{\hat{\nu}}\right\}$$

It is obvious that the dimension of the zero-action manifold is

$$\dim \mathcal{N}_0 = (V-1)(N^2-1) + \dim \mathcal{M}_0(z_{\hat{\mu}\hat{\nu}})$$

It can be shown [112] that, for the usual (untwisted) Wilson action

$$\dim \mathcal{M}_0 = (N-1)(N+d)$$

The toron manifold in this case is highly non-trivial: for example, we have both *regular* torons as well as *singular* torons [109, 108, 110]. The configuration $U_{\mathbb{1}}$ belongs to the second type. For this kind of configuration, the $d(N^2-1)$ eigenvectors with 0 eigenvalue correspond to directions along which the action has a quartic growth. Now let us consider the twisted action. In 2 dimensions, the general result concerning twist eaters is the following [112]: given a (simple) twist $z_{\hat{\mu}\hat{\nu}} = z = e^{2\pi i k/N} \neq 1$ with k coprime with N, we have

$$\dim \mathcal{M}_0 = N^2 - 1$$

and any configuration in $\mathcal{M}_0$ is equivalent to any other by a *global gauge transformation*. This is precisely the sought after result, as we have got rid of toronic degrees of freedom completely. It is thus to be expected that the Hessian of the twisted action, computed at a twist eater configuration, exhibits only $V(N^2-1)$ null eigenvalues, all corresponding to (local and global[61]) gauge transformations. Now let us construct a twist eating configuration for $\mathrm{SU}(N)$ in 2 dimensions [112]. First, choose a phase factor c such that

$$c^N = (-1)^{N-1}$$

then choose a set of N orthonormal vectors $\{|v_j\rangle\}_{j=0\cdots N-1}$. G_1 and G_2 are defined by

$$G_1|v_j\rangle = cz^{-j}|v_j\rangle$$

$$G_2|v_j\rangle = c|v_{j+1}\rangle$$

for $j = 0 \cdots N-1$ and $|v_N\rangle = |v_0\rangle$. It can be shown that the choice of c is irrelevant. For $\mathrm{SU}(2)$ (where $z = -1$ is the only possible twist) a possible choice is

$$G_1 = i\,\sigma_1 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$$

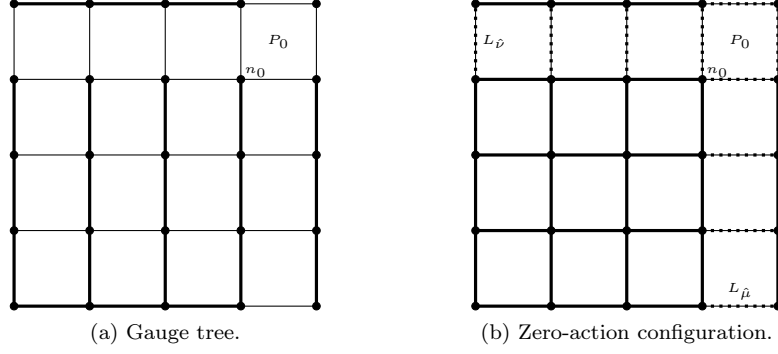$$G_2 = i\,\sigma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

(a) Gauge tree.   (b) Zero-action configuration.

Figure 10.1: Gauge tree and zero-action configurations for Yang-Mills theory in 2 dimensions with twisted action.

where σ_i is the i-th Pauli matrix.

We have already provided an expression for the twisted action, but we still have to compute the twisted drift as well as the twisted Hessian. Denoting n_0 the lattice site on which the twisted plaquette P_0 lies, we have

$$
\nabla^a_{n,\hat{\mu}} S^{(t)}[U] = -\frac{\beta}{2N} \sum_{\hat{\nu} \neq \hat{\mu}} \mathrm{Tr}\, \nabla^a_{n,\hat{\mu}} \left(c_U \, \rule{0pt}{0pt} + c_{\mathcal{U}} \, \rule{0pt}{0pt} + c_{\mathcal{U}}^{-1} \, \rule{0pt}{0pt} + c_U^{-1} \, \rule{0pt}{0pt} \right)
$$

$$
= -\frac{i\beta}{2N} \sum_{\hat{\nu} \neq \hat{\mu}} \mathrm{Tr}\, \left[T^a \left(c_U U_{\hat{\mu}\hat{\nu}}(n) + c_{\mathcal{U}} \mathcal{U}_{\hat{\mu}\hat{\nu}}(n) - c_U^{-1} U_{\hat{\mu}\hat{\nu}}^{-1}(n) - c_{\mathcal{U}}^{-1} \mathcal{U}_{\hat{\mu}\hat{\nu}}^{-1}(n) \right) \right]
$$

where the c coefficients are defined by (the marked point is n_0)

$$
c_U = \begin{cases} z \\ z^{-1} \\ 1 \end{cases} = 1 + \delta_{n,n_0} \delta_{\hat{\mu},\hat{1}}(z-1) + \delta_{n,n_0} \delta_{\hat{\mu},\hat{2}}(z^{-1}-1)
$$

$$
c_{\mathcal{U}} = \begin{cases} z \\ z^{-1} \\ 1 \end{cases} = 1 + \delta_{n,n_0+\hat{1}} \delta_{\hat{\mu},\hat{2}}(z-1) + \delta_{n,n_0+\hat{2}} \delta_{\hat{\mu},\hat{1}}(z^{-1}-1)
$$

The twisted Hessian is

---

[61] Twist eating configurations are not invariant under global gauge transformations, unlike $U_{\mathbb{1}}$.

$$\nabla^b_{m,\hat{\rho}}\nabla^a_{n,\hat{\mu}}S^{(\mathrm{t})}[U]$$

$$=-\frac{i}{2N}\frac{\beta}{\sum_{\hat{\nu}}}(1-\delta_{\hat{\nu},\hat{\mu}})\mathrm{Tr}\Big\{T^a\Big[c_U\big(i\,T^b U_{\hat{\mu}}(n)\big)U_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n)\delta_{n,m}\delta_{\hat{\mu},\hat{\rho}}+c_U U_{\hat{\mu}}(n)\big(i\,T^b U_{\hat{\nu}}(n+\hat{\mu})\big)U_{\hat{\mu}}^{-1}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n)\delta_{n+\hat{\mu},m}\delta_{\hat{\nu},\hat{\rho}}$$

$$+c_U U_{\hat{\mu}}(n)U_{\hat{\nu}}(n+\hat{\mu})\big(-i\,U_{\hat{\mu}}^{-1}(n+\hat{\nu})T^b\big)U_{\hat{\nu}}^{-1}(n)\delta_{n+\hat{\nu},m}\delta_{\hat{\mu},\hat{\rho}}+c_U U_{\hat{\mu}}(n)U_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})\big(-i\,U_{\hat{\nu}}^{-1}(n)T^b\big)\delta_{n,m}\delta_{\hat{\nu},\hat{\rho}}$$

$$+c_{\mathcal{U}}\big(i\,T^b U_{\hat{\mu}}(n)\big)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})U_{\hat{\nu}}(n-\hat{\nu})\delta_{n,m}\delta_{\hat{\mu},\hat{\rho}}+c_{\mathcal{U}} U_{\hat{\mu}}(n)\big(-i\,U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})T^b\big)U_{\hat{\mu}}^{-1}(n-\hat{\nu})U_{\hat{\nu}}(n-\hat{\nu})\delta_{n+\hat{\mu}-\hat{\nu},m}\delta_{\hat{\nu},\hat{\rho}}$$

$$+c_{\mathcal{U}} U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})\big(-i\,U_{\hat{\mu}}^{-1}(n-\hat{\nu})T^b\big)U_{\hat{\nu}}(n-\hat{\nu})\delta_{n-\hat{\nu},m}\delta_{\hat{\mu},\hat{\rho}}+c_{\mathcal{U}} U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})\big(i\,T^b U_{\hat{\nu}}(n-\hat{\nu})\big)\delta_{n-\hat{\nu},m}\delta_{\hat{\nu},\hat{\rho}}$$

$$-c_U^{-1}\big(i\,T^b U_{\hat{\nu}}(n)\big)U_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n)\delta_{n,m}\delta_{\hat{\nu},\hat{\rho}}-c_U^{-1}U_{\hat{\nu}}(n)\big(i\,T^b U_{\hat{\mu}}(n+\hat{\nu})\big)U_{\hat{\nu}}^{-1}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n)\delta_{n+\hat{\nu},m}\delta_{\hat{\mu},\hat{\rho}}$$

$$-c_U^{-1}U_{\hat{\nu}}(n)U_{\hat{\mu}}(n+\hat{\nu})\big(-i\,U_{\hat{\nu}}^{-1}(n+\hat{\mu})T^b\big)U_{\hat{\mu}}^{-1}(n)\delta_{n+\hat{\mu},m}\delta_{\hat{\nu},\hat{\rho}}-c_U^{-1}U_{\hat{\nu}}(n)U_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})\big(-i\,U_{\hat{\mu}}^{-1}(n)T^b\big)\delta_{n,m}\delta_{\hat{\mu},\hat{\rho}}$$

$$-c_{\mathcal{U}}^{-1}\big(-i\,U_{\hat{\nu}}^{-1}(n-\hat{\nu})T^b\big)U_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\delta_{n-\hat{\nu},m}\delta_{\hat{\nu},\hat{\rho}}-c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})\big(i\,T^b U_{\hat{\mu}}(n-\hat{\nu})\big)U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\delta_{n-\hat{\nu},m}\delta_{\hat{\mu},\hat{\rho}}$$

$$-c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})U_{\hat{\mu}}(n-\hat{\nu})\big(i\,T^b U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})\big)U_{\hat{\mu}}^{-1}(n)\delta_{n+\hat{\mu}-\hat{\nu},m}\delta_{\hat{\nu},\hat{\rho}}-c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})U_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})\big(-i\,U_{\hat{\mu}}^{-1}(n)T^b\big)\delta_{n,m}\delta_{\hat{\mu},\hat{\rho}}\Big]\Big\}$$

$$=\frac{\beta}{2N}\sum_{\hat{\nu}}(1-\delta_{\hat{\nu},\hat{\mu}})\Big\{\delta_{\hat{\mu},\hat{\rho}}\Big[\delta_{n,m}\mathrm{Tr}\Big[T^a T^b(c_U U_{\hat{\mu}\hat{\nu}}(n)+c_{\mathcal{U}}\mathcal{U}_{\hat{\mu}\hat{\nu}}(n))+T^b T^a\big(c_U^{-1}U_{\hat{\mu}\hat{\nu}}^{-1}(n)+c_{\mathcal{U}}^{-1}\mathcal{U}_{\hat{\mu}\hat{\nu}}^{-1}(n)\big)\Big]$$

$$-\delta_{n+\hat{\nu},m}\mathrm{Tr}\Big[T^a\big(c_U U_{\hat{\mu}}(n)U_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})T^b U_{\hat{\nu}}^{-1}(n)+c_U^{-1}U_{\hat{\nu}}(n)T^b U_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n)\big)\Big]$$

$$-\delta_{n-\hat{\nu},m}\mathrm{Tr}\Big[T^a\big(c_{\mathcal{U}}U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})T^b U_{\hat{\nu}}(n-\hat{\nu})+c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})T^b U_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\big)\Big]\Big]$$

$$+\delta_{\hat{\nu},\hat{\rho}}\Big[-\delta_{n,m}\mathrm{Tr}\Big[T^a T^b c_U^{-1}U_{\hat{\mu}\hat{\nu}}^{-1}(n)+T^b T^a c_U U_{\hat{\mu}\hat{\nu}}(n)\Big]$$

$$+\delta_{n+\hat{\mu},m}\mathrm{Tr}\Big[T^a\big(c_U U_{\hat{\mu}}(n)T^b U_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n)+c_U^{-1}U_{\hat{\nu}}(n)U_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})T^b U_{\hat{\mu}}^{-1}(n)\big)\Big]$$

$$+\delta_{n-\hat{\nu},m}\mathrm{Tr}\Big[T^a\big(c_{\mathcal{U}}U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})T^b U_{\hat{\nu}}(n-\hat{\nu})+c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})T^b U_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\big)\Big]$$

$$-\delta_{n+\hat{\mu}-\hat{\nu},m}\mathrm{Tr}\Big[T^a\big(c_{\mathcal{U}}U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})T^b U_{\hat{\mu}}^{-1}(n-\hat{\nu})U_{\hat{\nu}}(n-\hat{\nu})+c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})U_{\hat{\mu}}(n-\hat{\nu})T^b U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\big)\Big]\Big]\Big\}$$

10.2 Integration on a gauge-symmetric thimble

We have set up a zero-action configuration (that is, the twist eater) which is unique up to gauge transformations. We call this configuration U_0 and attach to it the (stable) thimble $\mathcal{J}_0$. Being U_0 part of the original domain of integration $\otimes_{n,\hat{\mu}}\mathrm{SU}(N)$, it has $\mathfrak{n}_0 = 1$. In this section we consider the problem of integrating over $\mathcal{J}_0$. Let us begin discussing the preparation of the initial condition near U_0 for the integration of SA equations. As discussed is Section 4.3, U_0 belongs to a critical manifold $\mathcal{M}_0$ of gauge-transformed copies of U_0, that is

$$\mathcal{M}_0 \equiv \Big\{\{U^G_{0\,\hat{\mu}}(n)\} \,\big|\, \exists\,\{G(n)\} \in \underset{n}{\otimes}\,\mathrm{SU}(N) : U^G_{0\,\hat{\mu}}(n) = G(n)U_{0\,\hat{\mu}}(n)G^\dagger(n+\hat{\mu}) \ \forall\,n,\hat{\mu}\Big\}$$

Suppose now that we start in the vicinity of U_0 (at $t_0 \to -\infty$) and integrate SA equations until a time t, calling the final configuration $U(t)$. Let us now consider a gauge-transformed starting configuration $U_0^G \in \mathcal{M}_0$ (so that $U^G_{0\hat{\mu}}(n) = G(n)U_{0\,\hat{\mu}}(n)G^\dagger(n+\hat{\mu})$ for some G); we can integrate SA equations starting near U_0^G as well, provided that we know the tangent space $T_{U_0^G}\mathcal{J}_0$ to the thimble at U_0^G. Let us call $U^G(t)$ the evolved configuration at time t. Being the gauge transformation G *rigid*, that is time independent, it "rotates" the whole thimble [26], so that we have $U^G_{\hat{\mu}}(n;t) = G(n)U_{\hat{\mu}}(n;t)G^\dagger(n+\hat{\mu})$, that is $U^G(t)$ is the same as $U(t)$ after the gauge transformation. This procedure is depicted in Figure 10.2.

These considerations teach us that, in order to cover the whole thimble, we have to start at every possible configuration in $\mathcal{M}_0$ and integrate the SA equations. Thus we need to compute the tangent space to the thimble at the configuration U_0^G. We know that, at U_0, $T_{U_0}\mathcal{J}_0 = T_{U_0}\mathcal{M}_0 \oplus N^+_{U_0}\mathcal{M}_0$, with $T_{U_0}\mathcal{M}_0$ spanned by
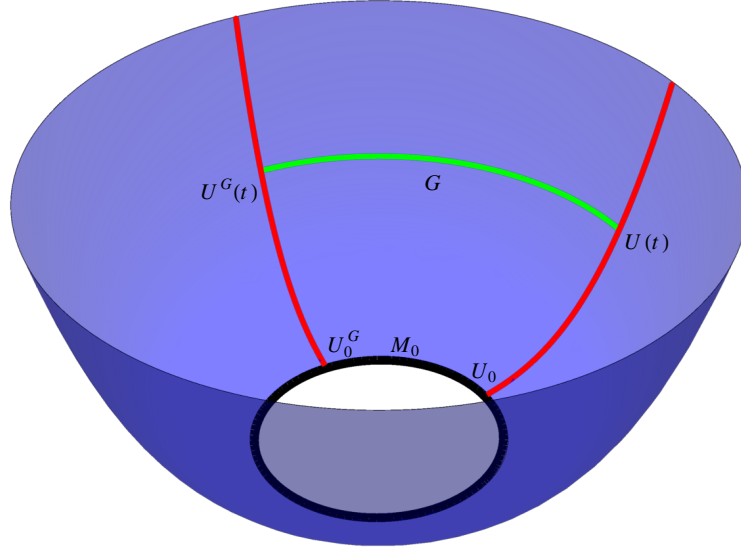
Figure 10.2: Integration of SA curves (in red) starting from U_0 as well as from a gauge-transformed configuration U_0^G, both belonging to the critical manifold $\mathcal{M}_0$ (in black). The thimble is pictorially represented with a bowl emanating from $\mathcal{M}_0$. The gauge transformation G connecting $U(t)$ and $U^G(t)$ is shown in green. The same gauge transformation connects U_0 and U_0^G in the critical manifold $\mathcal{M}_0$.

the n_G Takagi vectors of $H(S; U_0)$ with *zero* Takagi value[62] and $N_{U_0}^+ \mathcal{M}_0$ spanned by the n_+ Takagi vectors of $H(S; U_0)$ with *positive* Takagi value. The number of such vectors is $n_+ = n - n_G$, with $n = Vd(N^2 - 1)$ the total number of degrees of freedom and $n_G = V(N^2 - 1)$ the number of gauge degrees of freedom, which means that $n_+ = V(d - 1)(N^2 - 1)$. We can easily compute the Takagi vectors $\{v^{G(i)}\}$ spanning $T_{U_0^G} \mathcal{J}_0$ given the Takagi vectors $\{v^{(i)}\}$ spanning $T_{U_0} \mathcal{J}_0$. Consider a couple of configurations $U(t_0)$ and $U^G(t_0)$ with $|c_i| \ll 1$, so that they are close to $\mathcal{M}_0$, that is[63]

$$U_{\hat{\mu}}(n; t_0) = e^{i \sum_i c_i v_{n\hat{\mu},a}^{(i)} T^a} U_{0\,\hat{\mu}}(n)$$

$$U_{\hat{\mu}}^G(n; t_0) = e^{i \sum_i c_i v_{n\hat{\mu},a}^{G(i)} T^a} U_{0\,\hat{\mu}}^G(n)$$

Let us set

$$G(n) = e^{i\, g_{n,a} T^a}$$

The previous considerations lead to setting $U_{\hat{\mu}}^G(n; t_0) = G(n) U_{\hat{\mu}}(n; t_0) G^\dagger(n + \hat{\mu})$, which imply

---

[62]Directions tangent to $\mathcal{M}_0$ at U_0 represent infinitesimal gauge transformations around U_0.

[63]We generically take $|c_i| \ll 1$ in order not to leave $T_U \mathcal{J}_0$ while leaving the critical point U. This condition is automatically ensured for directions corresponding to $\lambda_i > 0$: for these directions $c_i = n_i e^{\lambda_i t_0}$ with $t_0 \to -\infty$, so that we can safely take $n_i = \mathcal{O}(1)$. For directions corresponding to $\lambda_i = 0$, however, the coefficients c_i have to be taken small explicitly.

$$e^{i\sum_i c_i v^{G(i)}_{n\hat{\mu},a} T^a} U^G_{0\,\hat{\mu}}(n) = G(n) e^{i\sum_i c_i v^{(i)}_{n\hat{\mu},a} T^a} U_{0\,\hat{\mu}}(n) G^\dagger(n+\hat{\mu})$$

$$\Rightarrow e^{i\sum_i c_i v^{G(i)}_{n\hat{\mu},a} T^a} G(n) U_{0\,\hat{\mu}}(n) G^\dagger(n+\hat{\mu}) = G(n) e^{i\sum_i c_i v^{(i)}_{n\hat{\mu},a} T^a} U_{0\,\hat{\mu}}(n) G^\dagger(n+\hat{\mu})$$

$$\Rightarrow G(n) e^{i\sum_i c_i v^{(i)}_{n\hat{\mu},a} T^a} G^{-1}(n) = e^{i\sum_i c_i v^{G(i)}_{n\hat{\mu},a} T^a}$$

$$\Rightarrow e^{i\,g_{n,a} T^a} e^{i\sum_i c_i v^{(i)}_{n\hat{\mu},a} T^a} e^{-i\,g_{n,a} T^a} = e^{i\sum_i c_i v^{G(i)}_{n\hat{\mu},a} T^a}$$

Now we can make use of the lemma in Appendix B, setting $g_a \rightarrow g_{n,a}$ and $x_b \rightarrow \sum_i c_i v^{(i)}_{n\hat{\mu},b}$. The conclusion is

$$v^{G(i)}_{n\hat{\mu},a} = M^{(n)}_{ab} v^{(i)}_{n\hat{\mu},b} \tag{10.3}$$

with

$$M^{(n)}_{ab} = \left(e^{i\,g_{n,c} t^c} \right)_{ab}$$

where $\{t^c\}$ are the generators of $\mathfrak{su}(N)$ in the adjoint representation. Notice that the "rotation" of $v^{(i)}$ does not mix different vectors; it also only affects color components. We have now a recipe to compute the tangent space to $\mathcal{J}_0$ at any configuration $U \in \mathcal{M}_0$. It is worth noting that the transformation law (10.3) holds for all vectors of $T_{U^G_0}\mathcal{J}_0$: those spanning $N^+_{U^G_0}\mathcal{M}_0$ as well as those spanning $T_{U^G_0}\mathcal{M}_0$. It is manifest that the previous proof extends beyond the vicinity of the critical point U_0: with a reasoning similar to that in Section 4.3, we can set

$$U'_{\hat{\mu}}(n) = e^{i\sum_i \delta y_i V^{(i)}_{n\hat{\mu},a}(t) T^a} U_{\hat{\mu}}(n)$$

$$U'^{G}_{\hat{\mu}}(n) = e^{i\sum_i \delta y_i V^{G(i)}_{n\hat{\mu},a}(t) T^a} U^G_{\hat{\mu}}(n)$$

where $\{V^{(i)}(t)\}$ is a local basis for $T_U \mathcal{J}_0$ and U' belongs to a neighbourhood of $U \in \mathcal{J}_0$. As we know from (5.11), $\delta y_i \in \mathbb{R}$ is only dependent on the choice of $\hat{n}$. The very same proof of (10.3) now leads to the transformation

$$V^{G(i)}_{n\hat{\mu},a} = \mathcal{M}_{n\hat{\mu}a,m\hat{\nu}b} V^{(i)}_{m\hat{\nu},b} \tag{10.4}$$

for the local tangent space basis at *any* point on $\mathcal{J}_0$ (we have set $\mathcal{M}_{n\hat{\mu}a,m\hat{\nu}b} \equiv \delta_{n,m}\delta_{\hat{\mu},\hat{\nu}} M^{(n)}_{ab}$). Equation (10.4) does not come as a surprise, given (10.3) and the linearity of PT equations. A consideration is now due: because gauge transformations rigidly rotate the whole thimble as described above, integrations of all the SA curves starting from every configuration in $\mathcal{M}_0$ is redundant, if we are concerned only with *gauge-invariant observables* (for example the action density). We can choose any configuration, say U_0, in $\mathcal{M}_0$ and integrate the SA equations starting only along the n_+ directions of $N^+_{U_0}\mathcal{M}_0$, as the other n_G directions of $T_{U_0}\mathcal{M}_0$ correspond to infinitesimal gauge transformations around U_0.[64]

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[64]Neglecting all gauge copies of U_0 in $\mathcal{M}_0$ (along with infinitesimal ones corresponding to directions in $T_{U_0}\mathcal{M}_0$) is effectively a *gauge fixing* (although an unusual one) and, where the action $S(U)$ as well as any other gauge-invariant observable $O(U)$ are manifestly unaffected by this, one could be concerned with the effect on $\det V(t)$. It is immediate to show that this is gauge-invariant as well. Consider (10.4) and the definition of the matrix $V(t)$

10.3 Tangent space at a twist-eating configuration

We have shown that for the computation of expectation values of gauge-invariant observables it is enough to fix a single critical point $U_0 \in \mathcal{M}_0$ (namely, the twist eater) and start integrating SA equation only along directions of $N_{U_0}^+ \mathcal{M}_0$, neglecting all the directions of $T_{U_0}\mathcal{M}_0$. Still, we have to parallel transport a whole n-dimensional basis of $T_U \mathcal{J}_0$ along the flow of SA equations. To this purpose, we compute Takagi vectors of $N_{U_0}^+ \mathcal{M}_0$ by numerically diagonalizing $H(S_R; U_0)$ and making use of the relation between eigenvectors of $H(S_R; U_0)$ and Takagi vectors of $H(S; U_0)$, as described in Section 3.6 and Appendix A. Vectors of $T_{U_0}\mathcal{M}_0$ have zero eigenvalue, so it is not trivial to extract the n_G eigenvectors of $H(S_R; U_0)$ corresponding to gauge transformations in $SU(N)$ from the (degenerate) set of $2n_G$ eigenvectors with zero eigenvalue.[65] Fortunately, we can easily compute such "gauge vectors" analytically. As described in Section 10.1, a basis of gauge vectors $\{v^{(i)}\}$ corresponds to a basis of functions $\{\delta g^{(i)}\}$ on the lattice respecting periodic boundary conditions. Considering local as well as global gauge transformations, we have a basis of $V(N^2 - 1)$ functions. Let v be a Takagi vector of $H(S; U_0)$ with zero Takagi value corresponding to the function δg parametrizing an infinitesimal gauge transformation around U_0. An infinitesimal displacement around U_0 along the direction of v realizes such gauge transformation, that is

$$e^{i\varepsilon v_{n\hat{\mu},a} T^a} U_{0\,\hat{\mu}}(n) = e^{i\delta g_a(n) T^a} U_{0\,\hat{\mu}}(n) e^{-i\delta g_a(n+\hat{\mu}) T^a}$$

with $\varepsilon \ll 1$. This, after setting

$$U_{0\,\hat{\mu}} = e^{i\phi_{0\,\hat{\mu}}^a(n) T^a} \tag{10.5}$$

as well as

$$M_{ab}(n, \hat{\mu}) = \left(e^{i\phi_{0\,\hat{\mu}}^c(n) t^c} \right)_{ab}$$

becomes (using again the lemma in Appendix B)

$$e^{i\varepsilon v_{n\hat{\mu},a} T^a} = e^{i\delta g_a(n) T^a} U_{0\,\hat{\mu}}(n) e^{-i\delta g_a(n+\hat{\mu}) T^a} U_{0\,\hat{\mu}}^{-1}(n) = e^{i\delta g_a(n) T^a} e^{i\phi_{0\,\hat{\mu}}^a(n) T^a} e^{-i\delta g_a(n+\hat{\mu}) T^a} e^{-i\phi_{0\,\hat{\mu}}^a(n) T^a}$$

$$= e^{i\delta g_a(n) T^a} e^{-i M_{ab} \delta g_b(n+\hat{\mu}) T^a} = e^{i\left[\delta g_a(n) - M_{ab}(n,\hat{\mu}) \delta g_b(n+\hat{\mu}) + \mathcal{O}(\delta g^2)\right] T^a}$$

Thus we have an expression for v

$$\varepsilon \, v_{n\hat{\mu},a} = \delta g_a(n) - \left(e^{i\phi_{0\,\hat{\mu}}^c(n) t^c} \right)_{ab} \delta g_b(n + \hat{\mu})$$

Let us now consider a 2-dimensional $L \times L$ lattice and a twist-eating configuration U_0 (such as that introduced in Section 10.1). Then $\phi_{0,\hat{\mu}}^a(n)$ (related to $U_{0,\hat{\mu}}(n)$ by (10.5)) is given by

$$\phi_{0,\hat{\mu}}^a(n) = \begin{cases} \Gamma_{\hat{\mu}}^a & \text{if } n_{\hat{\mu}} = L \\ 0 & \text{otherwise} \end{cases} = \delta(n_1 - L)\delta_{\hat{\mu},\hat{1}} \Gamma_{\hat{1}}^a + \delta(n_2 - L)\delta_{\hat{\mu},\hat{2}} \Gamma_{\hat{2}}^a$$

$$V_{ij}^G = V_i^{G(j)} = \mathcal{M}_{ik} V_k^{(j)} = \mathcal{M}_{ik} V_{kj} = (\mathcal{M}V)_{ij}$$

where we have made use of the multi-index $i = (n, \hat{\mu}, a)$ and $k = (m, \hat{\nu}, b)$. As a consequence, $\det V^G = \det \mathcal{M} \det V = \det V$, because

$$\det \mathcal{M} = \prod_n \prod_{\hat{\mu}} \det M^{(n)} = 1$$

where $\det M^{(n)} = 1$ thanks to t^c being traceless.

[65]The $2n_g$ eigenvectors of $H(S_R; U_0)$ correspond to all the possibile gauge transformations in $SL(N, \mathbb{C})$.

with $n = (n_1, n_2)$ and $G_{\hat{\mu}} = e^{i \Gamma^a_{\hat{\mu}} T^a}$ the (constant) links on the two ladders. For v it follows

$$\varepsilon\, v_{n\hat{\mu},a} = \begin{cases} \delta g_a(n) - \left(e^{i \Gamma^c_{\hat{\mu}} t^c}\right)_{ab} \delta g_b(n + \hat{\mu}) & \text{if } n_{\hat{\mu}} = L \\ \delta g_a(n) - \delta g_a(n + \hat{\mu}) & \text{otherwise} \end{cases} \tag{10.6}$$

where we immediately recover the usual expression for infinitesimal gauge transformations around $\mathbb{1}$ for the links in the bulk. In order to generate a set $\{v^{(i)}_{n\hat{\mu}a}\}$ of gauge vectors, we simply have to choose a basis of functions $\{\delta g^{(i)}_a(n)\}$. We can work in Fourier space and choose a basis of plane waves; then there is a single vector representing constant gauge transformations (corresponding to $k = 0$). However, it is simpler to work in configuration space and choose the canonical basis $\delta g^{(m,b)}_a(n) \sim \delta_{n,m} \delta_{a,b}$, where we have split the index $i = 1 \cdots n_G = V(N^2 - 1)$ into a spacetime and a colour component (with respect to this basis, constant gauge transformations correspond to linear combinations of all basis vectors). So far we have put ε in front of v to be consistent with δg being infinitesimal. What one actually does is computing v accordingly to (10.6) in the canonical basis $\{\delta g^{(i)}_a(n)\}$ in configuration space and then normalizing the vector.

Consider the case of SU(2). For our choice of twist matrices, that is $G_{\hat{\mu}} = i \sigma_{\hat{\mu}}$ with $\hat{\mu} = 1, 2$, we have $\Gamma^a_{\hat{\mu}} = \pi \delta_{\hat{\mu},a}$. This can be easily checked by writing

$$G_{\hat{\mu}} = e^{i \Gamma^a_{\hat{\mu}} T^a} = e^{i \Gamma^a_{\hat{\mu}} \sigma^a / 2} = e^{i \theta_{\hat{\mu}} (\hat{n}_{\hat{\mu}} \cdot \vec{\sigma})}$$

which holds after setting $2 \theta_{\hat{\mu}} \hat{n}^a_{\hat{\mu}} = \Gamma^a_{\hat{\mu}}$ ($\hat{n}_{\hat{\mu}}$ is a 3-dimensional unit vector and $\theta_{\hat{\mu}} \in [0, 2\pi]$). We now make use of the well-known relation for Pauli matrices

$$e^{i \theta (\hat{n} \cdot \vec{\sigma})} = \cos \theta\, \mathbb{1}_{2 \times 2} + i \sin \theta\, (\hat{n} \cdot \vec{\sigma})$$

In our case this leads to

$$e^{i \theta_{\hat{\mu}} (\hat{n}_{\hat{\mu}} \cdot \vec{\sigma})} = \cos \theta_{\hat{\mu}}\, \mathbb{1}_{2 \times 2} + i \sin \theta_{\hat{\mu}}\, (\hat{n}_{\hat{\mu}} \cdot \vec{\sigma}) = G_{\hat{\mu}} = i \sigma_{\hat{\mu}}$$

which implies $\theta_{\hat{\mu}} = \pi/2$ and $\hat{n}^a_{\hat{\mu}} = \delta_{\hat{\mu},a}$. We now compute $e^{i \Gamma^c_{\hat{\mu}} t^c} = e^{i \pi t^{\hat{\mu}}}$ using the adjoint representation of $\mathfrak{su}(2)$, that is $(t^c)_{ab} = -i\, f^{cab} = -i\, \epsilon^{cab}$. The explicit expression for the generators is

$$t^1 = -i \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \qquad t^2 = -i \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad t^3 = -i \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

which leads to

$$e^{i \pi t^1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$e^{i \pi t^2} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Thus we can set

$$\left(e^{i \Gamma^c_{\hat{\mu}} t^c}\right)_{ab} = \tau^a_{\hat{\mu}} \delta_{ab}$$

with

$$\tau_{\hat{\mu}}^a = \left(\delta_{\hat{\mu},\hat{1}} - \delta_{\hat{\mu},\hat{2}}\right)\delta_{a1} + \left(-\delta_{\hat{\mu},\hat{1}} + \delta_{\hat{\mu},\hat{2}}\right)\delta_{a2} + \left(-\delta_{\hat{\mu},\hat{1}} - \delta_{\hat{\mu},\hat{2}}\right)\delta_{a3}$$

The conclusion is that we can write, for SU(2) on a $L \times L$ lattice

$$\varepsilon\, v_{n\hat{\mu},a} = \begin{cases} \delta g_a(n) - \tau_{\hat{\mu}}^a \delta g_a(n+\hat{\mu}) & \text{if } n_{\hat{\mu}} = L \\ \delta g_a(n) - \delta g_a(n+\hat{\mu}) & \text{otherwise} \end{cases}$$

which holds in a neighbourhood of the twist eater. If we choose the aforementioned canonical basis for δg in configuration space, then it is manifest that such vectors are not orthonormal. A set of orthonormal gauge vectors spanning the same space can be obtained *e.g.* by means of Gram-Schmidt procedure.

11   Conclusions and outlook

Thimble regularization is still young enough to make us confront open problems. There are theoretical issues, among which the enumeration of critical points and the fundamental related question of how many of them do contribute to the solution. There are computational issues as well: since we lack a local characterization of these (non-trivial) manifolds, devising algorithms which efficiently sample them is a challenging task (even not leaving the manifold can be at some point an issue). In view of this, we do need extensive tests in models which are less and less trivial. In this spirit, we have in this work studied several models. Even the simpler ones (*e.g.* the ϕ^4 zero-dimensional model, $SU(N)$ one-link models and $0 + 1$ QCD) proved to be a very interesting setting for the discussion of the above mentioned non-trivial issues. We did encounter examples of the relevance of more than one critical point. We also had the chance to test new algorithmic solutions such as those discussed in Section 5.3. The Chiral Random Matrix model provided an example in which the dimensionality of the problem could be tuned explicitly. In this case, in the range of parameters we explored we found just one critical point to be relevant. While numerical simulations are not yet available, we also addressed thimble regularization of Yang-Mills theories, where a general framework for handling gauge symmetry has been pinned down.

The possible relevance of different critical points was discussed in Section 3.4, where universality as well as thermodynamic arguments were given in support of a scenario in which a single thimble could be dominant. This issue is of utmost importance when one faces realistic theories such as QCD, where an explicit enumeration of all critical points (in complexified space) is a very hard task [113]. On one hand, more and more results are becoming available from which it is clear that in many cases more than one thimble do contribute to the solution of the problem. On the other hand, we still lack a realistic model in which a real thermodynamic limit is in place; it is in this limit that one can expect the single thimble dominance scenario to hold.

As for algorithmic issues, in any case the most demanding task is solving parallel transport equations for the tangent space basis. Since the total number of basis vector components grows quadratically with the number of degrees of freedom of the system, it will be eventually mandatory to rely on heavy parallelization. More efficient ways to compute $\det V$ appearing in (5.15) that do not require parallel transport of the whole tangent space basis are under investigation [59, 114].

All in all, thimble regularization is a very powerful and general framework for the study of quantum field theories. Being based on first principles, its applications could in principle go far beyond a treating of the sign problem (any theory in any region of its parameter space can be regularized on thimbles). A great advantage of this method is its close connection to classical physics: it retains an immediate link with semiclassical expansion and perturbation theory around vacua which may well be non-trivial. Numerical computations on thimbles may also provide a valuable tool to relate perturbative and non-perturbative physics in the context of resurgence [53]. Besides being itself a very powerful tool to tackle the sign problem, the thimble approach may also shed some light on other approaches to the latter (*e.g.* an insight on the reasons behind occasional bad convergence of complex Langevin may come from an analysis in terms of thimbles [115, 116, 117, 86]).

A   Relation between eigenvectors and Takagi vectors

Let us introduce the vector notation

$$v = \begin{pmatrix} v_R \\ v_I \end{pmatrix} \in \mathbb{R}^{2n \times 1}$$

from which it follows that $\mathcal{P}v = (\mathbb{1}_{n\times n} \; i\,\mathbb{1}_{n\times n})\,v = v_R + i\,v_I \in \mathbb{C}^{n\times 1}$. Suppose that v is an eigenvector of $H(S_R; p_\sigma)$ with eigenvalue $\pm\lambda$. In vector notation this reads (we set $H \equiv H(S; p_\sigma) = \Re(H) + i\,\Im(H) \in \mathbb{C}^{n\times n}$)

$$\begin{pmatrix} \Re(H) & -\Im(H) \\ -\Im(H) & -\Re(H) \end{pmatrix} \begin{pmatrix} v_R \\ v_I \end{pmatrix} = \pm\lambda \begin{pmatrix} v_R \\ v_I \end{pmatrix}$$

which implies

$$\begin{cases} \Re(H)v_R - \Im(H)v_I = \pm\lambda v_R \\ -\Im(H)v_R - \Re(H)v_I = \pm\lambda v_I \end{cases}$$

Suppose that v is normalized so that $\sum_i v_i^2 = v_R^T v_R + v_I^T v_I = 1$. Now we show that $\mathcal{P}v$ is a Takagi vector of H with Takagi value $\pm\lambda$, that is $(\mathcal{P}v)^T H(\mathcal{P}v) = \pm\lambda$

$$\left(\mathcal{P}v\right)^T H(\mathcal{P}v) = (v_R + i\,v_I)^T \left(\Re(H) + i\,\Im(H)\right)(v_R + i\,v_I)$$

$$= \left(v_R^T + i\,v_I^T\right)\left[(\Re(H)v_R - \Im(H)v_I) - i\left(-\Im(H)v_R - \Re(H)v_I\right)\right]$$

$$= \left(v_R^T + i\,v_I^T\right)\left[(\pm\lambda)v_R - i(\pm\lambda)v_I\right] = \pm\lambda\left(v_R^T v_R + v_I^T v_I + i\,v_I^T v_R - i\,v_R^T v_I\right) = \pm\lambda$$

It is now immediate to see that, if $(\mathcal{P}v)^T H(\mathcal{P}v) = \lambda > 0$, then $(i\,\mathcal{P}v)^T H(i\,\mathcal{P}v) = -\lambda$.

B   An useful lemma for gauge theories

We want to prove the relation

$$e^{ig_a T^a} e^{ix_b T^b} e^{-ig_a T^a} = e^{iM_{ab}x_b T^a}$$

where T^a are the generators of a Lie algebra $\mathfrak{g}$ in the fundamental representation. The matrix M is given by

$$M_{ab} = \left(e^{ig_c t^c} \right)_{ab}$$

and $(t^c)_{ab} = -if^{cab}$ are the generators of $\mathfrak{g}$ in the adjoint representation. In general $g_a, x_a \in \mathbb{C}$. Making use of the Baker-Campbell-Hausdorff formula in the form

$$e^X e^Y = e^{Y + [X,Y] + \frac{1}{2!}[X,[X,Y]] + \frac{1}{3!}[X,[X,[X,Y]]] + \cdots} e^X$$

and the relations

$$\left[T^{a_1}, T^b \right] = i f^{a_1 ba} T^a$$

$$\left[T^{a_2}, \left[T^{a_1}, T^b \right] \right] = i^2 f^{a_1 bc_1} f^{a_2 c_1 a} T^a$$

$$\left[T^{a_3}, \left[T^{a_2}, \left[T^{a_1}, T^b \right] \right] \right] = i^3 f^{a_1 bc_1} f^{a_2 c_1 c_2} f^{a_3 c_2 a} T^a$$

$$\left[T^{a_j}, \left[T^{a_{j-1}}, \cdots, \left[T^{a_1}, T^b \right] \right] \right] = i^j f^{a_1 bc_1} f^{a_2 c_1 c_2} f^{a_3 c_2 c_3} \cdots f^{a_j c_{j-1} a} T^a$$

we have

$$e^{ig_a T^a} e^{ix_b T^b} e^{-ig_a T^a} = e^{ix_a T^a + [ig_{a_1} T^{a_1}, ix_b T^b] + \frac{1}{2!}[ig_{a_2} T^{a_2}, [ig_{a_1} T^{a_1}, ix_b T^b]] + \cdots}$$

$$= e^{ix_a T^a + (ix_b)(ig_{a_1})[T^{a_1}, T^b] + \frac{1}{2!}(ix_b)(ig_{a_1})(ig_{a_2})[T^{a_2}, [T^{a_1}, T^b]] + \cdots}$$

$$= e^{ix_a T^a + (ix_b) \sum\limits_{j=1}^{\infty} \frac{1}{j!} (ig_{a_1}) \cdots (ig_{a_j}) i f^{a_1 bc_1} i f^{a_2 c_1 c_2} \cdots i f^{a_j c_{j-1} a} T^a}$$

$$= e^{i\left\{ \delta^{ab} + \sum\limits_{j=1}^{\infty} \frac{1}{j!} \left(-ig_{a_1} t^{a_1} \right)_{bc_1} \left(-ig_{a_2} t^{a_2} \right)_{c_1 c_2} \cdots \left(-ig_{a_j} t^{a_j} \right)_{c_{j-1} a} \right\} x_b T^a}$$

$$= e^{i\left\{ \delta^{ab} + \sum\limits_{j=1}^{\infty} \frac{1}{j!} \left[(-ig_c t^c)^j \right]_{ba} \right\} x_b T^a} = e^{i\left\{ \sum\limits_{j=0}^{\infty} \frac{1}{j!} \left[(ig_c t^c)^j \right]_{ab} \right\} x_b T^a}$$

which is what we were to prove, as

$$\sum_{j=0}^{\infty} \frac{1}{j!} (ig_c t^c)^j = e^{ig_c t^c}$$

C   Hessian of the CRM model

Recall the notation introduced in Section 7. By deriving the drift (7.3), we obtain the entries of the Hessian at a generic configuration

$$\frac{\partial^2 S}{\partial a_{mn} \partial a_{ij}} = 2N\delta_{mi}\delta_{nj} + iN_f \cosh\mu \left(\frac{\partial R_{mn}}{\partial a_{ij}} + \frac{\partial T_{mn}}{\partial a_{ij}} \right)$$

$$\frac{\partial^2 S}{\partial b_{mn} \partial b_{ij}} = 2N\delta_{mi}\delta_{nj} - N_f \cosh\mu \left(\frac{\partial R_{mn}}{\partial b_{ij}} - \frac{\partial T_{mn}}{\partial b_{ij}} \right)$$

$$\frac{\partial^2 S}{\partial \alpha_{mn} \partial \alpha_{ij}} = 2N\delta_{mi}\delta_{nj} + N_f \sinh\mu \left(\frac{\partial R_{mn}}{\partial \alpha_{ij}} + \frac{\partial T_{mn}}{\partial \alpha_{ij}} \right)$$

$$\frac{\partial^2 S}{\partial \beta_{mn} \partial \beta_{ij}} = 2N\delta_{mi}\delta_{nj} + iN_f \sinh\mu \left(\frac{\partial R_{mn}}{\partial \beta_{ij}} - \frac{\partial T_{mn}}{\partial \beta_{ij}} \right)$$

$$\frac{\partial^2 S}{\partial a_{mn} \partial b_{ij}} = iN_f \cosh\mu \left(\frac{\partial R_{mn}}{\partial b_{ij}} + \frac{\partial T_{mn}}{\partial b_{ij}} \right)$$

$$\frac{\partial^2 S}{\partial a_{mn} \partial \alpha_{ij}} = iN_f \cosh\mu \left(\frac{\partial R_{mn}}{\partial \alpha_{ij}} + \frac{\partial T_{mn}}{\partial \alpha_{ij}} \right)$$

$$\frac{\partial^2 S}{\partial a_{mn} \partial \beta_{ij}} = iN_f \cosh\mu \left(\frac{\partial R_{mn}}{\partial \beta_{ij}} + \frac{\partial T_{mn}}{\partial \beta_{ij}} \right)$$

$$\frac{\partial^2 S}{\partial b_{mn} \partial \alpha_{ij}} = -N_f \cosh\mu \left(\frac{\partial R_{mn}}{\partial \alpha_{ij}} - \frac{\partial T_{mn}}{\partial \alpha_{ij}} \right)$$

$$\frac{\partial^2 S}{\partial b_{mn} \partial \beta_{ij}} = -N_f \cosh\mu \left(\frac{\partial R_{mn}}{\partial \beta_{ij}} - \frac{\partial T_{mn}}{\partial \beta_{ij}} \right)$$

$$\frac{\partial^2 S}{\partial \alpha_{mn} \partial \beta_{ij}} = N_f \sinh\mu \left(\frac{\partial R_{mn}}{\partial \beta_{ij}} + \frac{\partial T_{mn}}{\partial \beta_{ij}} \right)$$

with

$$\frac{\partial R_{mn}}{\partial a_{ij}} = i\cosh\mu \left[\sum_{k=1}^{N} \left(G_{ki}R_{mj} + T_{kj}G_{im} \right) Y_{nk} + G_{im}\delta_{nj} \right]$$

$$\frac{\partial R_{mn}}{\partial b_{ij}} = -\cosh\mu \left[\sum_{k=1}^{N} \left(G_{ki}R_{mj} - T_{kj}G_{im} \right) Y_{nk} - G_{im}\delta_{nj} \right]$$

$$\frac{\partial R_{mn}}{\partial \alpha_{ij}} = \sinh\mu \left[\sum_{k=1}^{N} \left(G_{ki}R_{mj} + T_{kj}G_{im} \right) Y_{nk} + G_{im}\delta_{nj} \right]$$

$$\frac{\partial R_{mn}}{\partial \beta_{ij}} = i\sinh\mu \left[\sum_{k=1}^{N} \left(G_{ki}R_{mj} - T_{kj}G_{im} \right) Y_{nk} - G_{im}\delta_{nj} \right]$$

and

$$\frac{\partial T_{mn}}{\partial a_{ij}} = i \cosh \mu \left[\sum_{k=1}^{N} (G_{mi} R_{kj} + T_{mj} G_{ik}) X_{kn} + G_{mi} \delta_{jn} \right]$$

$$\frac{\partial T_{mn}}{\partial b_{ij}} = - \cosh \mu \left[\sum_{k=1}^{N} (G_{mi} R_{kj} - T_{mj} G_{ik}) X_{kn} + G_{mi} \delta_{jn} \right]$$

$$\frac{\partial T_{mn}}{\partial \alpha_{ij}} = \sinh \mu \left[\sum_{k=1}^{N} (G_{mi} R_{kj} + T_{mj} G_{ik}) X_{kn} + G_{mi} \delta_{jn} \right]$$

$$\frac{\partial T_{mn}}{\partial \beta_{ij}} = i \sinh \mu \left[\sum_{k=1}^{N} (G_{mi} R_{kj} - T_{mj} G_{ik}) X_{kn} + G_{mi} \delta_{jn} \right]$$

The Hessian computed at the classical vacuum (given by $a = b = \alpha = \beta = 0$) has the entries

$$\left. \frac{\partial^2 S}{\partial a_{mn} \partial a_{ij}} \right|_0 = 2 \left(N - N_f \frac{\cosh^2 \mu}{m^2} \right) \delta_{mi} \delta_{nj}$$

$$\left. \frac{\partial^2 S}{\partial b_{mn} \partial b_{ij}} \right|_0 = 2 \left(N - N_f \frac{\cosh^2 \mu}{m^2} \right) \delta_{mi} \delta_{nj}$$

$$\left. \frac{\partial^2 S}{\partial \alpha_{mn} \partial \alpha_{ij}} \right|_0 = 2 \left(N + N_f \frac{\sinh^2 \mu}{m^2} \right) \delta_{mi} \delta_{nj}$$

$$\left. \frac{\partial^2 S}{\partial \beta_{mn} \partial \beta_{ij}} \right|_0 = 2 \left(N + N_f \frac{\sinh^2 \mu}{m^2} \right) \delta_{mi} \delta_{nj}$$

$$\left. \frac{\partial^2 S}{\partial a_{mn} \partial b_{ij}} \right|_0 = 0$$

$$\left. \frac{\partial^2 S}{\partial a_{mn} \partial \alpha_{ij}} \right|_0 = 2i N_f \frac{\cosh \mu \sinh \mu}{m^2} \delta_{mi} \delta_{nj}$$

$$\left. \frac{\partial^2 S}{\partial a_{mn} \partial \beta_{ij}} \right|_0 = 0$$

$$\left. \frac{\partial^2 S}{\partial b_{mn} \partial \alpha_{ij}} \right|_0 = 0$$

$$\left. \frac{\partial^2 S}{\partial b_{mn} \partial \beta_{ij}} \right|_0 = 2i N_f \frac{\cosh \mu \sinh \mu}{m^2} \delta_{mi} \delta_{nj}$$

$$\left. \frac{\partial^2 S}{\partial \alpha_{mn} \partial \beta_{ij}} \right|_0 = 0$$

The Hessian at this critical point, that is H_0, is diagonal with respect to the indices i, j, m, n and therefore it is block-diagonal (the fields being ordered a, b, α, β at fixed index (i, j))

$$H_0 = \bigoplus^{N^2} \mathcal{H}_0 \tag{C.1}$$

with

$$\mathcal{H}_0 = \begin{pmatrix} a_- & 0 & i\,b & 0 \\ 0 & a_- & 0 & i\,b \\ i\,b & 0 & a_+ & 0 \\ 0 & i\,b & 0 & a_+ \end{pmatrix}$$

and the coefficients are

$$a_- = 2\left(N - N_f \frac{\cosh^2\mu}{m^2}\right)$$

$$a_+ = 2\left(N + N_f \frac{\sinh^2\mu}{m^2}\right)$$

$$b = 2N_f \frac{\cosh\mu \sinh\mu}{m^2}$$

$\mathcal{H}_0$ has only two distinct (positive) Takagi values[66]

$$\lambda_\pm = \frac{1}{2}\left[\sqrt{(a_+ + a_-)^2 + 4b^2} \pm (a_+ - a_-)\right] = \frac{N_f}{m^2}\left[\sqrt{\left(\frac{2N}{N_f}m^2 - 1\right)^2 + \sinh^2(2\mu)} \pm \cosh(2\mu)\right]$$

with othonormal Takagi vectors

$$v_+^{(1)} = \frac{1}{\sqrt{c^2+1}}\begin{pmatrix} i \\ 0 \\ c \\ 0 \end{pmatrix} \qquad v_+^{(2)} = \frac{1}{\sqrt{c^2+1}}\begin{pmatrix} 0 \\ i \\ 0 \\ c \end{pmatrix}$$

$$v_-^{(1)} = \frac{1}{\sqrt{c^2+1}}\begin{pmatrix} c \\ 0 \\ i \\ 0 \end{pmatrix} \qquad v_-^{(2)} = \frac{1}{\sqrt{c^2+1}}\begin{pmatrix} 0 \\ c \\ 0 \\ i \end{pmatrix}$$

$$\text{(C.2)}$$

having defined

$$c \equiv -\frac{\sqrt{(a_+ + a_-)^2 + 4b^2} + a_+ + a_-}{2b}$$

Now, thanks to the structure of H_0 given by (C.1), we can construct its Takagi vectors given those of $\mathcal{H}_0$. The generic Takagi vector takes the form

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[66]Actually, things are a bit more involved. At low masses, λ_- changes sign, so it does not correspond to a stable direction on $\mathcal{J}_0$ anymore. The solution is quite simple: in this regime, the second Takagi value (other that λ_+, which is always positive) is $-\lambda_- > 0$ and its two Takagi vectors are

$$v_-^{(1)} = \frac{1}{\sqrt{\tilde{c}^2+1}}\begin{pmatrix} i \\ 0 \\ \tilde{c} \\ 0 \end{pmatrix} \qquad v_-^{(2)} = \frac{1}{\sqrt{\tilde{c}^2+1}}\begin{pmatrix} 0 \\ i \\ 0 \\ \tilde{c} \end{pmatrix}$$

with $\tilde{c} \equiv \frac{\sqrt{(a_+ + a_-^2)^2 + 4b^2} - a_+ - a_-}{2b}$ (orthogonality with $v_+^{(1,2)}$ follows from $c\tilde{c} = -1$). It is straightforward to show that this happens for $\tilde{m} < \sqrt{NN_f}$, regardless of the value of μ.

$$v^{(i)} = \begin{pmatrix} 0_{4\times1} \\ \vdots \\ v_{\pm}^{(1,2)} \\ \vdots \\ 0_{4\times1} \end{pmatrix}$$

with $v_{\pm}^{(1,2)}$ each of the 4 vectors appearing in (C.2). The whole set of Takagi vectors consists of the $4N^2$ vectors $\{v^{(i)}\}$, each of which has the only non-zero 4×1 block at position $j = 1 \cdots N^2$. Such vectors are automatically orthonormal. From this structure we can easily build the matrix W whose columns are the Takagi vectors of H_0. A suitable arrangement of the vectors $\{v^{(i)}\}$ (which amounts to a factor of ± 1 in $\det W$) gives

$$W = \bigoplus^{N^2} \mathcal{W}$$

with

$$\det \mathcal{W} = \frac{1}{(c^2+1)^2} \det \begin{pmatrix} i & 0 & c & 0 \\ 0 & i & 0 & c \\ c & 0 & i & 0 \\ 0 & c & 0 & i \end{pmatrix} = 1$$

so that $\det W = (\det \mathcal{W})^{N^2} = 1$. In conclusion, a suitable arrangement of the Takagi vectors, gives a residual phase at the classical vacuum $e^{i\,\omega_0} = 1$.[67]

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[67]The same considerations hold in the case $\tilde{m} < \sqrt{NN_f}$ as well. In this case we have (using $c\tilde{c} = -1$)

$$\det \mathcal{W} = \frac{1}{(c^2+1)(\tilde{c}^2+1)} \det \begin{pmatrix} i & 0 & i & 0 \\ 0 & i & 0 & i \\ c & 0 & \tilde{c} & 0 \\ 0 & c & 0 & \tilde{c} \end{pmatrix} = -\frac{(c-\tilde{c})^2}{(c^2+1)(\tilde{c}^2+1)} = -1$$

D Analytical results for 0+1 QCD

In this section we present analytical results for the partition function of $0 + 1$-dimensional QCD and for the expectation value of the Polyakov loop at different values of N_f. The chiral condensate can be obtained by $\Sigma = T\frac{\partial}{\partial m}\log Z$ and the quark number density by $n = T\frac{\partial}{\partial \mu}\log Z$. We recall that $A = 2\cosh(\mu_c/T)$ and $\mu_c = \sinh^{-1}(m)$. We also have the anti-Polyakov loop from the Polyakov loop using $\langle \operatorname{Tr} U^{\dagger}\rangle = \langle \operatorname{Tr} U\rangle_{\mu \to -\mu}$.

D.1 1 quark flavour

$$Z_1 = A^3 - 2A + 2\cosh\left(\frac{3\mu}{T}\right)$$

$$\langle \operatorname{Tr} U\rangle_1 = \frac{1}{Z_1}\left[e^{-\frac{\mu}{T}}\left(A\left(A + e^{\frac{3\mu}{T}}\right) - 1\right)\right]$$

D.2 2 quark flavours

$$Z_2 = A^6 - 2A^4 + 4\left(2A^2 - 3\right)A\cosh\left(\frac{3\mu}{T}\right) + 3A^2 + 2\cosh\left(\frac{6\mu}{T}\right) + 6$$

$$\langle \operatorname{Tr} U\rangle_2 = \frac{1}{Z_2}\left[e^{-\frac{4\mu}{T}}\left(3\left(A^4 - 1\right)e^{\frac{6\mu}{T}} + 3A^2 + 2\left(A^4 - A^2 + 3\right)Ae^{\frac{3\mu}{T}} + 2Ae^{\frac{9\mu}{T}} - 2\right)\right]$$

D.3 3 quark flavours

$$Z_3 = A^9 + 9A^5 + 36A^3 + 4\left(5A^2 - 6\right)A\cosh\left(\frac{6\mu}{T}\right) + \left(20A^6 - 30A^4 + 36A^2 + 36\right)\cosh\left(\frac{3\mu}{T}\right) - 54A + 2\cosh\left(\frac{9\mu}{T}\right)$$

$$\langle \operatorname{Tr} U\rangle_3 = \frac{1}{Z_3}\left[3e^{-\frac{7\mu}{T}}\left(2A^2 + \left(5A^4 - 4A^2 + 6\right)Ae^{\frac{3\mu}{T}} + \left(5A^4 - 2A^2 - 2\right)e^{\frac{12\mu}{T}} + \left(A^8 + A^6 + 11A^4 - 6\right)e^{\frac{6\mu}{T}}\right.\right.$$

$$\left.\left. + 2\left(A^6 + 2A^4 - A^2 + 6\right)Ae^{\frac{9\mu}{T}} + Ae^{\frac{15\mu}{T}} - 1\right)\right]$$

D.4 4 quark flavours

$$Z_4 = 40A\left(A^2 - 1\right)\cosh\left(\frac{9\mu}{T}\right) + 8A\left(5A^8 + 24A^4 + 40A^2 - 60\right)\cosh\left(\frac{3\mu}{T}\right) + 20\left(5A^6 - 6A^4 + 6A^2 + 4\right)\cosh\left(\frac{6\mu}{T}\right)$$

$$+ \left(A^4 + 6A^2 + 2\right)\left(A^8 - 2A^6 + 40A^4 - 60A^2 + 60\right) + 2\cosh\left(\frac{12\mu}{T}\right)$$

$$\langle \operatorname{Tr} U \rangle_4 = \frac{1}{Z_4} \left[e^{-\frac{10\mu}{T}} \left(10A^2 + 12 \left(5A^6 + 3A^4 + 10 \right) Ae^{\frac{15\mu}{T}} + 20 \left(3A^4 - 2A^2 + 2 \right) Ae^{\frac{3\mu}{T}} + 5 \left(9A^4 - 4A^2 - 2 \right) e^{\frac{18\mu}{T}} \right. \right.$$

$$+ 3 \left(15A^8 + 8A^6 + 60A^4 - 20 \right) e^{\frac{6\mu}{T}} + 10 \left(A^4 + 6A^2 + 2 \right) \left(A^6 + 6A^2 - 4 \right) e^{\frac{12\mu}{T}}$$

$$\left. \left. + 4 \left(A^{10} + 5A^8 + 36A^6 + 44A^4 - 20A^2 + 60 \right) Ae^{\frac{9\mu}{T}} + 4Ae^{\frac{21\mu}{T}} - 4 \right) \right]$$

D.5 5 quark flavours

$$Z_5 = 10A \left(7A^2 - 6 \right) \cosh\left(\frac{12\mu}{T} \right) + 50A \left(7A^8 + 21A^4 + 20A^2 - 30 \right) \cosh\left(\frac{6\mu}{T} \right)$$

$$+ 10 \left(\left(\left(7A^2 \left(A^6 + 3A^4 + 15A^2 + 40 \right) - 300 \right) A^2 + 300 \right) A^2 + 100 \right) \cosh\left(\frac{3\mu}{T} \right) + 50 \left(7A^6 - 7A^4 + 6A^2 + 3 \right) \cosh\left(\frac{9\mu}{T} \right)$$

$$+ A \left(A^4 + 10A^2 + 10 \right) \left(A^{10} + 80A^6 - 100A^4 + 300A^2 - 200 \right) + 2 \cosh\left(\frac{15\mu}{T} \right)$$

$$\langle \operatorname{Tr} U \rangle_5 = \frac{1}{Z_5} \left[5e^{-\frac{13\mu}{T}} \left(3A^2 + 5 \left(7A^4 - 4A^2 + 3 \right) Ae^{\frac{3\mu}{T}} + 5 \left(A^2 \left(A^2 \left(7 \left(A^4 + 3A^2 + 4 \right) A^2 + 65 \right) - 30 \right) - 10 \right) e^{\frac{18\mu}{T}} \right. \right.$$

$$+ 3 \left(7A^4 - 3A^2 - 1 \right) e^{\frac{24\mu}{T}} + 3 \left(21A^8 + 7A^6 + 45A^4 - 10 \right) e^{\frac{6\mu}{T}} + \left(63A^6 + 14A^4 + 10A^2 + 60 \right) Ae^{\frac{21\mu}{T}}$$

$$+ 3 \left(\left(A^8 + 12A^6 + 45A^4 + 160A^2 + 60 \right) A^4 + 100 \right) Ae^{\frac{15\mu}{T}} + \left(21A^{10} + 70A^8 + 280A^6 + 240A^4 - 100A^2 + 200 \right) Ae^{\frac{9\mu}{T}}$$

$$\left. \left. + \left(A^{14} + 11A^{12} + 102A^{10} + 325A^8 + 260A^6 + 600A^4 - 200A^2 - 100 \right) e^{\frac{12\mu}{T}} + Ae^{\frac{27\mu}{T}} - 1 \right) \right]$$

D.6 6 quark flavours

$$Z_6 = 28A \left(4A^2 - 3 \right) \cosh\left(\frac{15\mu}{T} \right) + 28A \left(70A^8 + 144A^4 + 90A^2 - 135 \right) \cosh\left(\frac{9\mu}{T} \right)$$

$$+ 4A \left(A^2 \left(\left(2 \left(7 \left(2A^6 + 15A^4 + 90A^2 + 350 \right) A^2 + 450 \right) A^2 + 7875 \right) A^2 + 1750 \right) - 5250 \right) \cosh\left(\frac{3\mu}{T} \right)$$

$$+ 14 \left(70A^6 - 60A^4 + 45A^2 + 18 \right) \cosh\left(\frac{12\mu}{T} \right)$$

$$+ 14 \left(70A^{12} + 168A^{10} + 630A^8 + 1040A^6 - 975A^4 + 900A^2 + 225 \right) \cosh\left(\frac{6\mu}{T} \right)$$

$$+ \left(A^6 + 15A^4 + 30A^2 + 5 \right) \left(A^{12} + 3A^{10} + 150A^8 - 35A^6 + 1050A^4 - 1050A^2 + 700 \right) + 2 \cosh\left(\frac{18\mu}{T} \right)$$

$$\langle \mathrm{Tr}\, U \rangle_6 = \frac{1}{Z_6} \left[3 e^{-\frac{16\mu}{T}} \left(7A^2 + 14 \left(10A^4 - 5A^2 + 3 \right) A e^{\frac{3\mu}{T}} + 7 \left(10A^4 - 4A^2 - 1 \right) e^{\frac{30\mu}{T}} + 7 \left(70A^8 + 16A^6 + 95A^4 - 15 \right) e^{\frac{6\mu}{T}} \right. \right.$$

$$+ 14 \left(28A^6 + 2A^4 + 5A^2 + 15 \right) A e^{\frac{27\mu}{T}} + 14 \left(28A^{10} + 70A^8 + 200A^6 + 130A^4 - 50A^2 + 75 \right) A e^{\frac{9\mu}{T}}$$

$$+ 7 \left(A^6 + 15A^4 + 30A^2 + 5 \right) \left(A^{10} + 5A^8 + 35A^6 + 50A^2 - 25 \right) e^{\frac{18\mu}{T}}$$

$$+ 7 \left(70A^{10} + 140A^8 + 176A^6 + 280A^4 - 135A^2 - 30 \right) e^{\frac{24\mu}{T}}$$

$$+ 2 \left(\left(A^{12} + 19A^{10} + 245A^8 + 1400A^6 + 3200A^4 + 6075A^2 + 1575 \right) A^4 + 1750 \right) A e^{\frac{15\mu}{T}}$$

$$+ 2 \left(70A^{12} + 476A^{10} + 1400A^8 + 3240A^6 + 455A^4 + 350A^2 + 1050 \right) A e^{\frac{21\mu}{T}}$$

$$\left. \left. + \left(70A^{14} + 532A^{12} + 2828A^{10} + 6120A^8 + 3465A^6 + 5950A^4 - 1750A^2 - 700 \right) e^{\frac{12\mu}{T}} + 2A e^{\frac{33\mu}{T}} - 2 \right) \right]$$

D.7 12 quark flavours

$$Z_{12} = A^{36} + 108A^{34} + 6138A^{32} + 243936A^{30} + 5741010A^{28} + 86631336A^{26} + 876297708A^{24} + 5899484448A^{22}$$

$$+ 27113316516A^{20} + 84986169840A^{18} + 178513767432A^{16} + 255813313536A^{14} + 234466082136A^{12} + 132619604832A^{10}$$

$$+ 59537546640A^{8} + 1255782528A^{6} - 941836896A^{4} + \left(728A^{3} - 312A\right)\cosh\left(\frac{33\mu}{T}\right) + 3767347584A^{2}$$

$$+ \left(1145144A^{9} + 576576A^{5} + 82368A^{3} - 123552A\right)\cosh\left(\frac{27\mu}{T}\right) + \left(52052A^{6} - 24024A^{4} + 10296A^{2} + 1872\right)\cosh\left(\frac{30\mu}{T}\right)$$

$$+ \left(9447438A^{12} + 10306296A^{10} + 15459444A^{8} + 6694688A^{6} - 3586440A^{4} + 2265120A^{2} + 226512\right)\cosh\left(\frac{24\mu}{T}\right)$$

$$+ \left(32391216A^{15} + 97173648A^{13} + 194347296A^{11} + 188948760A^{9} + 29899584A^{7} + 59799168A^{5} - 5536960A^{3}\right.$$

$$\left. - 8305440A\right)\cosh\left(\frac{21\mu}{T}\right) + \left(48586824A^{18} + 291520944A^{16} + 947443068A^{14} + 1700538840A^{12} + 1360431072A^{10}\right.$$

$$\left. + 1046485440A^{8} + 152612460A^{6} - 93436200A^{4} + 93436200A^{2} + 6921200\right)\cosh\left(\frac{18\mu}{T}\right)$$

$$+ \left(32391216A^{21} + 340107768A^{19} + 1797712488A^{17} + 5484912576A^{15} + 9069540480A^{13} + 10203233040A^{11}\right.$$

$$\left. + 5862256400A^{9} + 1245816000A^{7} + 1308106800A^{5} - 259545000A^{3} - 155727000A\right)\cosh\left(\frac{15\mu}{T}\right)$$

$$+ \left(9447438A^{24} + 161956080A^{22} + 1360431072A^{20} + 6751769024A^{18} + 19625027994A^{16} + 37120333536A^{14}\right.$$

$$\left. + 42891368520A^{12} + 28010926944A^{10} + 15571142730A^{8} + 959278320A^{6} - 654053400A^{4} + 1121234400A^{2}\right.$$

$$\left. + 70077150\right)\cosh\left(\frac{12\mu}{T}\right) + \left(1145144A^{27} + 30918888A^{25} + 406362528A^{23} + 3212619696A^{21} + 15459444000A^{19}\right.$$

$$\left. + 48604491936A^{17} + 99081785088A^{15} + 126520089696A^{13} + 110373295032A^{11} + 50698482120A^{9} + 11705687136A^{7}\right.$$

$$\left. + 8947450512A^{5} - 2354592240A^{3} - 1009110960A\right)\cosh\left(\frac{9\mu}{T}\right) + \left(52052A^{30} + 2186184A^{28} + 44972928A^{26}\right.$$

$$\left. + 567515520A^{24} + 4442883588A^{22} + 22910896008A^{20} + 78767584896A^{18} + 177598092672A^{16} + 270716949360A^{14}\right.$$

$$\left. + 261358153056A^{12} + 153018596016A^{10} + 72252344736A^{8} + 2145295152A^{6} - 1569728160A^{4} + 4709184480A^{2}\right.$$

$$\left. + 269096256\right)\cosh\left(\frac{6\mu}{T}\right) + \left(728A^{33} + 48048A^{31} + 1585584A^{29} + 33153120A^{27} + 430640496A^{25} + 3684814848A^{23}\right.$$

$$\left. + 21267362688A^{21} + 82107881856A^{19} + 216479783520A^{17} + 381992554944A^{15} + 438076368576A^{13} + 343774544256A^{11}\right.$$

$$\left. + 144185760576A^{9} + 34085525760A^{7} + 22604085504A^{5} - 6697506816A^{3} - 2511565056A\right)\cosh\left(\frac{3\mu}{T}\right)$$

$$+ 2\cosh\left(\frac{36\mu}{T}\right) + 209297088$$

$$\langle \operatorname{Tr} U \rangle_{12} = \frac{1}{Z_{12}} \Big[3e^{-\frac{34\mu}{T}} \Big(26A^2 + 52(77A^4 - 22A^2 + 6)e^{\frac{3\mu}{T}}A + 6292((A^2(7(39(A^4 + A^2) + 44)A^2 + 76) - 20)A^2 + 12)e^{\frac{9\mu}{T}}A$$

$$+ 69212(3(((13(6A^6 + 33A^4 + 93A^2 + 136)A^2 + 1240)A^2 + 675)A^2 + 45)A^4 + 50)e^{\frac{15\mu}{T}}A + 69212((((((13(6A^{10} + 96A^8 + 728A^6 + 3135A^4 + 7932A^2 + 12642)A^2$$

$$+ 155316)A^2 + 86790)A^2 + 32670)A^2 + 630)A^2 + 900)A^2 + 675)e^{\frac{21\mu}{T}}A + 572(((((((13(7A^{14} + 280A^{12} + 5328A^{10} + 59346A^8 + 408771A^6 + 1831368A^4$$

$$+ 5377680A^2 + 10348272)A^2 + 170236836)A^2 + 133737516)A^2 + 66076164)A^2 + 20255400)A^2 + 91476)A^2 + 914760)A^2 + 392040)e^{\frac{27\mu}{T}}A$$

$$+ 4(((A^{28} + 109A^{26} + 6248A^{24} + 208890A^{22} + 4192518A^{20} + 54236754A^{18} + 463103784A^{16} + 2647132488A^{14} + 10274489940A^{12} + 26914665492A^{10}$$

$$+ 47368816704A^8 + 55424254248A^6 + 40840226856A^4 + 19366209720A^2 + 5396874912)A^4 + 313945632)A^2 + 104648544)e^{\frac{33\mu}{T}}A$$

$$+ 44(((A^2(((((13(((((((7(A^4 + 59A^2 + 1544)A^2 + 166896)A^2 + 1606365)A^2 + 10030185)A^2 + 41725992)A^2 + 115304112)A^2 + 212326884)A^2 + 3350946060)A^2$$

$$+ 2541052800)A^2 + 1249610076)A^2 + 348092316) - 1189188)A^2 + 23783760)A^2 + 7135128)e^{\frac{39\mu}{T}}A + 6292(((A^2(((13(21A^{12} + 474A^{10} + 4848A^8 + 28840A^6$$

$$+ 103188A^4 + 233220A^2 + 335538)A^2 + 3760428)A^2 + 2098965)A^2 + 648450) - 6930)A^2 + 49500)A^2 + 14850)e^{\frac{45\mu}{T}}A + 69212(((A^2 + 1)(A^2(13(18A^8 + 132A^6$$

$$+ 450A^4 + 831A^2 + 625)A^2 + 5595) - 135)A^2 + 450)A^2 + 150)e^{\frac{51\mu}{T}}A + 6292(((3A^2(286A^6 + 611A^4 + 767A^2 + 540) - 76)A^2 + 140)A^2 + 60)e^{\frac{57\mu}{T}}A$$

$$+ 572(91A^6 - 7A^4 + 8A^2 + 6)e^{\frac{63\mu}{T}}A + 4e^{\frac{69\mu}{T}}A + 143(1001A^8 + 56A^6 + 292A^4 - 12)e^{\frac{6\mu}{T}} + 3146(A^2(A^2(3(858A^8 + 2340A^6 + 3887A^4 + 2826A^2 + 576)A^2 + 1360)$$

$$- 220) - 40)e^{\frac{12\mu}{T}} + 17303(A^2(A^2((((39(21A^8 + 204A^6 + 958A^4 + 2480A^2 + 3542)A^2 + 125048)A^2 + 55020)A^2 + 13440)A^2 + 5175) - 1500) - 150)e^{\frac{18\mu}{T}}$$

$$+ 3146(A^2(A^2(((((13(21A^{12} + 534A^{10} + 6414A^8 + 44548A^6 + 188020A^4 + 508728A^2 + 873468)A^2 + 12280464)A^2 + 8489613)A^2 + 3030390)A^2 + 772002)A^2$$

$$+ 180180) - 80190) - 5940)e^{\frac{24\mu}{T}} + 11(A^2(A^2((((((13((((((7(A^4 + 64A^2 + 1992)A^2 + 255888)A^2 + 2910555)A^2 + 21642312)A^2 + 106933596)A^2 + 353433696)A^2$$

$$+ 786585492)A^2 + 15000511680)A^2 + 14366956032)A^2 + 8800444224)A^2 + 2877325308)A^2 + 751566816)A^2 + 118918800) - 76108032) - 4756752)e^{\frac{30\mu}{T}}$$

$$+ 26(A^{12} + 66A^{10} + 990A^8 + 4620A^6 + 6930A^4 + 2772A^2 + 132)(A^2((A^{16} + 44A^{14} + 1100A^{12} + 12408A^{10} + 81840A^8 + 281424A^6 + 585156A^4 + 566280A^2$$

$$+ 396396)A^4 + 60984) - 17424)e^{\frac{36\mu}{T}} + 1573(A^2(A^2((((((13(7A^{14} + 252A^{12} + 4086A^{10} + 38880A^8 + 228144A^6 + 861168A^4 + 2131848A^2 + 3393792)A^2$$

$$+ 45612315)A^2 + 29497644)A^2 + 10021374)A^2 + 3027024)A^2 + 353430) - 320760) - 17820)e^{\frac{42\mu}{T}} + 34606(A^2(A^2((((39(6A^{10} + 84A^8 + 537A^6 + 1974A^4$$

$$+ 4160A^2 + 5432)A^2 + 167398)A^2 + 64020)A^2 + 22890)A^2 + 3300) - 2625) - 150)e^{\frac{48\mu}{T}} + 17303(A^2(3A^2(((13(21A^6 + 96A^4 + 216A^2 + 272)A^2 + 1665)A^2 + 792)A^2$$

$$+ 180) - 320) - 20)e^{\frac{54\mu}{T}} + 286(3003A^{10} + 2002A^8 + 1624A^6 + 800A^4 - 324A^2 - 24)e^{\frac{60\mu}{T}} + 13(77A^4 - 20A^2 - 2)e^{\frac{66\mu}{T}} - 4\Big) \Big]$$

E Reflection symmetry in thimble decomposition

In this section we go into detail describing the reflection symmetry discussed in [42]. Consider the partition function of a generic field theory consisting of n real (scalar, for the sake of simplicity) degrees of freedom $\{x_i\}$ on a domain $\mathcal{C}$

$$Z = \int_{\mathcal{C}} \mathrm{d}^n x \, e^{-S(x)}$$

Before complexifying the degrees of freedom, we note that, in order for Z to be the partition function of a *physical* system, it must be real even when $S(x)$ is complex. A sufficient condition for this to hold is the existence of a "reflection" symmetry L, which is a *real* operator on the fields so that $L = L^T$, $L^2 = \mathbb{1}$ and L satisfies

$$\overline{S(x)} = S(L\,x)$$

This ensures the reality of Z, as

$$\bar{Z} = \overline{\int_{\mathcal{C}} \mathrm{d}^n x \, e^{-S(x)}} = \int_{\mathcal{C}} \mathrm{d}^n x \, e^{-\overline{S(x)}} = \int_{\mathcal{C}} \mathrm{d}^n \left(L^{-1} L \, x \right) e^{-S(L\,x)} = \int_{\mathcal{C}} \mathrm{d}^n x \, e^{-S(x)} = Z$$

We now turn to the decomposition of Z in terms of thimbles, that is

$$Z = \sum_{\sigma \in \Sigma} \mathfrak{n}_\sigma \int_{\mathcal{J}_\sigma} \mathrm{d}^n z \, e^{-S(z)} \tag{E.1}$$

In order for Z to be real, integrals over $\{\mathcal{J}_\sigma\}$ must either be real or appear in complex conjugate pairs. We shall see that this is ensured by the reflection symmetry. When the fields are complexified $(x \to z)$, L is extended to an *antilinear* map $K : z \mapsto L\,\bar{z}$ satisfying

$$\overline{S(z)} = S(L\,\bar{z})$$

We now show covariance of the steepest ascent flow under the action of K, that is, if the flow $z(t)$ is a solution to

$$\frac{\mathrm{d}z_i(t)}{\mathrm{d}t} = \frac{\partial \overline{S(z)}}{\partial \bar{z}_i}$$

then $z'(t) \equiv K(z(t)) = L\,\bar{z}(t)$ solves the SA equations as well

$$\frac{\mathrm{d}z'_i}{\mathrm{d}t} = \sum_{j=1}^n L_{ij} \frac{\mathrm{d}\bar{z}_j(t)}{\mathrm{d}t} = \sum_{j=1}^n L_{ij} \frac{\partial S(z)}{\partial z_j} = \sum_{j=1}^n L_{ij} \frac{\partial \overline{S(L\,\bar{z})}}{\partial z_j} = \sum_{j=1}^n L_{ij} \sum_{k=1}^n \left(\frac{\partial z'_k}{\partial z_j} \frac{\partial}{\partial z'_k} + \frac{\partial \bar{z}'_k}{\partial z_j} \frac{\partial}{\partial \bar{z}'_k} \right) \overline{S(z')}$$

$$= \sum_{j=1}^n L_{ij} \sum_{k=1}^n L_{kj} \frac{\partial \overline{S(z')}}{\partial \bar{z}'_k} = \sum_{k=1}^n \sum_{j=1}^n L_{ij} L_{jk} \frac{\partial \overline{S(z')}}{\partial \bar{z}'_k} = \sum_{k=1}^n \delta_{ik} \frac{\partial \overline{S(z')}}{\partial \bar{z}'_k} = \frac{\partial \overline{S(z')}}{\partial \bar{z}'_i}$$

As a consequence, if z_σ is a critical point of S, so is $K(z_\sigma)$ and the thimble associated to $K(z_\sigma)$ is

$$\mathcal{J}_\sigma^K \equiv \mathcal{J}_{K(z_\sigma)} = \left\{ K(z) \,\middle|\, z \in \mathcal{J}_\sigma \right\}$$

(up to a choice of orientation). We also note that covariance of the SA flow under K ensures that $\mathfrak{n}_\sigma^K = \langle \mathcal{C}, \mathcal{J}_\sigma^K \rangle = \langle \mathcal{C}, \mathcal{J}_\sigma \rangle = \mathfrak{n}_\sigma$ up to a change of orientation. The most useful property of two conjugated thimbles, $\mathcal{J}_\sigma$ and $\mathcal{J}_\sigma^K$, is the following

$$\int_{\mathcal{J}_\sigma^K} \mathrm{d}^n z \, e^{-S(z)} = \int_{\mathcal{J}_\sigma^K} \mathrm{d}^n z \, \overline{e^{-S(L\,\bar{z})}} = \overline{\int_{\mathcal{J}_\sigma^K} \mathrm{d}^n \left(L^{-1} L\bar{z}\right) e^{-S(L\,\bar{z})}} = \pm \overline{\int_{\mathcal{J}_\sigma} \mathrm{d}^n z \, e^{-S(z)}}$$

where the sign depends on whether K changes the orientation of the thimbles. As a consequence, complex conjugate pairs of critical points appearing in the decomposition (E.1) either yield an overall real contribution to Z or a purely imaginary contribution, in which case they have $\mathfrak{n}_\sigma = 0$. We also note that self-conjugate critical points (those for which $K(z_\sigma) = z_\sigma$) give a contribution which is purely real or imaginary (in the latter case, they cannot contribute to Z). The reflection symmetry we have described holds also at every order in perturbation theory, in particular it is to be recovered in a semiclassical expansion around thimbles.

F The partition function of Yang-Mills theory in 2 dimensions

In this section we compute the partition function for the action (10.1) in 2 dimensions, following [29] and [118]. Here fields need not to be complexified, as we integrate over the original (compact) group $\otimes_{n,\hat{\mu}}\mathrm{SU}(N)$ and eventually continue $Z(\beta)$ to complex values of the coupling. Neglecting the additive constant βV in the action, we compute the partition function

$$Z(\beta) = \int \mathcal{D}U\, e^{-S[U]} = \int \mathcal{D}U\, e^{\beta \sum_{\square} \frac{1}{2N}\mathrm{Tr}(U_\square + U_\square^\dagger)} = \int \mathcal{D}U \prod_\square e^{\beta f(U_\square)}$$

where $\square$ labels different plaquettes (they are products of U that we label $U_\square$) and the group invariant measure is

$$\mathcal{D}U = \prod_{n,\hat{\mu}} \mathrm{d}U_{\hat{\mu}}(n)$$

As $f(U_\square)$ is obviously a (real valued) gauge-invariant function of the plaquette variables, we have that $e^{\beta f(U_\square)}$ is a class function on $\mathrm{SU}(N)$ and therefore it can be expanded in terms of irreducible characters of $U_\square$

$$e^{\beta f(U_\square)} = \sum_r d_r \lambda_r(\beta)\chi_r(U_\square)$$

where r labels the r-th irreducible representation of $\mathrm{SU}(N)$ (d_r being its dimension) and χ_r is the character of $U_\square$ in the r-th representation. Now, for U, U_1, U_2 in $\mathrm{SU}(N)$, we have the following relations for group integrals of the characters [96]

$$\int \mathrm{d}U\, \chi_r(U)\chi_{r'}(U^\dagger) = \delta_{rr'}$$

$$\int \mathrm{d}U\, \chi_r(U_1 U)\chi_{r'}(U^\dagger U_2) = \frac{1}{d_r}\delta_{rr'}\chi_r(U_1 U_2)$$

$$\int \mathrm{d}U\, \chi_r(U U_1 U^\dagger U_2) = \frac{1}{d_r}\chi_r(U_1)\chi_r(U2)$$

By integrating the character expansion after multiplying it with $\chi_r(U^\dagger)$, we extract the coefficients $\{\lambda_r\}$

$$\lambda_r = \frac{1}{d_r}\int \mathrm{d}U\, \chi_r(U^\dagger)\, e^{\beta f(U)}$$

Now let us consider the partition function, where a given link U appears only in two plaquettes $U_{\square_1} = V_1 U$ and $U_{\square_2} = U^\dagger V_2$,where V_1 and V_2 are the (path-ordered) staples corresponding to the link U. The integration with respect to U is therefore

$$\int \mathrm{d}U\, e^{\beta f(U_{\square_1})}e^{\beta f(U_{\square_2})} = \sum_r \sum_{r'} d_r d_{r'} \lambda_r(\beta)\lambda_{r'}(\beta) \int \mathrm{d}U\, \chi_r(V_1 U)\chi_{r'}(U^\dagger V_2)$$

$$= \sum_r \sum_{r'} d_r d_{r'} \lambda_r(\beta)\lambda_{r'}(\beta)\frac{1}{d_r}\delta_{rr'}\chi_r(V_1 V_2) = \sum_r d_r \left[\lambda_r(\beta)\right]^2 \chi_r(V_1 V_2)$$

We have glued the two plaquettes sharing the link U together to form a new "double plaquette", whose (path-ordered) boundary V_1V_2 we call $U_{\square_{12}}$; the power of 2 of $\lambda_r(\beta)$ matches the number of plaquettes that have been glued together. The generalization of this procedure is straightforward: if we now glue another plaquette (sharing one link with $U_{\square_{12}}$), thus forming $U_{\square_{123}}$, we pick another factor of $\lambda_r(\beta)$ (the additional d_r cancels out during integration in the new common link variable). In general, if we pick a closed, non self-intersecting contour Γ enclosing N_Γ plaquettes of a two-dimensional lattice, by integrating over the internal link variables, we get a functional $Z(\Gamma)$ of the (path-ordered) product of link variables on the boundary, which we call U_Γ

$$Z(U_\Gamma) = \sum_r d_r \left[\lambda_r(\beta)\right]^{N_\Gamma} \chi_r(U_\Gamma)$$

We now consider the particular case in which the contour Γ consists of only the links on the lattice boundaries, that is $U \in \partial\Lambda$ (all the internal links have already been integrated out)

$$Z(\beta) = \int \mathcal{D}U \, Z(U_{\partial\Lambda}) = \int \mathrm{d}U_1 \mathrm{d}U_2 \mathrm{d}U_3 \mathrm{d}U_4 \, Z(U_1 U_2 U_3 U_4) \tag{F.1}$$

where, thanks to the invariance of the group measure and its normalization $\int \mathrm{d}U = 1$, we have expressed the remaining integrations over boundary links as only 4 integrations over link products on the four boundaries, that is $U_{\partial\Lambda} = U_1 U_2 U_3 U_4$. We now impose *periodic boundary conditions*, thus making the identifications $U_3 \equiv U_1^\dagger$ and $U_4 \equiv U_2^\dagger$ and then integrating over U_1 and U_2 (V is the total number of plaquettes, that is the total lattice area measured in lattice units)

$$Z^{\mathrm{(pbc)}}(\beta) = \int \mathrm{d}U_1 \mathrm{d}U_2 \, Z(U_1 U_2 U_1^\dagger U_2^\dagger) = \int \mathrm{d}U_2 \sum_r d_r \left[\lambda_r(\beta)\right]^V \int \mathrm{d}U_1 \, \chi_r(U_1 U_2 U_1^\dagger U_2^\dagger)$$

$$= \int \mathrm{d}U_2 \sum_r d_r \left[\lambda_r(\beta)\right]^V \frac{1}{d_r} \chi_r(U_2) \chi_r(U_2^\dagger) = \sum_r \left[\lambda_r(\beta)\right]^V \int \mathrm{d}U_2 \, \chi_r(U_2) \chi_r(U_2^\dagger) = \sum_r \left[\lambda_r(\beta)\right]^V$$

If we consider *free boundary conditions* instead, we have

$$Z^{\mathrm{(fbc)}}(\beta) = \int \mathrm{d}U_1 \mathrm{d}U_2 \mathrm{d}U_3 \mathrm{d}U_4 \, Z(U_1 U_2 U_3 U_4) = \sum_r d_r \left[\lambda_r(\beta)\right]^V \int \mathrm{d}U_1 \mathrm{d}U_2 \mathrm{d}U_3 \int \mathrm{d}U_4 \, \chi_r(U_1 U_2 U_3 U_4)$$

$$= \sum_r d_r \left[\lambda_r(\beta)\right]^V \int \mathrm{d}U_1 \mathrm{d}U_2 \mathrm{d}U_3 \, \delta_{r,0} = \left[\lambda_0(\beta)\right]^V$$

where $r = 0$ labels the trivial representation of the group, with dimension $d_0 = 1$ and we have used the character integral relations as well as the normalization of the group measure.

We now perform the explicit computation of $Z(\beta)$ for U(1) and SU(2). First, remember that $f(U_\square) = \frac{1}{2N}\mathrm{Tr}(U_\square + U_\square^\dagger)$, where the trace is understood in the fundamental representation of the gauge group. For U(1) we have the parametrization $U = e^{i\theta}$ and $\mathrm{d}U = \mathrm{d}\theta/2\pi$, therefore $f(U_\square) = \frac{1}{2}(e^{i\theta} + e^{-i\theta}) = \cos\theta$. The irreducible representations are labelled by the integer $\nu \in \mathbb{Z}$, with $\chi_\nu(U_\square) = e^{i\nu\theta}$ and they are all 1-dimensional, that is $d_\nu = 1$. Thus the coefficients $\{\lambda_r\}$ are

$$\lambda_\nu(\beta) = \frac{1}{d_\nu} \int \mathrm{d}U \, \chi_\nu(U^\dagger) e^{\beta f(U)} = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\theta \, e^{-i\nu\theta} e^{\beta\cos\theta} = \frac{1}{\pi} \int_0^\pi \mathrm{d}\theta \, e^{\beta\cos\theta} \cos(\nu\theta) - \frac{i}{2\pi} \int_0^{2\pi} \mathrm{d}\theta \, e^{\beta\cos\theta} \sin(\nu\theta) = I_\nu(\beta)$$

where $I_\nu(\beta)$ is the modified Bessel function of the first kind. To summarize (restoring the additive constant βV in the action)

$$Z^{(\text{fbc})}_{\text{U}(1)}(\beta) = e^{-\beta V}\left[I_0(\beta)\right]^V$$

$$Z^{(\text{pbc})}_{\text{U}(1)}(\beta) = e^{-\beta V}\sum_{\nu=-\infty}^{+\infty}\left[I_\nu(\beta)\right]^V$$

For SU(2) in the fundamental representation, we employ the parametrization

$$U = \cos\left(\frac{\psi}{2}\right)\mathbb{1} + i\,\sin\left(\frac{\psi}{2}\right)\hat{n}\cdot\vec{\sigma}$$

where $\{\sigma_i\}$ are the three Pauli matrices, $|\hat{n}| = 1$ and $\psi \in [0, 4\pi)$. The Haar measure is given by

$$dU = \frac{1}{8\pi^2}\sin^2\left(\frac{\psi}{2}\right)d\psi\,d\Omega$$

with $d\Omega = \sin\theta\,d\theta\,d\phi$ and $\theta \in [0,\pi]$, $\phi \in [0,2\pi)$. Each irreducible representation is labelled by its spin j, which takes integer or half-integer values: $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \cdots$ and its dimension $d_j = 2j+1$. The character in the j-th representation is given by [119]

$$\chi_j(U) = \frac{\sin\left[(2j+1)\frac{\psi}{2}\right]}{\sin\left(\frac{\psi}{2}\right)}$$

From the parametrization of U, it follows

$$f(U_\square) = \frac{1}{2N}\text{Tr}\left(U_\square + U_\square^\dagger\right) = \frac{1}{4}\left[2\cos\left(\frac{\psi}{2}\right)\right]\text{Tr}\,\mathbb{1} = \cos\left(\frac{\psi}{2}\right)$$

Being $f(U)$ a real class function, the weights of conjugate representations are the same ($\lambda_j = \lambda_{\bar{j}}$); moreover, irreducible representations of SU(2) are real (so that $\chi_j(U) = \chi_{\bar{j}}(U)$), so we simply sum over j. We are ready to compute the coefficients $\{\lambda_j\}$

$$\lambda_j(\beta) = \frac{1}{d_j}\int dU\,\chi_j(U^\dagger)e^{\beta f(U)} = \frac{1}{2j+1}\frac{1}{8\pi^2}\int_\Omega d\Omega\int_0^{4\pi}d\psi\,\sin^2\left(\frac{\psi}{2}\right)\frac{\sin\left[(2j+1)\frac{\psi}{2}\right]}{\sin\left(\frac{\psi}{2}\right)}e^{\beta\cos\left(\frac{\psi}{2}\right)}$$

$$= \frac{1}{2j+1}\frac{1}{\pi}\int_0^{2\pi}d\psi\,e^{\beta\cos\psi}\sin\psi\sin\left[(2j+1)\psi\right] = \frac{1}{2j+1}\left[\frac{1}{\pi}\int_0^\pi d\psi\,e^{\beta\cos\psi}\cos\left[(2j)\psi\right] - \frac{1}{\pi}\int_0^\pi d\psi\,e^{\beta\cos\psi}\cos\left[(2j+2)\psi\right]\right]$$

$$= \frac{1}{2j+1}\left[I_{2j}(\beta) - I_{2j+2}(\beta)\right] = \frac{1}{2j+1}\left[\frac{2(2j+1)}{\beta}I_{2j+1}(\beta)\right] = \frac{2}{\beta}I_{2j+1}(\beta)$$

Thus, to summarize, we have

$$Z_{\mathrm{SU(2)}}^{(\mathrm{fbc})}(\beta) = e^{-\beta V}\left[\frac{2}{\beta}I_1(\beta)\right]^V$$

$$Z_{\mathrm{SU(2)}}^{(\mathrm{pbc})}(\beta) = e^{-\beta V}\sum_{n=1}^{\infty}\left[\frac{2}{\beta}I_n(\beta)\right]^V$$

F.1 The twisted case

We now compute the partition function of 2-dimensional Yang-Mills theory in the *twisted* case. The computational scheme is the same as before, but we must keep in mind that there is a *single* twisted plaquette (P_0) in the lattice, whose action density $-f(U_\square)$ undergoes a multiplication by a center element of $\mathrm{SU}(N)$, that is $f(U_\square) \to f(zU_\square)$ with $z = \zeta_k\mathbb{1} = e^{2\pi i k/N}\mathbb{1}$. This plaquette is the only one whose character expansion differs from the one which has already been computed, in particular we call its coefficients $\lambda_r^{(\mathrm{t})}(\beta)$. The obvious result for the partition function is thus

$$Z^{(\mathrm{pbc,t})}(\beta) = \sum_r [\lambda_r(\beta)]^{V-1}\,\lambda_r^{(\mathrm{t})}(\beta)$$

So all is left is the computation of the twisted coefficients

$$\lambda_r^{(\mathrm{t})} = \frac{1}{d_r}\int \mathrm{d}U\,\chi_r(U^\dagger)e^{\beta f(zU)} = \frac{1}{d_r}\int \mathrm{d}(zU)\,\chi_r\left(U^\dagger z^\dagger z\right)e^{\beta f(zU)} = \zeta_k\frac{1}{d_r}\int \mathrm{d}(zU)\,\chi_r\left((zU)^\dagger\right)e^{\beta f(zU)} = \zeta_k\lambda_r(\beta)$$

where we have used the invariance of the group measure $\mathrm{d}(zU) = \mathrm{d}U$. Thus, for the partition function, we have

$$Z^{(\mathrm{pbc,t})}(\beta) = \zeta_k\,Z^{(\mathrm{pbc})}(\beta)$$

As stated in Section 10.1, twisting the action is equivalent to simply considering twisted periodic boundary conditions along with an untwisted action. We will check this explicitly for the 2-dimensional case. Twisted periodic boundary conditions correspond to taking $U_3 = \Omega_1 U_1^\dagger\Omega_1^\dagger$ and $U_4 = \Omega_2 U_2^\dagger\Omega_2^\dagger$ in (F.1). Then, using the previously given expressions for group integrals of characters as well as the twisted commutation relation $\Omega_2\Omega_1 = z\,\Omega_1\Omega_2$ and $d_r = \chi_r(\mathbb{1})$

$$Z^{(\mathrm{pbc,t})}(\beta) = \int \mathcal{D}U\,Z(U_{\partial\Lambda}) = \int \mathrm{d}U_1\mathrm{d}U_2\,Z(U_1U_2\Omega_1U_1^\dagger\Omega_1^\dagger\Omega_2U_2^\dagger\Omega_2^\dagger)$$

$$= \int \mathrm{d}U_2\sum_r d_r\,[\lambda_r(\beta)]^V\int \mathrm{d}U_1\,\chi_r(U_1U_2\Omega_1U_1^\dagger\Omega_1^\dagger\Omega_2U_2^\dagger\Omega_2^\dagger) = \int \mathrm{d}U_2\sum_r d_r\,[\lambda_r(\beta)]^V\frac{1}{d_r}\chi_r(U_2\Omega_1)\chi_r(\Omega_1^\dagger\Omega_2U_2^\dagger\Omega_2^\dagger)$$

$$= \sum_r [\lambda_r(\beta)]^V\int \mathrm{d}U_2\,\chi_r(\Omega_1U_2)\chi_r(U_2^\dagger\Omega_2^\dagger\Omega_1^\dagger\Omega_2) = \sum_r [\lambda_r(\beta)]^V\frac{1}{d_r}\chi_r(\Omega_1\Omega_2^\dagger\Omega_1^\dagger\Omega_2) = \sum_r [\lambda_r(\beta)]^V\frac{1}{d_r}\chi_r(\Omega_2\Omega_1\Omega_2^\dagger\Omega_1^\dagger)$$

$$= \sum_r [\lambda_r(\beta)]^V\frac{1}{d_r}\chi_r(z\,\Omega_1\Omega_2\Omega_2^\dagger\Omega_1^\dagger)) = \zeta_k\sum_r [\lambda_r(\beta)]^V\frac{1}{d_r}\chi_r(\mathbb{1}) = \zeta_k\sum_r [\lambda_r(\beta)]^V = \zeta_k\,Z^{(\mathrm{pbc})}(\beta)$$

which agrees with the previous result.

G   Matrix form of complex Yang-Mills theory equations

In this section we compute SA equations as well as PT equations for complex $\mathrm{SU}(N)$ Yang-Mills theory in 2 dimensions in matrix form, that is getting rid of colour indices completely. This form is more suitable for computer simulations. Recall the definitions of Section 10 and consider the action for the (twisted) theory: the number of distinct plaquettes is given by $Vd(d-1)/2 = V$, where V is the lattice volume, so that

$$S[U] = \beta \left[V - \frac{1}{2N} \sum_n \sum_{\hat{\mu} < \hat{\nu}} \mathrm{Tr}\left(\mathcal{Z}(n) U_{\hat{\mu}\hat{\nu}}(n) + \mathcal{Z}^{-1}(n) U_{\hat{\mu}\hat{\nu}}^{-1}(n) \right) \right]$$

with $\mathcal{Z}(n) \equiv 1 + \delta_{n,n_0}(z-1)$ (z being the twist). We now make use of the following fact: any matrix $A \in \mathrm{SL}(N,\mathbb{C})$ can be decomposed as $A = a_{\mathbb{1}}\mathbb{1} + a_b T^b$. From this decomposition, it follows

$$T^a \mathrm{Tr}\left(T^a A \right) = T^a \mathrm{Tr}\left(T^a \left(a_{\mathbb{1}}\mathbb{1} + a_b T^b \right) \right) = a_{\mathbb{1}} T^a \mathrm{Tr}(T^a) + a_b T^a \mathrm{Tr}\left(T^a T^b \right) = \frac{1}{2} a_b T^b$$

where we have used $\mathrm{Tr}(T^a) = 0$ and $\mathrm{Tr}(T^a T^b) = \frac{1}{2}\delta^{ab}$. The decomposition of A can be used to compute $a_{\mathbb{1}}$

$$\mathrm{Tr}(A) = \mathrm{Tr}\left(a_{\mathbb{1}}\mathbb{1} + a_b T^b \right) = a_{\mathbb{1}} \mathrm{Tr}\,\mathbb{1} + a_b \mathrm{Tr}(T^b) = N a_{\mathbb{1}}$$

so that

$$T^a \mathrm{Tr}\left(T^a A \right) = \frac{1}{2}\left(A - a_{\mathbb{1}}\mathbb{1} \right) = \frac{1}{2}\left(A - \frac{1}{N}\mathrm{Tr}(A)\,\mathbb{1} \right) = \frac{1}{2}[A]_{\mathrm{T}}$$

with $[A]_{\mathrm{T}} \equiv A - \frac{1}{N}\mathrm{Tr}(A)\,\mathbb{1}$.

Our SA equations read

$$\frac{\mathrm{d}}{\mathrm{dt}} U_{\hat{\mu}}(n;t) = i\,\bar{\nabla}_{n,\hat{\mu}}\overline{S[U(t)]}\,U_{\hat{\mu}}(n;t)$$

with $\bar{\nabla}_{n,\hat{\mu}}\bar{S} \equiv T^a \bar{\nabla}_{n,\hat{\mu}}^a \bar{S}$. Thus, after defining

$$D_{\hat{\mu}\hat{\nu}}(n) \equiv c_U U_{\hat{\mu}\hat{\nu}}(n) + c_{\mathcal{U}}\mathcal{U}_{\hat{\mu}\hat{\nu}}(n) - c_U^{-1} U_{\hat{\mu}\hat{\nu}}^{-1}(n) - c_{\mathcal{U}}^{-1}\mathcal{U}_{\hat{\mu}\hat{\nu}}^{-1}(n)$$

we can write (recall that $\beta \in \mathbb{C}$)

$$\bar{\nabla}_{n,\hat{\mu}}^a \overline{S[U]} = \overline{\nabla_{n,\hat{\mu}}^a S[U]} = \overline{-\frac{i\beta}{2N} \sum_{\hat{\nu}\neq\hat{\mu}} \mathrm{Tr}\left[T^a D_{\hat{\mu}\hat{\nu}}(n) \right]} = \frac{i\bar{\beta}}{2N} \sum_{\hat{\nu}\neq\hat{\mu}} \mathrm{Tr}\left[T^a D_{\hat{\mu}\hat{\nu}}^\dagger(n) \right]$$

which yields

$$\bar{\nabla}_{n,\hat{\mu}}\overline{S[U]} = \frac{i\bar{\beta}}{4N} \sum_{\hat{\nu}\neq\hat{\mu}} \left[D_{\hat{\mu}\hat{\nu}}^\dagger(n) \right]_{\mathrm{T}}$$

Now let us come to PT equations. We immediately see that we can rewrite the Hessian as

$$\bar{\nabla}^b_{m,\hat{\rho}} \bar{\nabla}^a_{n,\hat{\mu}} \overline{S[U]} = \overline{\nabla^b_{m,\hat{\rho}} \nabla^a_{n,\hat{\mu}} S[U]} = \text{Tr}\left(T^a M^{b\,\dagger}_{(m,\hat{\rho}),(n,\hat{\mu})} \right)$$

with

$$M^b_{(m,\hat{\rho}),(n,\hat{\mu})} \equiv \tfrac{\beta}{2N} \sum_{\hat{\nu}} (1-\delta_{\hat{\nu},\hat{\mu}}) \Big\{ \delta_{\hat{\mu},\hat{\rho}} \Big[\delta_{n,m} \big[T^b(c_U U_{\hat{\mu}\hat{\nu}}(n) + c_{\mathcal{U}} \mathcal{U}_{\hat{\mu}\hat{\nu}}(n)) + \big(c_U^{-1} U_{\hat{\mu}\hat{\nu}}^{-1}(n) + c_{\mathcal{U}}^{-1} \mathcal{U}_{\hat{\mu}\hat{\nu}}^{-1}(n) \big) T^b \big]$$

$$-\delta_{n+\hat{\nu},m} \big[c_U U_{\hat{\mu}}(n) U_{\hat{\nu}}(n+\hat{\mu}) U_{\hat{\mu}}^{-1}(n+\hat{\nu}) T^b U_{\hat{\nu}}^{-1}(n) + c_U^{-1} U_{\hat{\nu}}(n) T^b U_{\hat{\mu}}(n+\hat{\nu}) U_{\hat{\nu}}^{-1}(n+\hat{\mu}) U_{\hat{\mu}}^{-1}(n) \big]$$

$$-\delta_{n-\hat{\nu},m} \big[c_{\mathcal{U}} U_{\hat{\mu}}(n) U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu}) U_{\hat{\mu}}^{-1}(n-\hat{\nu}) T^b U_{\hat{\nu}}(n-\hat{\nu}) + c_{\mathcal{U}}^{-1} U_{\hat{\nu}}^{-1}(n-\hat{\nu}) T^b U_{\hat{\mu}}(n-\hat{\nu}) U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu}) U_{\hat{\mu}}^{-1}(n) \big] \Big]$$

$$+\delta_{\hat{\nu},\hat{\rho}} \Big[-\delta_{n,m} \big[T^b c_U^{-1} U_{\hat{\mu}\hat{\nu}}^{-1}(n) + c_U U_{\hat{\mu}\hat{\nu}}(n) T^b \big]$$

$$+\delta_{n+\hat{\mu},m} \big[c_U U_{\hat{\mu}}(n) T^b U_{\hat{\nu}}(n+\hat{\mu}) U_{\hat{\mu}}^{-1}(n+\hat{\nu}) U_{\hat{\nu}}^{-1}(n) + c_U^{-1} U_{\hat{\nu}}(n) U_{\hat{\mu}}(n+\hat{\nu}) U_{\hat{\nu}}^{-1}(n+\hat{\mu}) T^b U_{\hat{\mu}}^{-1}(n) \big]$$

$$+\delta_{n-\hat{\nu},m} \big[c_{\mathcal{U}} U_{\hat{\mu}}(n) U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu}) U_{\hat{\mu}}^{-1}(n-\hat{\nu}) T^b U_{\hat{\nu}}(n-\hat{\nu}) + c_{\mathcal{U}}^{-1} U_{\hat{\nu}}^{-1}(n-\hat{\nu}) T^b U_{\hat{\mu}}(n-\hat{\nu}) U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu}) U_{\hat{\mu}}^{-1}(n) \big]$$

$$-\delta_{n+\hat{\mu}-\hat{\nu},m} \big[c_{\mathcal{U}} U_{\hat{\mu}}(n) U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu}) T^b U_{\hat{\mu}}^{-1}(n-\hat{\nu}) U_{\hat{\nu}}(n-\hat{\nu}) + c_{\mathcal{U}}^{-1} U_{\hat{\nu}}^{-1}(n-\hat{\nu}) U_{\hat{\mu}}(n-\hat{\nu}) T^b U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu}) U_{\hat{\mu}}^{-1}(n) \big] \Big] \Big\}$$

which enables us to write

$$T^a \bar{\nabla}^b_{m,\hat{\rho}} \bar{\nabla}^a_{n,\hat{\mu}} \overline{S[U]} = \bar{\nabla}^b_{m,\hat{\rho}} \bar{\nabla}_{n,\hat{\mu}} \overline{S[U]} = T^a \text{Tr}\left(T^a M^{b\,\dagger}_{(m,\hat{\rho}),(n,\hat{\mu})} \right) = \frac{1}{2}\left[M^{b\,\dagger}_{(m,\hat{\rho}),(n,\hat{\mu})} \right]_{\text{T}}$$

Next, we write the components of tangent basis vectors as matrices, that is $V_{n,\hat{\mu}} \equiv V_{n\hat{\mu},a} T^a$ (along with $\bar{V}_{n,\hat{\mu}} \equiv \bar{V}_{n\hat{\mu},a} T^a$). Consider our PT equations

$$\frac{\mathrm{d}}{\mathrm{d}t} V_{n\hat{\mu},a}(t) = \sum_{m,\hat{\rho},b} \bar{V}_{m\hat{\rho},b}(t)\, \bar{\nabla}^b_{m,\hat{\rho}} \bar{\nabla}^a_{n,\hat{\mu}} \overline{S[U(t)]} + \sum_{b,c} f^{cba} V_{n\hat{\mu},c}(t)\, \bar{\nabla}^b_{n,\hat{\mu}} \overline{S[U(t)]}$$

We can multiply both sides by T^a and sum over a

$$\frac{\mathrm{d}}{\mathrm{d}t} V_{n\hat{\mu},a} T^a = \sum_{m,\hat{\rho},b} \bar{V}_{m\hat{\rho},b}\, T^a \bar{\nabla}^b_{m,\hat{\rho}} \bar{\nabla}^a_{n,\hat{\mu}} \overline{S[U]} + \sum_{b,c} f^{cba} T^a V_{n\hat{\mu},c}\, \bar{\nabla}^b_{n,\hat{\mu}} \overline{S[U]}$$

$$\Rightarrow \frac{\mathrm{d}}{\mathrm{d}t} V_{n,\hat{\mu}} = \bar{\nabla}_V \bar{\nabla}_{n,\hat{\mu}} \overline{S[U]} - i \sum_{b,c} \left[T^c, T^b \right] V_{n\hat{\mu},c}\, \bar{\nabla}^b_{n,\hat{\mu}} \overline{S[U]}$$

$$\Rightarrow \frac{\mathrm{d}}{\mathrm{d}t} V_{n,\hat{\mu}} = \bar{\nabla}_V \bar{\nabla}_{n,\hat{\mu}} \overline{S[U]} - i \left[V_{n,\hat{\mu}}\,, \bar{\nabla}_{n,\hat{\mu}} \overline{S[U]} \right]$$

where we have introduced the directional derivative with respect to V

$$\bar{\nabla}_V \equiv \sum_{m,\hat{\rho},b} \bar{V}_{m\hat{\rho},b} \bar{\nabla}^b_{m,\hat{\rho}}$$

We have reached an expression which is quite general. However, we are interested in complex Yang-Mills theory: when one contracts $\bar{\nabla}^b_{m,\hat{\rho}} \bar{\nabla}^a_{n,\hat{\mu}} \overline{S[U]}$ with $\bar{V}_{m\hat{\rho},b}$, the effect of summing over b is that each T^b in the Hessian is substituted with $V_{m,\hat{\rho}}$. Thus we can rephrase PT equations as

$$\frac{\mathrm{d}}{\mathrm{d}t}V_{n,\hat{\mu}}(t) = \frac{\bar{\beta}}{4N}\sum_{\hat{\nu}\neq\hat{\mu}}\left\{\left[\mathcal{M}_{\hat{\mu}\hat{\nu}}^{\dagger}(n)\right]_{\mathrm{T}} + \left[V_{n,\hat{\mu}}(t),\left[D_{\hat{\mu}\hat{\nu}}^{\dagger}(n)\right]_{\mathrm{T}}\right]\right\}$$

having defined

$$\mathcal{M}_{\hat{\mu}\hat{\nu}}(n) \equiv \sum_{m,\hat{\rho}}\left\{\delta_{\hat{\mu},\hat{\rho}}\left[\delta_{n,m}\left[V_{m,\hat{\rho}}(t)(c_U U_{\hat{\mu}\hat{\nu}}(n)+c_{\mathcal{U}}\mathcal{U}_{\hat{\mu}\hat{\nu}}(n))+\left(c_U^{-1}U_{\hat{\mu}\hat{\nu}}^{-1}(n)+c_{\mathcal{U}}^{-1}\mathcal{U}_{\hat{\mu}\hat{\nu}}^{-1}(n)\right)V_{m,\hat{\rho}}(t)\right]\right.\right.$$

$$-\delta_{n+\hat{\nu},m}\left[c_U U_{\hat{\mu}}(n)U_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})V_{m,\hat{\rho}}(t)U_{\hat{\nu}}^{-1}(n)+c_U^{-1}U_{\hat{\nu}}(n)V_{m,\hat{\rho}}(t)U_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n)\right]$$

$$-\delta_{n-\hat{\nu},m}\left[c_{\mathcal{U}}U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})V_{m,\hat{\rho}}(t)U_{\hat{\nu}}(n-\hat{\nu})+c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})V_{m,\hat{\rho}}(t)U_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\right]\right]$$

$$+\delta_{\hat{\nu},\hat{\rho}}\left[-\delta_{n,m}\left[V_{m,\hat{\rho}}(t)c_U^{-1}U_{\hat{\mu}\hat{\nu}}^{-1}(n)+c_U U_{\hat{\mu}\hat{\nu}}(n)V_{m,\hat{\rho}}(t)\right]\right.$$

$$+\delta_{n+\hat{\mu},m}\left[c_U U_{\hat{\mu}}(n)V_{m,\hat{\rho}}(t)U_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n)+c_U^{-1}U_{\hat{\nu}}(n)U_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})V_{m,\hat{\rho}}(t)U_{\hat{\mu}}^{-1}(n)\right]$$

$$+\delta_{n-\hat{\nu},m}\left[c_{\mathcal{U}}U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})V_{m,\hat{\rho}}(t)U_{\hat{\nu}}(n-\hat{\nu})+c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})V_{m,\hat{\rho}}(t)U_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\right]$$

$$\left.\left.-\delta_{n+\hat{\mu}-\hat{\nu},m}\left[c_{\mathcal{U}}U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})V_{m,\hat{\rho}}(t)U_{\hat{\mu}}^{-1}(n-\hat{\nu})U_{\hat{\nu}}(n-\hat{\nu})+c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})U_{\hat{\mu}}(n-\hat{\nu})V_{m,\hat{\rho}}(t)U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\right]\right]\right\}$$

$$=\sum_{\hat{\rho}}\left\{\delta_{\hat{\mu},\hat{\rho}}\left[V_{n,\hat{\rho}}(t)(c_U U_{\hat{\mu}\hat{\nu}}(n)+c_{\mathcal{U}}\mathcal{U}_{\hat{\mu}\hat{\nu}}(n))+\left(c_U^{-1}U_{\hat{\mu}\hat{\nu}}^{-1}(n)+c_{\mathcal{U}}^{-1}\mathcal{U}_{\hat{\mu}\hat{\nu}}^{-1}(n)\right)V_{n,\hat{\rho}}(t)\right.\right.$$

$$-c_U U_{\hat{\mu}}(n)U_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})V_{n+\hat{\nu},\hat{\rho}}(t)U_{\hat{\nu}}^{-1}(n)-c_U^{-1}U_{\hat{\nu}}(n)V_{n+\hat{\nu},\hat{\rho}}(t)U_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n)$$

$$\left.-c_{\mathcal{U}}U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})V_{n-\hat{\nu},\hat{\rho}}(t)U_{\hat{\nu}}(n-\hat{\nu})-c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})V_{n-\hat{\nu},\hat{\rho}}(t)U_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\right]$$

$$+\delta_{\hat{\nu},\hat{\rho}}\left[-V_{n,\hat{\rho}}(t)c_U^{-1}U_{\hat{\mu}\hat{\nu}}^{-1}(n)-c_U U_{\hat{\mu}\hat{\nu}}(n)V_{n,\hat{\rho}}(t)\right.$$

$$+c_U U_{\hat{\mu}}(n)V_{n+\hat{\mu},\hat{\rho}}(t)U_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n)+c_U^{-1}U_{\hat{\nu}}(n)U_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})V_{n+\hat{\mu},\hat{\rho}}(t)U_{\hat{\mu}}^{-1}(n)$$

$$+c_{\mathcal{U}}U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})V_{n-\hat{\nu},\hat{\rho}}(t)U_{\hat{\nu}}(n-\hat{\nu})+c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})V_{n-\hat{\nu},\hat{\rho}}(t)U_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)$$

$$\left.\left.-c_{\mathcal{U}}U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})V_{n+\hat{\mu}-\hat{\nu},\hat{\rho}}(t)U_{\hat{\mu}}^{-1}(n-\hat{\nu})U_{\hat{\nu}}(n-\hat{\nu})-c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})U_{\hat{\mu}}(n-\hat{\nu})V_{n+\hat{\mu}-\hat{\nu},\hat{\rho}}(t)U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)\right]\right\}$$

$$= V_{n,\hat{\mu}}(t)(c_U U_{\hat{\mu}\hat{\nu}}(n)+c_{\mathcal{U}}\mathcal{U}_{\hat{\mu}\hat{\nu}}(n))+\left(c_U^{-1}U_{\hat{\mu}\hat{\nu}}^{-1}(n)+c_{\mathcal{U}}^{-1}\mathcal{U}_{\hat{\mu}\hat{\nu}}^{-1}(n)\right)V_{n,\hat{\mu}}(t)$$

$$- c_U U_{\hat{\mu}}(n)U_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})V_{n+\hat{\nu},\hat{\mu}}(t)U_{\hat{\nu}}^{-1}(n)-c_U^{-1}U_{\hat{\nu}}(n)V_{n+\hat{\nu},\hat{\mu}}(t)U_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n)$$

$$- c_{\mathcal{U}}U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})V_{n-\hat{\nu},\hat{\mu}}(t)U_{\hat{\nu}}(n-\hat{\nu})-c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})V_{n-\hat{\nu},\hat{\mu}}(t)U_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)$$

$$- V_{n,\hat{\nu}}(t)c_U^{-1}U_{\hat{\mu}\hat{\nu}}^{-1}(n)-c_U U_{\hat{\mu}\hat{\nu}}(n)V_{n,\hat{\nu}}(t)$$

$$+ c_U U_{\hat{\mu}}(n)V_{n+\hat{\mu},\hat{\nu}}(t)U_{\hat{\nu}}(n+\hat{\mu})U_{\hat{\mu}}^{-1}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n)+c_U^{-1}U_{\hat{\nu}}(n)U_{\hat{\mu}}(n+\hat{\nu})U_{\hat{\nu}}^{-1}(n+\hat{\mu})V_{n+\hat{\mu},\hat{\nu}}(t)U_{\hat{\mu}}^{-1}(n)$$

$$+ c_{\mathcal{U}}U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n-\hat{\nu})V_{n-\hat{\nu},\hat{\nu}}(t)U_{\hat{\nu}}(n-\hat{\nu})+c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})V_{n-\hat{\nu},\hat{\nu}}(t)U_{\hat{\mu}}(n-\hat{\nu})U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)$$

$$- c_{\mathcal{U}}U_{\hat{\mu}}(n)U_{\hat{\nu}}^{-1}(n+\hat{\mu}-\hat{\nu})V_{n+\hat{\mu}-\hat{\nu},\hat{\nu}}(t)U_{\hat{\mu}}^{-1}(n-\hat{\nu})U_{\hat{\nu}}(n-\hat{\nu})-c_{\mathcal{U}}^{-1}U_{\hat{\nu}}^{-1}(n-\hat{\nu})U_{\hat{\mu}}(n-\hat{\nu})V_{n+\hat{\mu}-\hat{\nu},\hat{\nu}}(t)U_{\hat{\nu}}(n+\hat{\mu}-\hat{\nu})U_{\hat{\mu}}^{-1}(n)$$

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