Chemical potential in lattice QCD

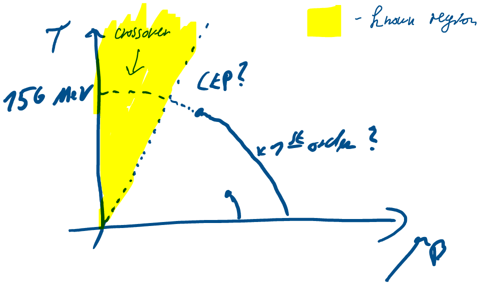
Motivations:

Matter under extreme conditions:

- Heavy Ion collisions
- Neutron stars

} Need QCD at non-vanishing Quark number density n_q.

QCD Phasediagram:



So how do we introduce it?

Reminder: grand canonical ensemble:

$$Z(T,\mu) = \mathrm{tr}\left(e^{-(\hat{H}-\mu \hat{N}_q)/T}\right)$$

In the continuum: $\hat{N}_q = \int d^3x\, \bar{\psi}(x)\gamma_4 \psi(x)$

$$\Rightarrow \mathcal{L}(\mu) = \mathcal{L}(0) - \mu \bar{\psi}\gamma_4\psi$$

$$\Rightarrow S(\mu) = \int_0^{1/T} dx^0 \int d^3x \left(\mathcal{L}(0) - \mu\bar{\psi}\gamma_4\psi\right) = S(0) - \mu \frac{\hat{N}_q}{T}$$

This suggests to simply modify the lattice Dirac Operator as follows: $D(n|m) \to D(n|m) + \mu\gamma_4\delta_{n,m}$

Unfortunately this leads to a diverging energy density in the continuum limit:

$$\varepsilon = -\frac{1}{V}\frac{\partial}{\partial\beta}\ln(Z)$$

(*) consider free theory $\Rightarrow Z = \det(D)$

$$\overset{(*)}{=} -\frac{1}{V}\frac{\partial}{\partial\beta}\ln(\det(D))\Big|_{a_T\mu = \text{const.}}$$

$$\overset{(**)}{=} -\frac{1}{(aN_S)^3 N_T}\frac{\partial}{\partial a_T}\ln(\det(D))\Big|_{a_T\mu = \text{const}}$$

(**) introduce anisotropic lattice with temporal lattice spacing a_T

Since the FT of $D(n|m)$ is diagonal in the momentum, use FT to evaluate $\det(D)$:

$$\ln(\det(D)) = \ln\Big(\prod_p \det_d[\tilde{D}(p)]\Big) \overset{!}{=} \sum_p \ln\big(\det_d[\tilde{D}(p)]\big)$$

$$\overset{!}{=} \sum_p \mathrm{tr}_d \ln(\tilde{D}(p))$$

$$\Rightarrow \frac{\partial}{\partial a_T} \ln(\det(D)) = \sum_p \mathrm{tr}_d\Big(\frac{\partial}{\partial a_T} \ln[\tilde{D}(p)]\Big)$$

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

$$\Rightarrow \sum_p \mathrm{tr}_d\Big(\frac{\partial}{\partial a_T} \ln[\tilde{D}(p)]\Big) = \frac{-4N^3N_4}{a_T} + \sum_p \mathrm{tr}_d\Big[(\tilde{D}(p)a_T)^{-1}\Big(\frac{i}{a}\sum_{j=1}^{3}\gamma_j \sin(p_j a) + m\mathbb{1}\Big)\Big]$$

$a_T = a$

$$\Rightarrow \varepsilon(\mu) = C - \frac{4}{N^3 N_4 a^4} \sum_p \underbrace{\frac{\sum_{j=1}^{3}\sin^2(ap_j) + (am)^2}{\sum_{j=1}^{3}\sin^2(ap_j) + (am)^2 + \boxed{(\sin(ap_4) - ia\mu)^2}}}_{\equiv \mathcal{F}(ap, am, \mu)}$$

causes quadratic divergence in $a \to 0$ limit.

Normalize and take $N_T, N \to \infty$

$$\Rightarrow \varepsilon(\mu) - \varepsilon(0) = -\frac{4}{(2\pi)^4}\int_{-\pi}^{\pi} d^4p\, \big(\mathcal{F}(ap, am, \mu) - \mathcal{F}(ap, am, 0)\big)$$

$$\Rightarrow \lim_{a \to 0} \varepsilon(\mu) - \varepsilon(0) \sim \Big(\frac{\mu}{a}\Big)^2$$

What went wrong?

In the continuum, the quark number is the conserved charge of the $U(1)$ global symmetry.
It is constructed from the Noether current that fulfills $\partial_\mu J^\mu = 0$
We need to find the lattice equivalent of this conservation law.

We transform $\psi(n) \to e^{i\varepsilon(n)}\psi(n) \Rightarrow \delta\psi(n) = i\varepsilon(n)\psi(n)$

$\bar{\psi}(n) \to e^{-i\varepsilon(n)}\bar{\psi}(n) \Rightarrow \delta\bar{\psi}(n) = -i\varepsilon(n)\bar{\psi}(n)$

$$S = \sum_{n,m} \bar{\psi}(n) D(n|m) \psi(m)$$

$$\Rightarrow \delta S = i\sum_{n,m} \bar{\psi}(n) D(n|m) \varepsilon(m)\psi(m) - \bar{\psi}(n)\varepsilon(n) D(n|m)\psi(m) \overset{!}{=} 0 \quad \forall \varepsilon(n)$$

e.g. naive fermions : $D(n|m) = \sum_{\nu=1}^{4} \frac{\gamma_\nu}{2a}(\delta_{m,n+\hat{\nu}} - \delta_{m,n-\hat{\nu}}) + m\,\delta_{m,n}$

$$= i\sum_n \Big[\sum_\nu \bar{\psi}(n)\frac{\gamma_\nu}{2a}\big(\psi(n+\hat{\nu})\varepsilon(n+\hat{\nu}) - \psi(n-\hat{\nu})\varepsilon(n-\hat{\nu})\big) - \bar{\psi}(n)\frac{\gamma_\nu}{2a}\big(\psi(n+\hat{\nu}) - \psi(n-\hat{\nu})\big)\varepsilon(n)$$

shift indices

$$\Rightarrow \sum_\nu \frac{1}{2a}\big(\bar{\psi}(n-\hat{\nu})\gamma_\nu\psi(n) - \bar{\psi}(n+\hat{\nu})\gamma_\nu\psi(n) - \bar{\psi}(n)\gamma_\nu\psi(n+\hat{\nu}) + \bar{\psi}(n)\psi(n-\hat{\nu})\big) \overset{!}{=} 0$$

$$\Rightarrow \sum_\nu \frac{1}{a}\big(J_\nu(n-\hat{\nu}) - J_\nu(n)\big) \overset{!}{=} 0 \quad (\simeq \partial_\mu J^\mu = 0 \text{ in continuum})$$

with $J_\nu(n) = \bar{\psi}(n)\frac{\gamma_\nu}{2}\psi(n+\hat{\nu}) + \bar{\psi}(n+\hat{\nu})\frac{\gamma_\nu}{2}\psi(n)$

Setting $\mu = 4$ and integrating over the spatial volume then gives the correct form of the chemical potential term.

Now: Use "control knob" $f(a\mu)$ to introduce this term into the temporal hopping term

$$\Rightarrow \quad \sum_n \bar\psi(n) \frac{\gamma_4}{2a}\left(f(a\mu)\, U_4(n)\, \psi(n+\hat 4) - f(a\mu)^{-1}\, U^{\dagger}_{-4}(n)\, \psi(n-\hat 4)\right)$$

Conditions to $f(a\mu)$:

- at $\mu = 0$ recover original theory
  $\Rightarrow \quad f(0) \equiv 1$
- around $\mu = 0$ recover density term:
  $\Rightarrow \quad f(a\mu) \sim 1 + a\mu + \mathcal{O}((a\mu)^2)$
- time reversal symmetry:
  $f(a\mu) = \frac{1}{f(-a\mu)}$

regarding divergence in $\varepsilon(\mu)$: $\quad \varepsilon(\mu) \sim \dfrac{\sum_j (\ldots)}{\sum_j(\ldots) + \sin^2(ap_4 - ia\mu)}$ $\Rightarrow$ no divergence!

previously $(\sin(ap_4) - ia\mu)^2$

Simple solution to these conditions:

$$f(a\mu) = \exp(a\mu)$$

$\Rightarrow$ To implement chemical potential on the lattice, modify temporal gauge link with a factor $\exp(\pm a\mu)$!

The sign problem

At $\mu = 0$, most lattice Dirac operators are γ^5 hermitian:

$$\gamma^5 D \gamma^5 = D^{\dagger}$$

This implies that the determinant $\det(D)$ is real:

$$\det(D) = \underbrace{\det(\gamma^5)}_{=1} \det(D) \det(\gamma^5) = \det(\gamma^5 D \gamma^5) = \det(D^{\dagger}) = \det(D)^*$$

At $\mu > 0$ we have $\gamma^5 D(f) \gamma^5 = D^\dagger(1/f^*)$

$$\Rightarrow \det(D(f)) = \det(D(1/f^*))^*$$

$\det(D)$ is only real for $f = 1/f^*$

$\Rightarrow$ for real f this implies $f = 1/f = 1 \Rightarrow a\mu = 0$

$\Rightarrow$ At $\mu > 0$, $\det(D)$ is complex and cannot be used for importance sampling!

Methods to circumvent the sign problem:

- Taylor Expansion around $\mu = 0$:

  Expand your Observable of interest around $\mu = 0$.

  E.g. $$\frac{P(T,\mu)}{T^4} = \sum_{i,j,k=0}^{\infty} \frac{1}{i!j!k!} \chi^{BQS}_{ijk}(T)\, \hat{\mu}_B^i \hat{\mu}_Q^j \hat{\mu}_S^k$$

  $\uparrow$ finite μ formulation generates Observables that can be evaluated at $\mu = 0$

- Analytical continuation from imaginary μ:

  for $\mu = i\eta$, $\eta \in \mathbb{R}$ $\quad f(a\mu) = f(ia\eta) = 1/f(ia\eta)^* = \frac{1}{f(-ia\eta)}$

  $\Rightarrow D$ is γ^5 hermitian $\rightarrow$ Standard techniques applicable!

  Since μ enters through $\exp(a\mu) = \exp(ia\eta)$, thermodynamic functions are 2π-periodic! One can limit the η range to $\eta \in [0, 2\pi)$

- $\exists$ many more potential techniques: Reweighting, complex Langevin, Thimbles, dual representations, ...