Towards Lefschetz thimbles regularization of heavy-dense QCD

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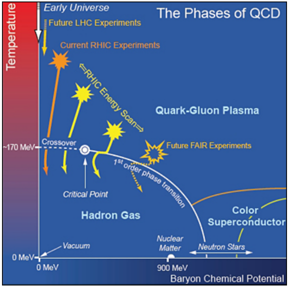
Outline

Introduction

The sign problem



- At finite density, M loses γ_5-hermitianicity and $det M$ becomes complex $\rightarrow$ sign problem
- Some techniques are available to investigate QCD at finite density, but mostly limited to small chemical potential.
- A currently active area of research is the study of alternative approaches to attack the sign problem.

- One of such approaches is thimble regularization. Idea: complexify the degrees of freedom of the theory and deform the integration paths. Picard-Lefschetz theory: attached to each critical point p_σ exists a manifold $\mathcal{J}_\sigma$ s.t.

$$\int_{\mathcal{C}} dz^n\, O(z)\, e^{-S(z)} = \sum_\sigma n_\sigma e^{-iS^I_\sigma} \int_{\mathcal{J}_\sigma} dz^n\, O(z)\, e^{-S^R_\sigma}$$

- The thimble $\mathcal{J}_\sigma$ attached to a critical point p_σ is the union of the steepest ascent paths leaving the critical points

$$\frac{dz_i}{dt} = \frac{\partial \bar{S}}{\partial \bar{z}_i}\ , \text{ with i.c. } z_i(-\infty) = z_{\sigma,i}$$

Along the flow, the imaginary part of the action is constant.

- The tangent space at p_σ is spanned by the Takagi vectors, which can be found by diagonalizing the Hessian at the critical point

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

- A natural parametrization for a point on the thimble is $z \in \mathcal{J}_\sigma \leftrightarrow (\hat{n}, t)$, where $\hat{n}$ defines the direction along which the path leaves the critical point and t is the integration time.

- Using this parametrization, the thimbles decomposition of an expectation value $\langle O \rangle$ takes the form

$$\langle O \rangle = \frac{\sum_\sigma n_\sigma \int D\hat{n}\, 2\sum_i \lambda_i^\sigma n_i^2 \int dt\; e^{-S_{eff}(\hat{n},t)}\; O\; e^{i\omega(\hat{n},t)}}{\sum_\sigma n_\sigma \int D\hat{n}\, 2\sum_i \lambda_i^\sigma n_i^2 \int dt\; e^{-S_{eff}(\hat{n},t)}\; e^{i\omega(\hat{n},t)}}$$

  where $V(\hat{n}, t)$ is the parallel transported basis, $S_{eff}(\hat{n}, t) = S_R(\hat{n}, t) - log\,|detV(\hat{n}, t)|$ and $\omega(\hat{n}, t) = arg(detV(\hat{n}, t)))$.

- The above expression may be estimated by a "crude" Montecarlo or . . .

- Observe that, when only a thimble contributes, one can rewrite $\langle O \rangle = \frac{\langle O e^{i\omega} \rangle_\sigma}{\langle e^{i\omega} \rangle_\sigma}$, having defined

$$\langle f \rangle_\sigma = \int D\hat{n} \, \frac{Z_{\hat{n}}}{Z_\sigma} \, f_{\hat{n}}$$

$$Z_\sigma = \int D\hat{n} \, Z_{\hat{n}}, \; Z_{\hat{n}} = (2 \textstyle\sum_i \lambda_i^\sigma n_i^2) \int dt \, e^{-S_{eff}(\hat{n},t)}$$

$$f_{\hat{n}} = \frac{1}{Z_{\hat{n}}} (2 \textstyle\sum_i \lambda_i^\sigma n_i^2) \int dt \, f(\hat{n}, t) e^{-S_{eff}(\hat{n},t)}$$

$\rightarrow$ importance sampling, $P_{acc}(\hat{n}' \leftarrow \hat{n}) = min\left(1, \frac{Z_{\hat{n}'}}{Z_{\hat{n}}}\right)$.

- Can be generalized to more than one thimble:

$$\langle O \rangle = \frac{\sum_\sigma n_\sigma Z_\sigma \langle O e^{i\omega} \rangle_\sigma}{\sum_\sigma n_\sigma Z_\sigma \langle e^{i\omega} \rangle_\sigma}$$

- We wanted to investigate the feasibility of thimble regularization for heavy-dense QCD, whose action is

$$S = S_G + S_F^0 + S_F^1 = -\lambda \sum_{<x,y>} \left(TrW_x \, TrW_y^\dagger + TrW_x^\dagger \, TrW_y \right)$$

$$-2 \sum_x ln \left(1 + h_1 \, TrW_x + h_1^2 \, TrW_x^\dagger + h_1^3 \right)$$

$$+2h_2 \sum_{<x,y>} \left(\frac{h_1 \, TrW_x + 2h_1^2 \, TrW_x^\dagger + 3h_1^3}{1 + h_1 \, TrW_x + h_1^2 \, TrW_x^\dagger + h_1^3} \right) \left(\frac{h_1 \, TrW_y + 2h_1^2 \, TrW_y^\dagger + 3h_1^3}{1 + h_1 \, TrW_y + h_1^2 \, TrW_y^\dagger + h_1^3} \right)$$

- Above, $h_1 = (2ke^\mu)^{N_t}$, $h_2 = k^2 \frac{N_t}{3}$ and $\lambda = (\frac{\beta}{18})^{N_t}$. At low temperatures, $\lambda \ll 1$, and the contribution of the gauge action is numerically negligible.

- We work in a convenient gauge, where $W_x = U_x$. The first step is to complexify the degrees of freedom and to find the critical points.
- I.e. for the leading term of the action, one finds

$$\nabla_z^a S_F^0 = \frac{-2i\left(h_1 \, Tr[T^a U_z] - h_1^2 \, Tr[U_z^{-1} T^a]\right)}{\left(1 + h_1 \, TrU_z + h_1^2 \, TrU_z^{-1} + h_1^3\right)}$$

  $\rightarrow$ the critical points are mixtures of center elements of $SU(3)$. This remains true after taking into account S_F^1.

- The number of critical points grows as 3^{volume}. How many of them are relevant and which is the most relevant?

- The second step in thimble regularization is to solve the Takagi problem, by determining the Takagi vectors and values.

  After that, one is able to obtain some hints from the semiclassical approximation:

$$Z = (2\pi)^{\frac{n}{2}} \sum_{\sigma} n_{\sigma} \frac{e^{-S(z_{\sigma})}}{\sqrt{\prod_i \lambda_i^{\sigma}}} \, e^{i\omega_{\sigma}} = (2\pi)^{\frac{n}{2}} \sum_{\sigma} n_{\sigma} e^{-S_{eff}^{\sigma}} \, e^{i\omega_{\sigma}}$$

- I.e. for the leading action, one finds

$$ReS_0^{\sigma} = (N - n)\,\delta S_0 + n\,\delta S_1$$

$$\sqrt{\prod_i \lambda_i^{\sigma}} = e^{-[(N-n)\,\delta d_0 + n\,\delta d_1]}$$

- At fixed (k, μ, N_t), S_{eff}^{σ} only depends on the number n of links $\neq$ identity.

- Relative weight of the degenerate thimbles:

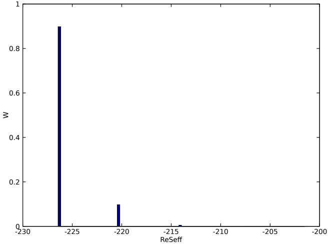
$$r = \frac{deg\ e^{-S_{eff}}}{e^{-S_{eff}[0]}} = \frac{2^n \binom{N}{n} e^{-S_{eff}}}{e^{-S_{eff}[0]}} = 2^n \binom{N}{n} e^{-n\,\delta\tilde{S}_{eff}}$$

By maximizing $ln(r)$,

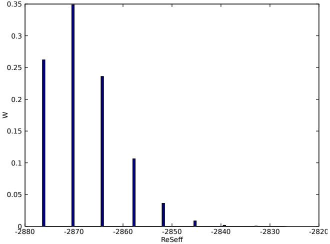
$$\rightarrow 0 = -H(n) + H(N-n) + ln(2) - \delta\tilde{S}_{eff} = f(n) - \delta\tilde{S}'_{eff}$$

$f(n)$ is a decreasing function, having value $H(N)$ at $n = 0$ and 0 at $n = \frac{N}{2}$.

- In general, if we define the weight of a degenerate thimble as $r = \frac{deg\ e^{-S_{eff}}}{\sum_\sigma e^{S_{eff}[\sigma]}}$, we can reconstruct the weights by importance sampling, sampling critical points $\propto e^{-S_{eff}}$.
- Example: histograms obtained for $\mu = 0.999\mu_c$, $V = 3^3$, 8^3



(a) $V = 3^3$



(b) $V = 8^3$

- Once we have determined which are the thimbles giving a non negligibile contribution, a problem remains to be solved: how do we determine Z_σ?
- Directly computing Z_σ might be difficult, but what about the ratio between Z_σ and Z_σ^G (where Z_σ^G is Z_σ in the gaussian approximation)?
- Take
  1. $Z_\sigma^G = \int D\hat{n} \frac{Z_{\hat{n}}^G}{Z_{\hat{n}}} Z_{\hat{n}} = Z_\sigma \int D\hat{n} \frac{Z_{\hat{n}}^G}{Z_{\hat{n}}} \frac{Z_{\hat{n}}}{Z_\sigma} = Z_\sigma \langle \frac{Z_{\hat{n}}^G}{Z_{\hat{n}}} \rangle \rightarrow \frac{Z_\sigma}{Z_\sigma^G} = \langle \frac{Z_{\hat{n}}^G}{Z_{\hat{n}}} \rangle^{-1}$
  2. $\frac{Z_\sigma^G}{\sum_{\sigma'} Z_{\sigma'}^G}$ (i.e. by the histogram method illustrated before)

  From 1) and 2) we obtain $\frac{Z_\sigma}{\sum_{\sigma'} Z_{\sigma'}^G}$, which is what we want up to a normalization factor.

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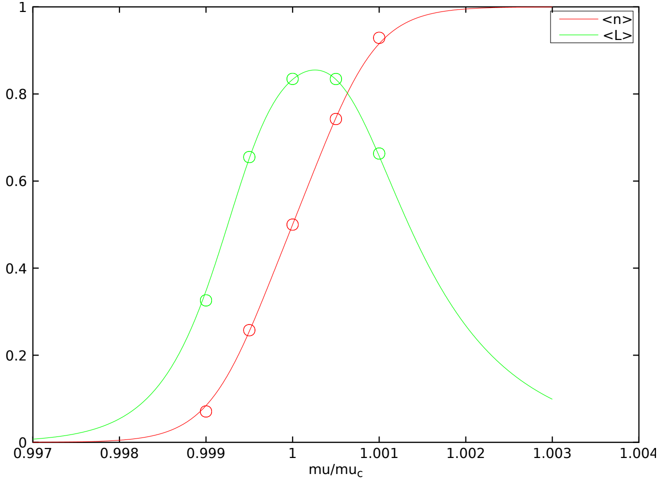
Preliminary results: single-site lattice (one thimble)



- $L(0.9990) = 0.313(2)$ ($L_{th} = 0.348$)
- $n(0.9990) = 0.0709(2)$ ($n_{th} = 0.0845$)

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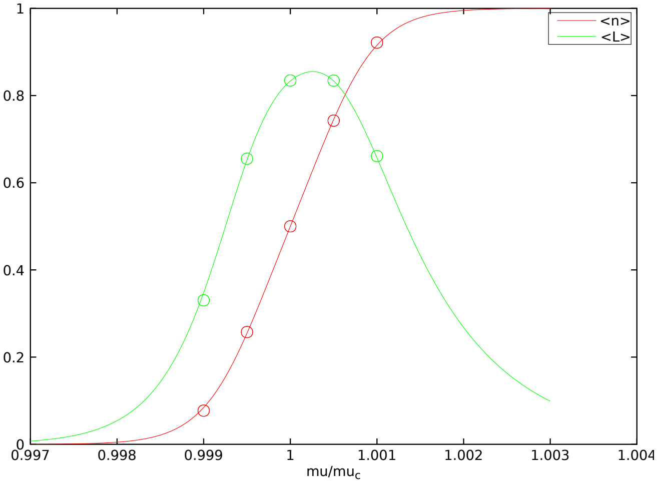
Preliminary results: single-site lattice (three thimbles)



- $L(0.9990) = 0.346(7)$ ($L_{th} = 0.348$)
- $n(0.9990) = 0.083(2)$ ($n_{th} = 0.0845$)

We had a first look at Lefschetz thimbles regularization for heavy-dense QCD:

- by a semiclassical analysis, we have found a region of parameters of physical interest where few thimbles contribute (for small lattices, up to $\approx 4^3$)
- we proposed a first-principles method to determine the weights of the contributing thimbles
- we have tested such method on a one-site simulation, recovering the expected results from theory
- in the near future, we plan to extend the simulation on a L^3 lattice and to include the $O(k^2)$ term S_F^1