Lattice QCD at non-zero temperature and density

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- QCD in a nutshell, non-perturbative physics, lattice-regularized QCD, Monte Carlo simulations
- the phase diagram on strongly interacting matter, chiral symmetry restoration, the equation of state
- finite density QCD, cumulants of conserved charge fluctuations, thermal masses & transport properties

Discretization of fermion fields

$$
\mathcal{L}_E = \frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a + \bar{\psi}_{j,a} \left(\sum_{\nu=0}^3 \gamma_\nu \left(\partial_\nu - i \frac{g}{2} \mathcal{A}_\nu^a \lambda^a \right) + m_j \right)^{a,b} \psi_{j,b} \nonumber \\ \psi(x) \rightarrow \psi_n \;\; , \;\; \bar{\psi}(x) \rightarrow \bar{\psi}_n
$$

discretization of first order derivative in fermionic part is straightforward:

$$
\bar{\psi}(x)\partial_{\mu}\psi(x) \rightarrow \bar{\psi}_n\left(\frac{\psi_{n+\mu}-\psi_{n-\mu}}{2a}\right)
$$

$$
\bar{\psi}_n\psi_{n+\mu}-\bar{\psi}_n\psi_{n-\mu}
$$

discretization of derivative generates point-split terms \Rightarrow local gauge invariance?

transformation of parallel transporter: $\; U_{\mu}(n) \; \rightarrow \; G_n U_{\mu}(n) G^{-1}_{n+\mu}$ gauge transformation: $\bar{\psi}_n \psi_{n+\mu} \Rightarrow \bar{\psi}_n G_n^{-1} G_{n+\mu} \psi_{n+\mu}$

$$
\bar{\psi}(x)\gamma_\mu\left(\partial_\mu +i\frac{g}{2}{\cal A}^a_\mu\lambda^a\right)\psi(x)\ \ \rightarrow\ \ \bar{\psi}_n\gamma_\mu U_\mu(n)\psi_{n+\mu}
$$

– symmetrize discretized derivative using forward and backward differences:

$$
\bar{\psi}(x)\gamma_{\mu}\left(\partial_{\mu}+i\frac{g}{2}\mathcal{A}_{\mu}^{a}\lambda^{a}\right)\psi(x) \;\;\rightarrow\;\; \bar{\psi}_{n}\gamma_{\mu}U_{\mu}(n)\psi_{n+\mu}-\bar{\psi}_{n}\gamma_{\mu}U_{\mu}^{\dagger}(n-\mu)\psi_{n-\mu}
$$

Fermion doubler:

$$
S_F = -\int_0^t dt' \int d^3x \, \bar{\psi}(t',\vec{x}) \left[\sum_{\mu=0}^3 \gamma_\mu (\partial_\mu + igA_\mu(t',\vec{x})) + m \right] \psi(t',\vec{x})
$$

lattice regularization $\psi(x) \to \psi_n \equiv \psi_n^{a,\nu,f}$ $a = 1,..., N_c$, color

$$
S_F = \sum_{n,m} \bar{\psi}_n M_{nm} \psi_m
$$
 Grassmann
variables:
 $\psi_n \psi_m = -\psi_m \psi_n$
 $\psi_n^2 = 0$
naïve discretization scheme
 $M[U]_{nm} = m \delta_{nm} + D[U]_{nm}$
 $D[U]_{nm} = \frac{1}{2} \sum_{\mu=0}^3 \gamma_\mu \left(U_\mu(n) \delta_{n,m-\mu} - U_\mu^\dagger(n-\mu) \delta_{n,m+\mu} \right)$

The fermion doubler problem:

consider free fermions: $U_{\mu}(n) \equiv 1$ $M_{nm} = m \delta_{nm} + D_{nm}$ $\begin{split} M_{nm}&=m\,\,\delta_{nm}+D_{nm}\ D_{nm}&=\frac{1}{2}\sum_{\mu=0}^{3}\gamma_{\mu}\left(\delta_{n,m-\mu}-\delta_{n,m+\mu}\right) \end{split}$ introduce Grassmann fields in momentum space: $\boxed{p_i = \frac{2\pi}{N_\sigma} n_i}$

$$
\bar{\psi}_x = \frac{1}{\sqrt{N_\sigma^3 N_\tau}} \sum_p e^{-ipx} \bar{\psi}_p \quad , \quad x \equiv (t, \vec{x})
$$
\n
$$
\psi_x = \frac{1}{\sqrt{N_\sigma^3 N_\tau}} \sum_p e^{ipx} \psi_p
$$
\n
$$
\Rightarrow S = \frac{1}{N_\sigma^3 N_\tau} \sum_x \sum_{p, p'} e^{ix(p-p')} \bar{\psi}_{p'}^{\alpha} \left[\frac{1}{2} \sum_\mu \gamma_\mu (e^{ip_\mu} - e^{-ip_\mu}) + m \cdot 1 \right]^{\alpha \beta} \psi_p^{\beta}
$$
\n
$$
= \sum_p \bar{\psi}_p^{\alpha} \left[i \sum_\mu \gamma_\mu \sin p_\mu + m \cdot 1 \right]^{\alpha \beta} \psi_p^{\beta} \qquad \langle \bar{\psi}_p^{\alpha} \psi_p^{\beta} \rangle = (M^{-1})^{\alpha \beta}
$$
\n
$$
(M_p)_{\alpha \beta} \text{ diagonal in momentum space}
$$

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consequences become apparent in 2-particle correlation function:

$$
M_p^{-1} = (M_p^{\dagger} M_p)^{-1} M_p^{\dagger} = \frac{1}{m^2 + \sum_{\mu} \sin^2 p_{\mu}} M_p^{\dagger}
$$

\n
$$
G(t, \vec{p}) = \sum_{\vec{x}} e^{i\vec{p}\vec{x}} \langle \bar{\psi}(t, \vec{x})^{\alpha} \psi(0, \vec{0})^{\beta} \rangle
$$

\n
$$
= \sum_{p_0} e^{-ip_0 t} \frac{[m \cdot 1 - i\gamma_{\mu} \sin p_{\mu}]^{\alpha \beta}}{\sin^2 p_0 + \omega^2(\vec{p})}, \quad \omega(\vec{p}) = \left(m^2 + \sum_{i=1}^3 \sin^2 p_i\right)^{1/2}
$$

\n
$$
\sim e^{-tE(\vec{p})}
$$

\n16 poles for m=0 - 16 massless states
\n $t \to \infty$
\n
$$
\begin{array}{|l|l|}\n1.0 & \sin(p) \\
0.5 & \sin(p) \\
\hline\n0.5 & p = 0 : (Ea)^2 = (pa)^2\n\end{array}
$$

\n0.0
\n0.5
\n0.6
\n0.7
\n1.0
\n0.8
\n0.9
\n0.9
\n0.1
\n0.9
\n0.1
\n0.1
\n0.9
\n0.1
\n0.1
\n0.9
\n0.1
\n0.1

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Wilson-fermions:

introduce heavy fermions with mass $ma \sim 1$ to remove doublers

$$
m\sim 1/a\rightarrow\infty
$$

will decouple in the continuum limit

$$
S_{naive}=\sum_{n,m}\bar{\psi}_n\left[\frac{1}{2}\sum_{\mu=0}^3\gamma_{\mu}\left(\delta_{n,m-\mu}-\delta_{n,m+\mu}\right)+\hat{m}\delta_{n,m}\right]\psi_m
$$

$$
S_{Wilson} = S_{naive} - \sum_{n,m} \bar{\psi}_n \left[\frac{1}{2} \sum_{\mu=0}^3 \left(\delta_{n,m-\mu} + \delta_{n,m+\mu} \right) - 4 \delta_{n,m} \right] \psi_m
$$

$$
S_{Wilson} = \sum_{n,m} \bar{\psi}_n \left[\begin{array}{c} \frac{1}{2\kappa} \delta_{n,m} - \\ \frac{1}{2} \sum_{\mu=0}^3 \left((1+\gamma_\mu) \delta_{n,m-\mu} + (1-\gamma_\mu) \delta_{n,m+\mu} \right) \right] \psi_m \end{array}
$$

$$
\kappa = \frac{1}{8+2\hat{m}}
$$

dispersion relation for Wilson fermions

Wilson fermions remove doublers but break fundamental symmetries of continuum QCD (chiral symmetry): distortion of particle spectrum

Phys. Lett B105 (1981) 219

Nielsen-Ninomiya theorem: any 4-d lattice discretization scheme for fermions either introduces doublers or breaks chiral symmetry

staggered fermions <>>
Kogut-Susskind fermions:

J.B. Kogut and L. Susskind, Phys. Rev. D11 (1975) 395

"naïve" fermion action:

$$
\begin{array}{ll} S_{naive}=\sum\limits_{n,m}\bar{\psi}_{n}\left[\frac{1}{2}\sum\limits_{\mu=0}^{3}\gamma_{\mu}\left(\delta_{n,m-\mu}-\delta_{n,m+\mu}\right)+\hat{m}\delta_{n,m}\right]\psi_{m}\\ &\\ \psi_{n}\equiv\psi_{n}^{\alpha,i}\ \ ,\ \ \alpha=0,...,3\ \ ,\ \ i=1,...,n_{f}\end{array}
$$

perform variable transformation on fermion fields:

$$
\psi' = \Gamma \psi \quad \bar{\psi}' = \bar{\psi} \Gamma^{\dagger} \qquad \qquad \Gamma = \gamma_0^{n_0} \gamma_1^{n_1} \gamma_2^{n_2} \gamma_3^{n_3}
$$
\n
$$
\Gamma^{\dagger} = \gamma_3^{n_3} \gamma_2^{n_2} \gamma_1^{n_1} \gamma_0^{n_0}
$$
\n
$$
\implies \text{mass term is invariant:} \quad \bar{\psi}' \psi' = \bar{\psi} \psi
$$

kinetic term changes:

$$
\bar{\psi}'_n\gamma_\mu\psi'_{n\pm{\hat{\mu}}}=\bar{\psi}_n\Gamma^\dagger\gamma_\mu\tilde{\Gamma}\psi_{n\pm{\hat{\mu}}}\qquad\tilde{\Gamma}=\gamma_0^{n_0}...\gamma_\mu^{n_\mu\pm1}..\gamma_3^{n_3}
$$

all gamma matrices appear an even number of times in

$$
\Gamma^{\dagger} \gamma_{\mu} \tilde{\Gamma} \qquad \text{i.e., this product is just +/- 1.}
$$
\n
$$
\Gamma^{\dagger} \gamma_{\mu} \tilde{\Gamma} = (-1)^{x_0 + \dots + x_{\mu - 1}} \cdot 1_{spinor} \qquad i = 1, \dots n_f
$$
\n
$$
\implies \bar{\psi}^{\alpha, i} \gamma_{\alpha\beta} \psi^{\beta, i} \implies \eta_{n, \mu} \bar{\psi}^{\alpha, i} \psi^{\alpha, i} \qquad \alpha, \ \beta = 1, \dots 4
$$
\nwith $\eta_{n, \mu} = (-1)^{n_0 + \dots + n_{\mu - 1}}$

the action now is diagonal in flavor AND spinor space!!

$$
Z = \int \prod dU_{n,\mu} \left[\det M_{KS} \right]^{4n_f} e^{-S_G}
$$

J.B. Kogut and L. Susskind, Phys. Rev. D11 (1975) 395

drop 3 out of 4 ''spinor'' components; reduce fermion doubling from 16 to 4

 $n_f = 1$ (drop 3 components):

$$
Z=\int \prod dU_{n,\mu} \left[\det \, M_{KS} \right] {\rm e}^{-S_G}
$$

describes in the continuum limit a 4-flavor theory

$$
\begin{aligned} M_{KS}&=m\cdot 1+D_{KS} \\ \left(M_{KS}\right)^{nm}&=\frac{1}{2}\sum_{\mu=0}^{3}\eta_{n,\mu}\left(U_{n,\mu}\delta_{n,m-\mu}-U_{n-\mu,\mu}^{\dagger}\delta_{n,m+\mu}\right) \end{aligned}
$$

 $\eta_{n,\mu}$ does not change sign when 'moving' in μ direction

$$
D_{KS}=\left(\begin{array}{cc} 0 & D_{eo} \\ D_{oe} & 0 \end{array}\right) \qquad \text{with} \quad \begin{array}{cc} D_{oe}=-D_{eo}^{\dagger} \\ \text{i.e.} & D^{\dagger}=-D \end{array}
$$

eigenvalues are purely imaginary and come in complex conjugate pairs \Rightarrow $\det M_{KS} \geq 0$

Monte Carlo Simulations

Observables = Expectation values

$$
Z = \int \mathcal{D} \mathcal{A} \mathcal{D} \psi \mathcal{D} \bar{\psi} e^{-S_E} \qquad \qquad \langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D} \mathcal{A} \mathcal{D} \psi \mathcal{D} \bar{\psi} \, \mathcal{O} e^{-S_E}
$$

integrate out fermions:

$$
Z = \int \mathcal{D}A \mathcal{D} \psi \mathcal{D} \bar{\psi} e^{-S_E} = \int \mathcal{D}A \prod_f \det M(m_f) e^{-S_G} = \int \mathcal{D}A e^{-S}
$$

$$
S = S_G - \sum_f \text{Tr} \ln M(m_f)
$$

distribute gauge field configurations $\{\mathcal{A}^{(i)}\}_{i=1}^{N_{tot}}$ according to the probability distribution $P({A}) = Z^{-1}e^{-S({A})}$ Monte Carlo algorithms (detailed balance) generates Markov chain

$$
\text{calculate expectation values: } \langle \mathcal{O} \rangle = \lim_{N_{tot} \to \infty} \frac{1}{N_{tot}} \sum_{i=1}^{N_{tot}} \mathcal{O}(\{\mathcal{A}^{(i)}\})
$$

Dealing with the fermion determinant

partition function again:

$$
Z(V,T) = \int \mathcal{D}\mathcal{A} \int \prod_{n \text{fermions}} \mathrm{d}\psi_n \mathrm{d}\bar{\psi}_n \,\,\mathrm{e}^{\bar{\psi}_n M(A,m_q)_{nm}\psi_m} \,\,\mathrm{e}^{-S_G}
$$
\n
$$
= \int \mathcal{D}\mathcal{A} \,\,\mathrm{det} M(\mathcal{A}, m_q) \,\,\mathrm{e}^{-S_G}
$$
\n"fermion matrix"\n
$$
\mathrm{det} M(\mathcal{A}, m_q) = \int \prod_{\substack{n \text{bosons} \\ \text{bosons}}} \mathrm{d}\phi_n \,\,\mathrm{e}^{-\sum_{nm} \phi_n^* M_{nm}^{-1} (\mathcal{A}, m_q) \phi_m}
$$
\n
$$
= \text{need} \quad x_n = M_{nm}^{-1} \phi_m
$$
\n
$$
- \text{node} \quad M_{nm} x_m = \phi_n
$$

Computational resources for Lattice QCD

Cori@NERSC

Intel Xeon Phi processor Knights Landing 9300 compute nodes #5, top500, 2016 peak: 29 Petaflops $=29 \times 10^{15}$ Flops

Titan@ORNL

Cray with NVIDIA graphics cards K20X 18688 GPUs #3, top500, 2016 peak: 20 Petaflops =20 Mill. Gflops

QCD as a video game,

G.I. Egri et al, Comp. Phys. Com, **177**, 631 (2007)

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1980/81:

first lattice calculation of an equation of state for gluon matter

Thermodynamics of strong-interaction matter

reminder:

Euclidean path integrals and thermodynamics (in quantum mechanics)

Time evolution operator:
$$
U(t, t') = \exp\left(-\frac{i}{\hbar}(t - t')H\right)
$$

$$
\psi_n(x, t) \equiv \langle x|U(t, 0)|\psi_n\rangle
$$

$$
= e^{-iE_n t/\hbar}\langle x|\psi_n\rangle
$$

Green's functions:
$$
G(y, t''; x, t') \equiv \langle y|U(t'', t')|x\rangle
$$

$$
= \sum_{n} e^{-\frac{i}{\hbar}E_n(t''-t)} \psi_n(y) \psi_n^*(x)
$$

Special case – periodic paths: $y = q(t) = q(0) = x$

$$
\begin{array}{lcl} \tilde{Z}(t) & = & \displaystyle \int dx\ G(x,t;x,0) = \int dx \langle x| \mathrm{e}^{-itH/\hbar} |x \rangle \\ \\ & = & \displaystyle \int dx\sum_n \mathrm{e}^{-\frac{i}{\hbar} E_n t} \psi_n(x) \psi_n^*(x) = \sum_n \mathrm{e}^{-\frac{i}{\hbar} E_n t} = \ \textrm{Tr}\ \mathrm{e}^{-itH/\hbar} \\ \\ \tilde{Z}(it) & = Z(\beta) \ \ \textrm{with} \ \ t = -i\hbar/T \ \ , \ \ \beta = 1/T \end{array}
$$

Simulating strongly interacting matter on a discrete space-time grid (lattice QCD)

 \boldsymbol{a} the lattice: $N_{\tau}^3 \times N_{\tau}$ lattice spacing: \boldsymbol{a} temperature: $T = 1/N_{\tau} a$ $1/T = N_{\tau} a$ bulk thermodynamics: $\frac{p}{T^4} = \frac{1}{VT^3} \ln Z$ \sim $V^{1/3}$ =N_oa $\frac{\epsilon}{T^4} = -\frac{1}{VT^4}\frac{\partial\ln Z}{\partial T^{-1}}$ partition function: $Z(\boldsymbol{V},\boldsymbol{T},\mu)=\int \mathcal{D}\mathcal{A}\mathcal{D}\psi\mathcal{D}\bar{\psi}\,\,\mathrm{e}^{-S_E},$ n_B 1 $\partial \ln Z$ $\frac{\overline{1}}{T^3} = \frac{\overline{1}}{V T^3} \frac{\partial \mu_B}{\partial T}$ $\frac{\chi_B}{\chi_B} = \frac{1}{\chi_B} \frac{\partial^2 \ln Z}{\partial Z}$ $\frac{\delta \Gamma}{T^2} = \frac{1}{V T^3} \frac{1}{\partial (\mu_B/T)^2}$

Simulating strongly interacting matter on a discrete space-time grid (lattice QCD)

 \boldsymbol{a} the lattice: $N_{\tau}^3 \times N_{\tau}$ lattice spacing: \boldsymbol{a} temperature: $T = 1/N_{\tau} a$ $1/T = N_\tau a$ bulk thermodynamics: $V^{1/3} = N_0 a$ $\frac{p}{T^4} = \frac{1}{VT^3} \ln Z$ $\frac{\epsilon}{T^4} = - \frac{1}{VT^4} \frac{\partial \ln Z}{\partial T^{-1}}$ phase structure: order parameter: $\displaystyle{\frac{\langle \bar{\psi}\psi \rangle_l}{T^3}=\frac{1}{VT^3}\frac{1}{4}\frac{\partial\ln Z}{\partial m_l/T}}$ n_B 1 $\partial \ln Z$ $\frac{E}{T^3} = \frac{1}{VT^3} \frac{\partial \mu_B}{T}$ chiral susceptibility: $\displaystyle{\frac{\chi_l}{T^2}=\frac{\partial \langle \bar{\psi}\psi \rangle_l/T^3}{\partial m_l/T}}$ $\frac{\chi_B}{\chi_B} = \frac{1}{\chi_B} \frac{\partial^2 \ln Z}{\partial Z}$ $\overline{\overline{T^2}} \equiv \overline{VT^3}\, \overline{\partial (\mu_B/T)^2}$

Calculating the equation of state on lines of constant physics (LCPs)

pressure (not an expectation value): $\frac{p}{T^4} = \frac{1}{V T^3} \ln Z$

trace anomaly (sometimes called interaction measure):

$$
\frac{\epsilon - 3p}{T^4} = T \frac{d}{dT} \left(\frac{p}{T^4} \right) = \left(a \frac{d\beta}{da} \right)_{LCP} \frac{\partial p/T^4}{\partial \beta}
$$

$$
= \left(\frac{\epsilon - 3p}{T^4} \right)_{gluon} + \left(\frac{\epsilon - 3p}{T^4} \right)_{fermion} + \left(\frac{\epsilon - 3p}{T^4} \right)_{\hat{m}_s/\hat{m}_l}
$$
pressure (reconstructed):
$$
\frac{p}{T^4} \Big|_{\beta_0}^{\beta} = \int_{T_0}^{T} dT \frac{1}{T} \left(\frac{\epsilon - 3p}{T^4} \right)
$$

lines of constant physics (LCP):

need T-scale $aT = 1/N_\tau$ and its relation to the gauge coupling $a \equiv a(\beta)$

LCP: for given $\boldsymbol{\beta}$ choose $m_{u/d}, m_s$ such that the "known hadron spectrum **gets reproduced at T=0''**

Calculating the equation of state on lines of constant physics (LCPs)

trace anomaly:
$$
\frac{\epsilon - 3p}{T^4} = T \frac{d}{dT} \left(\frac{p}{T^4} \right) \equiv a \left(\frac{N_\tau}{N_\sigma} \right)^3 \frac{d \ln Z(T, V)}{da} \qquad T \equiv \frac{1}{N_\tau a}
$$

$$
\frac{\epsilon - 3p}{T^4} \equiv \frac{\Theta_G^{\mu\mu}(T)}{T^4} + \frac{\Theta_F^{\mu\mu}(T)}{T^4} \qquad \langle ... \rangle_{0(\tau)}
$$
expectation values

$$
\frac{\Theta_G^{\mu\mu}(T)}{T^4} = R_\beta \left[\langle s_G \rangle_0 - \langle s_G \rangle_\tau \right] N_\tau^4 \qquad \text{temperature}
$$

$$
\frac{\Theta_F^{\mu\mu}(T)}{T^4} = -R_\beta R_m [2m_l \left(\langle \bar{\psi} \psi \rangle_{l,0} - \langle \bar{\psi} \psi \rangle_{l,\tau} \right)
$$

$$
+ m_s \left(\langle \bar{\psi} \psi \rangle_{s,0} - \langle \bar{\psi} \psi \rangle_{s,\tau} \right)] N_\tau^4
$$

beta-functions:
68.2 scale setting:
$$
r_1
$$
-scale: $r^2 \frac{dV_{\bar{q}q}}{dr}\Big|_{r_1} = 1$
 $R_2(3) = \frac{r_1}{r_1} \left(\frac{d(r_1/a)}{dr}\right)^{-1}$ $r_1 = 0.3106$ fm

F. Karsch, NNPSS 2017 19 bare strange quark mass: $m_s(\beta)$ keep a strange hadron mass const.
 $m_{sH}r_1 \equiv m_{sH}a \cdot \frac{r_1}{r_1} = \text{const.}$

$$
R_{\boldsymbol{\beta}}(\boldsymbol{\beta}) = \frac{r_1}{a} \left(\frac{\mathrm{d}(r_1/a)}{\mathrm{d}\beta} \right)^{-1} \nonumber \\ R_m(\boldsymbol{\beta}) = \frac{1}{m_s(\boldsymbol{\beta})} \frac{\mathrm{d}m_s(\boldsymbol{\beta})}{\mathrm{d}\beta}
$$

– calculate the heavy quark potential
 $V_{\bar{q}q}(r/a)a$ A)

– extract r_1/a

Heavy Quark potential

– tune the bare quark mass(es) such that $m_H r_1 = m_H a \cdot r_1/a$ takes on its physical value

 $\longrightarrow m_l(\beta), m_s(\beta)$

Equation of state of (2+1)-flavor QCD

– up to the crossover region the QCD EoS agrees quite well with hadron resonance gas (HRG) model calculations; **However**, QCD results are systematically above HRG

Equation of state of (2+1)-flavor QCD

Crossover transition parameters

PDG: Particle Data Group hadron spectrum

Crossover transition parameters

Crossover transition parameters

