

Propagator matrix for nonzero chemical potential

Journal club - Lattice field theory

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Why $\mu \neq 0$?

- μ introduces an *imbalance* between q and \bar{q} .
- Quark number density:

$$n_q = \frac{T}{V} \frac{\partial \log \mathcal{Z}(\mu, T)}{\partial \mu}.$$

- Study of (dense) baryonic matter. Examples:
 - Quark-Gluon Plasma (RHIC).
 - Neutron stars.
 - QCD phase diagram.

QCD phase diagram

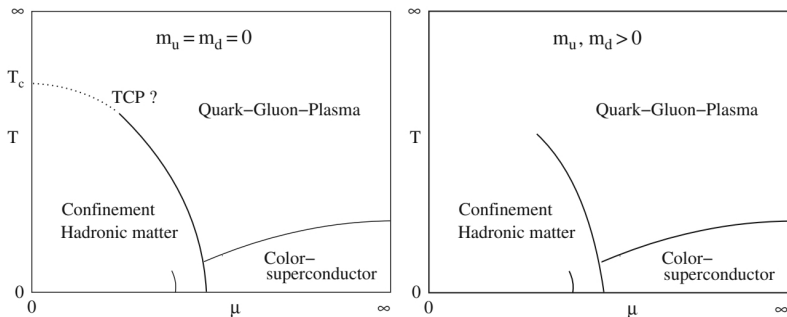


Figure: Conjectured QCD phase diagram [1].

Introduction of μ on the lattice

- Goal: introduce on the lattice a term

$$\mu \bar{\psi}(x) \gamma_4 \psi(x).$$

- Linear way:

$$D_{\text{free}}(n|m, \mu) = \sum_{j=1}^4 \gamma_j \frac{\delta_{n+\hat{j},m} - \delta_{n-\hat{j},m}}{2a} + m\delta_{nm} + \mu\gamma_4\delta_{nm}.$$

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- Divergence in the energy density appears:

$$\epsilon(\mu) - \epsilon(0) \propto \left(\frac{\mu}{a}\right)^2 \xrightarrow{a \rightarrow 0} \infty.$$

■ Alternative approach: (a la Hasenfratz-Karsch [2])

Like the QED interaction term :

- QED: $ig\bar{\psi}(x)\psi A_\nu\gamma^\nu(x)$.
- μ term: $ig\bar{\psi}(x)\psi A_\nu^{\text{ext.}}\gamma^\nu(x)\delta_{\nu,4}$.

with $A_4^{\text{ext.}} = -ia\mu/g$.

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■ Appears in the temporal term:

$$D_{\text{free}}(n|m, \mu) = \sum_{j=1}^3 \gamma_j \frac{\delta_{n+\hat{j},m} - \delta_{n-\hat{j},m}}{2a} + \gamma_4 \frac{e^\mu \delta_{n+\hat{j},m} - e^{-\mu} \delta_{n-\hat{j},m}}{2a} + m\delta_{nm}.$$

From now on $\mu \equiv \mu a$.

Sign problem

- Another problem appears:

$$\gamma_5 D(\mu) \gamma_5 = D^\dagger(-\mu).$$

$D(\mu)$ is not γ_5 -hermitian $\Rightarrow \det(D(\mu)) \in \mathbb{C}$.

- Several consequences:
 - $e^{-S_G} \det(D)$ is not a probability distribution.
 - Oscillations.

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 - Oscillations.
- Possible approaches:
 - Imaginary μ : $\mu_{\text{im}} = i\mu$ with $\mu \in \mathbb{R}$.
 - Reweighting

Dirac operator determinant

- Measurement:

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}U e^{-S_G} \det(M(\mu)) \mathcal{O}}{\int \mathcal{D}U e^{-S_G} \det(M(\mu))}$$

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- We can evaluate it stochastically, e.g. pseudofermions:

$$\det[DD^\dagger] \propto \int \mathcal{D}[\phi_R] \mathcal{D}[\phi_I] e^{-\phi^\dagger (DD^\dagger)^{-1} \phi}$$

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- Exact calculation \Rightarrow different strategies, e.g., *propagator matrix*.

Staggered formulation

- Staggered formulation:

$$D_{\text{stag.}}(n|m, \mu) = \underbrace{\sum_{j=1}^3 \eta_j \frac{U_j(n) \delta_{n+\hat{j},m} - U_{-j}(n) \delta_{n-\hat{j},m}}{2a}}_{\equiv D_{\text{stag.}}^{(3)}} + \eta_4 \frac{e^{\mu a} U_4(n) \delta_{n+\hat{j},m} - e^{-\mu a} U_{-4}(n) \delta_{n-\hat{j},m}}{2a}$$

$$M = D_{\text{stag.}} + m$$

- Definitions:

$$B_i = \eta_4 (D^{(3)} + m)|_{t=i}$$

$$U_{N_t-1} = U_4|_{t=N_t-1}$$

Propagator matrix derivation

- The derivation is in [3] with a missing factor of 3 in final exponential!
- Axial (temporal) gauge: $U_t(n) = 1 \quad \forall t \neq N_t - 1$.
- Take μ to the last time slice.
- We get $\det(M) =$

$$\det \begin{pmatrix} B_0 & 1 & 0 & \dots & U_{N_t-1}^\dagger e^{-\mu N_t} \\ -1 & B_1 & 1 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & -1 & B_{N_t-2} & 1 \\ -U_{N_t-1} e^{\mu N_t} & 0 & \dots & -1 & B_{N_t-1} \end{pmatrix}$$

Propagator matrix derivation

- Multiply by $U_{N_t-1} e^{N_t \mu}$ last column: $\det(M) = e^{-3V_s N_t \mu} \times$

$$\times \det \begin{pmatrix} B_0 & 1 & 0 & \dots & U_{N_t-1}^\dagger e^{-i\mu N_t} \\ -1 & B_1 & 1 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & -1 & B_{N_t-2} & 1 \\ -U_{N_t-1} e^{i\mu N_t} & 0 & \dots & -1 & B_{N_t-1} \end{pmatrix}$$

with $V_s = N_x N_y N_z$ spatial (dimensionless) volume.

Propagator matrix derivation

- Multiply from the left by:

$$\begin{pmatrix} 1 & B_0 & 0 & \dots & & & \\ 0 & 1 & 0 & \ddots & & & \\ 0 & 0 & 1 & B_2 & 0 & \dots & \\ 0 & 0 & 0 & 1 & 0 & \dots & \\ & & & & & \ddots & \\ 0 & 0 & \dots & 0 & 0 & 1 & B_{N_t-2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Propagator matrix derivation

- This determinant is easily calculable:

$$\det(M) = e^{3N_t V_s \mu} \det(P - e^{-N_t \mu})$$

with P the **propagator/reduced matrix**:

$$\begin{aligned} P &= - \left(\prod_{j=0,2,4}^{N_t-2} \Omega_{i,j+1} \right) U_{N_t-1} \\ &= - \left(\prod_{j=0}^{N_t-1} \begin{pmatrix} B_j & 1 \\ 1 & 0 \end{pmatrix} \right) U_{N_t-1}. \end{aligned}$$

- Then:

$$\det(M) = e^{3N_t V_s \mu} \prod_{i=1}^{6V_s} (\xi_i - e^{-N_t \mu}).$$

Properties of P

- Advantages:
 - Reduced matrix dimension $\rightarrow 6N_s^3$.
 - Independent of μ .
 - Nice properties.

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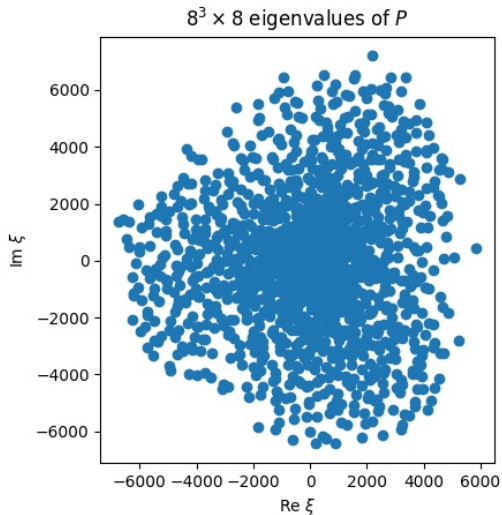
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- $\prod_i \xi_i$ with $|\xi_i| < 1$ is real positive.

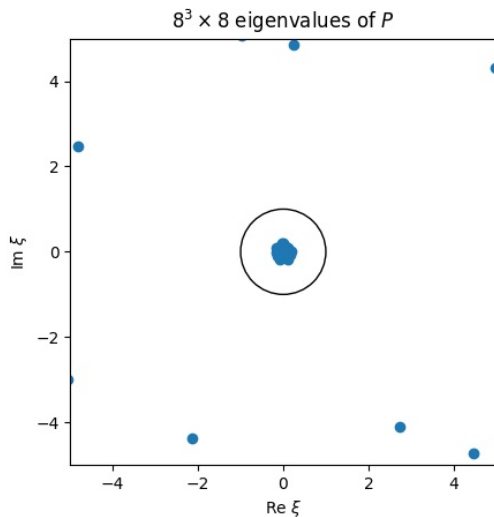
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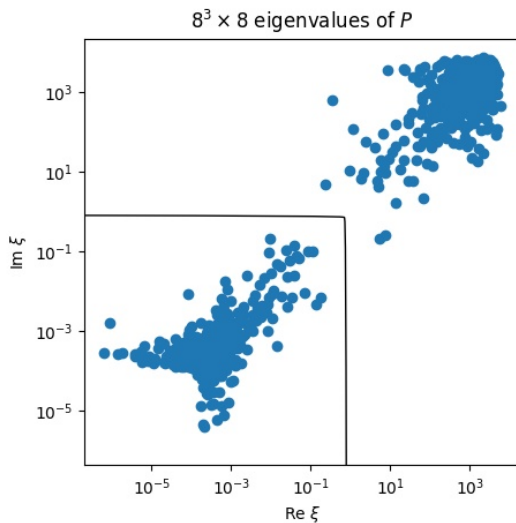
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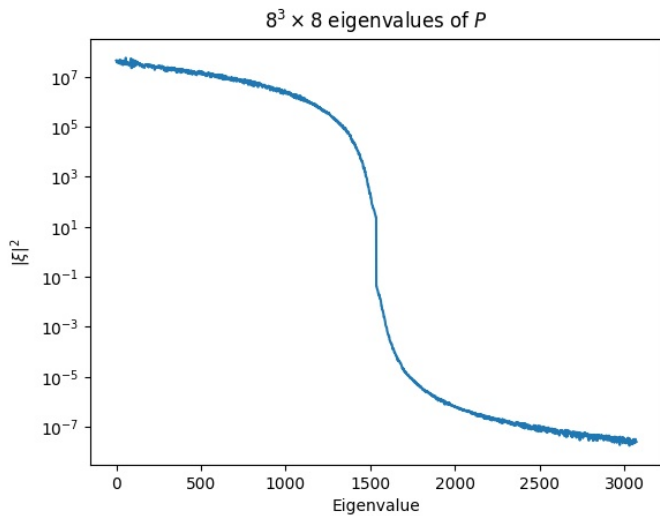
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- $\prod_i \xi_i$ with $|\xi_i| < 1$ is real positive.
- Eigenvalues of P are not in the unit circle.









Reweighting

- Allows to determine $\mathcal{Z}(T', \mu')$ from results evaluated at another T, μ :

$$\mathcal{Z}(T', \mu') = \mathcal{Z}(T, \mu) \left\langle \frac{e^{-S_G[T', \mu']} \det[M(\mu', U)]}{e^{-S_G[T, \mu']} \det[M(\mu, U)]} \right\rangle_{T, \mu}$$

- Require to evaluate $\det(M(\mu))$ exactly \Rightarrow Propagator matrix.
- Fodor, Katz [5]: $\mu = 0, T = T_c \rightarrow$ explore QCD critical point.

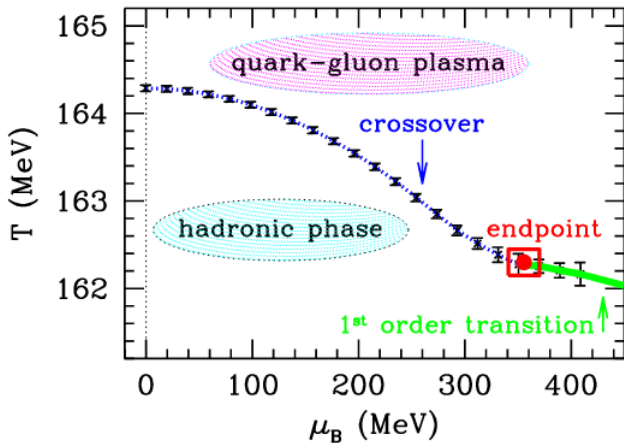


Figure: Study of the QCD critical point [5].

Lee-Yang zeros

- *Lee-Yang zeros*: $\mathcal{Z} = 0 \Rightarrow \ln \mathcal{Z} \rightarrow -\infty$: phase transitions.
- These can be related with the propagator matrix.

$$0 = \frac{\mathcal{Z}(\mu)}{\mathcal{Z}(0)} = \left\langle \frac{\det[M(\mu)]}{\det[M(0)]} \right\rangle_{\mu=0} = e^{3N_t V_s \mu} \left\langle \prod_{i=1}^{6V_s} \frac{\xi_i - e^{-N_t \mu}}{\xi_i - 1} \right\rangle_{\mu=0}.$$

- For μ_{im} , look for the zeros and check the behaviour with $1/V$.
- If in $V \rightarrow \infty$ there is a zero in $\mu \in \mathbb{R} \Rightarrow$ endpoint.
- Rooting is a technical problem here.

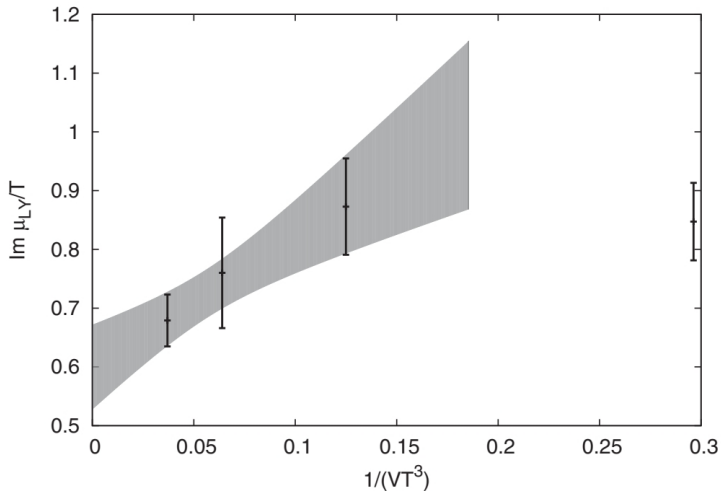


Figure: Behaviour of $\text{Im } \mu$ of the YL zeros with $1/V$ [4].

Canonical partition functions

- For μ_{im} , fugacity expansion:

$$\mathcal{Z}(T, \mu) = \sum_{n=-l_{\max}}^{l_{\max}} e^{i\mu n/T} \mathcal{Z}_n(T)$$

where n quark number, $z = e^{i\mu/T}$ fugacity. Coefficients:

$$\mathcal{Z}_n(T) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d(\mu/T) e^{-i\mu n/T} \mathcal{Z}(T, i\mu)$$

Hadron masses

- The \mathcal{Z}_n can be associated with the ξ 's:

$$\mathcal{Z}_n(T) = \mathcal{Z}(0) \cdot \left\langle \frac{1}{2\pi} \int_{-\pi}^{\pi} d(\mu/T) e^{-i\mu n/T} \left(\frac{\det M(i\mu)}{\det M(0)} \right)^{1/4} \right\rangle.$$

- They can be related with the masses of particles

$$F_{n_1, \dots, n_f} = -T \ln \mathcal{Z}_{n_1, \dots, n_f}$$
$$m_0^{n_1, \dots, n_f} = \lim_{T \rightarrow 0} F_{n_1, \dots, n_f} - F_{0, \dots, 0}$$

so they can be used for studying meson and baryon masses [6]:

$$am_\pi = \lim_{L_t \rightarrow \infty} -\frac{1}{L_t} \ln \left\langle \frac{N_t^2}{64} \left| \sum_{k=1}^{3V} \xi_k \right|^2 \right\rangle.$$

Conclusions

- Introducing μ on the lattice creates some technical problems, e.g., the sign problem.
- The propagator matrix is an exact and μ -independent way of dealing with the fermion determinant.
- Several applications to finite density QCD, e.g.:
 - Reweighting.
 - Lee-Yang zeros.
 - Meson/Baryon masses.

References I

- [1] Quantum Chromodynamics on the Lattice. An Introductory Presentation., C. Gattringer, C.B. Lang, SpringerLink (2010).
- [2] Hasenfratz P, Karsch F. Chemical potential on the lattice. Physics Letters, B . 1983; 125(4):308-310.
- [3] A. Hasenfratz and D. Toussaint, Canonical ensembles and nonzero density quantum chromodynamics, Nucl. Phys. B **371** (1992), 539-549, doi:10.1016/0550-3213(92)90247-9.
- [4] M. Giordano, K. Kapas, S. D. Katz, D. Negradi and A. Pasztor, Radius of convergence in lattice QCD at finite μ_B with rooted staggered fermions, Phys. Rev. D **101** (2020) no.7, 074511 doi:10.1103/PhysRevD.101.074511 [arXiv:1911.00043 [hep-lat]].

References II

- [5] Z. Fodor, S. Katz. Critical point of QCD at finite T and μ , lattice results for physical quark masses. Journal of High Energy Physics, Volume 2004, JHEP04 (2004).
- [6] Z. Fodor, K.K. Szabó, C. Tóth. Hadron spectroscopy from canonical partition functions. Journal of High Energy Physics, Volume 2007, JHEP08 (2007).
- [7] P.E. Gibbs, The fermion propagator matrix in lattice QCD 1986 Phys. Lett. B 172 53
- [8] I.M. Barbour and Z.A. Sabeur, Simulations with lattice QCD at finite density, Nucl. Phys. B **342** (1990), 269-278 doi:10.1016/0550-3213(90)90578-2.