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

$$\mathcal{L}_E = rac{1}{4} F^a_{\mu
u} F^a_{\mu
u} + ar{\psi}_{j,a} \left(\sum_{
u=0}^3 \gamma_
u \left(\partial_
u - i rac{g}{2} \mathcal{A}^a_
u \lambda^a
ight) + m_j
ight)^{a,b} \psi_{j,b}$$

$$\psi(x) o \psi_n \;\;,\;\; \psi(x) o \psi_n$$

discretization of first order derivative in fermionic part is straightforward: $-\sqrt{\eta/m} + \mu - \eta/m$

forward:
$$ar{\psi}(x)\partial_\mu\psi(x) o ar{\psi}_n\left(rac{\psi_{n+\mu}-\psi_{n-\mu}}{2a}
ight)$$

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

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

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

$$ar{\psi}(x)\gamma_{\mu}\left(\partial_{\mu}+irac{g}{2}\mathcal{A}^{a}_{\mu}\lambda^{a}
ight)\psi(x) ~
ightarrow ~ar{\psi}_{n}\gamma_{\mu}U_{\mu}(n)\psi_{n+\mu}$$

- symmetrize discretized derivative using forward and backward differences:

$$ar{\psi}(x)\gamma_{\mu}\left(\partial_{\mu}+irac{g}{2}\mathcal{A}^{a}_{\mu}\lambda^{a}
ight)\psi(x) ~
ightarrow ~ar{\psi}_{n}\gamma_{\mu}U_{\mu}(n)\psi_{n+\mu}-ar{\psi}_{n}\gamma_{\mu}U^{\dagger}_{\mu}(n-\mu)\psi_{n-\mu}$$

Fermion doubler:

$$\begin{split} S_{F} &= -\int_{0}^{t} \mathrm{d}t' \int \mathrm{d}^{3}x \; \bar{\psi}(t', \vec{x}) \left[\sum_{\mu=0}^{3} \gamma_{\mu}(\partial_{\mu} + igA_{\mu}(t', \vec{x})) + m \right] \psi(t', \vec{x}) \\ & \left[\text{lattice regularization } \psi(x) \rightarrow \psi_{n} \equiv \psi_{n}^{a,\nu,f} \quad a = 1, ..., \; N_{c}, \; \text{color} \\ \nu = 1, ..., \; 4, \; \text{spinor} \\ S_{F} &= \sum_{n,m} \bar{\psi}_{n} M_{nm} \psi_{m} \quad \underset{\text{variables:} \\ \psi_{n} \psi_{m} = -\psi_{m} \psi_{n} \\ \psi_{n}^{2} = 0 \\ \\ & \mathsf{na\"ive discretization \; scheme} \quad M[U]_{nm} \; = \; m \; \delta_{nm} + D[U]_{nm} \\ D[U]_{nm} &= \frac{1}{2} \sum_{\mu=0}^{3} \gamma_{\mu} \left(U_{\mu}(n) \delta_{n,m-\mu} - U_{\mu}^{\dagger}(n-\mu) \delta_{n,m+\mu} \right) \end{split}$$

The fermion doubler problem:

consider free fermions: $U_{\mu}(n) \equiv 1$ $M_{nm} = m \ \delta_{nm} + D_{nm}$ $D_{nm} = rac{1}{2} \sum_{\mu=0}^{3} \gamma_{\mu} \left(\delta_{n,m-\mu} - \delta_{n,m+\mu}\right)$

introduce Grassmann fields in momentum space: $\int p_i = rac{2\pi}{N_\sigma} n_i$

$$\begin{split} \bar{\psi}_{x} &= \frac{1}{\sqrt{N_{\sigma}^{3}N_{\tau}}} \sum_{p} e^{-ipx} \bar{\psi}_{p} \quad , \ x \equiv (t, \vec{x}) \\ \psi_{x} &= \frac{1}{\sqrt{N_{\sigma}^{3}N_{\tau}}} \sum_{p} e^{ipx} \psi_{p} \\ \Rightarrow \quad S &= \frac{1}{N_{\sigma}^{3}N_{\tau}} \sum_{x} \sum_{p,p'} e^{ix(p-p')} \bar{\psi}_{p'}^{\alpha} \left[\frac{1}{2} \sum_{\mu} \gamma_{\mu} (e^{ip\mu} - e^{-ip\mu}) + m \cdot 1 \right]^{\alpha\beta} \psi_{p}^{\beta} \\ &= \sum_{p} \bar{\psi}_{p}^{\alpha} \left[i \sum_{\mu} \gamma_{\mu} \sin p_{\mu} + m \cdot 1 \right]^{\alpha\beta} \psi_{p}^{\beta} \qquad \langle \bar{\psi}_{p}^{\alpha} \psi_{p}^{\beta} \rangle = (M^{-1})^{\alpha\beta} \\ & (M_{p})_{\alpha\beta} \quad \text{diagonal in momentum space} \end{split}$$

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consequences become apparent in 2-particle correlation function:

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

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

$$= \sum_{p_{0}} e^{-ip_{0}t} \frac{[m \cdot 1 - i\gamma_{\mu}\sin p_{\mu}]^{\alpha\beta}}{\sin^{2}p_{0} + \omega^{2}(\vec{p})} , \quad \omega(\vec{p}) = \left(m^{2} + \sum_{i=1}^{3}\sin^{2}p_{i}\right)^{1/2}$$

$$\approx e^{-tE(\vec{p})} \qquad 16 \text{ poles for } m=0 \rightarrow 16 \text{ massless states}$$

$$t \rightarrow \infty \qquad (\text{continuum dispersion relation})$$

$$(m_{0,5}) \qquad (m_{1,0}) \qquad$$

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Wilson-fermions:

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

$$\checkmark m \sim 1/a
ightarrow \infty$$

will decouple in the continuum limit

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

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

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:

$$egin{aligned} S_{naive} &= \sum_{n,m} ar{\psi}_n \left[rac{1}{2} \sum_{\mu=0}^3 \gamma_\mu \left(\delta_{n,m-\mu} - \delta_{n,m+\mu}
ight) + \hat{m} \delta_{n,m}
ight] \psi_m \ &\psi_n \equiv \psi_n^{lpha,i} \ , \ lpha &= 0,...,3 \ , \ i = 1,..,n_f \end{aligned}$$

perform variable transformation on fermion fields:

$$\psi' = \Gamma \psi \ \bar{\psi}' = \bar{\psi} \Gamma^{\dagger}$$

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

kinetic term changes:

$$ar{\psi}'_n \gamma_\mu \psi'_{n\pm\hat{\mu}} = ar{\psi}_n \Gamma^\dagger \gamma_\mu ilde{\Gamma} \psi_{n\pm\hat{\mu}} \qquad ilde{\Gamma} = \gamma_0^{n_0} ... \gamma_\mu^{n_\mu\pm 1} ... \gamma_3^{n_3}$$

all gamma matrices appear an even number of times in

$$\begin{split} \Gamma^{\dagger}\gamma_{\mu}\tilde{\Gamma} & \text{ i.e., this product is just +/- 1.} \\ \Gamma^{\dagger}\gamma_{\mu}\tilde{\Gamma} &= (-1)^{x_{0}+...x_{\mu-1}} \cdot 1_{spinor} & i = 1,..n_{f} \\ & & \downarrow \tilde{\psi}^{\alpha,i}\gamma_{\alpha\beta}\psi^{\beta,i} \Rightarrow \eta_{n,\mu}\bar{\psi}^{\alpha,i}\psi^{\alpha,i} & \alpha, \ \beta = 1,..4 \\ & \text{ with } \eta_{n,\mu} = (-1)^{n_{0}+...n_{\mu-1}} \end{split}$$

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

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

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):

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

describes in the continuum limit a 4-flavor theory

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

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

$$D_{KS} = \begin{pmatrix} 0 & D_{eo} \\ \hline D_{oe} & 0 \end{pmatrix} \quad \text{with} \quad D_{oe} = -D_{eo}^{\dagger}$$

i.e. $D^{\dagger} = -D$

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

Monte Carlo Simulations

Observables = Expectation values

$$Z \;\;=\;\; \int {\cal D} {\cal A} {\cal D} \psi {\cal D} ar \psi \; {
m e}^{-S_E} \qquad \qquad \langle {\cal O}
angle \;\;=\;\; {1\over Z} \int {\cal D} {\cal A} {\cal D} \psi {\cal D} ar \psi \; {\cal O} {
m e}^{-S_E}$$

integrate out fermions:

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

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

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:

$$Z(V,T) = \int \mathcal{D}\mathcal{A} \int \prod_{n} d\psi_{n} d\bar{\psi}_{n} e^{\bar{\psi}_{n}M(A,m_{q})_{nm}\psi_{m}} e^{-S_{G}}$$
fermions
(anti-commuting))
$$= \int \mathcal{D}\mathcal{A} \det M(\mathcal{A}, m_{q}) e^{-S_{G}}$$
"fermion matrix"
$$det M(\mathcal{A}, m_{q}) = \int \prod_{n} d\phi_{n} e^{-\sum_{nm} \phi_{n}^{*}M_{nm}^{-1}(\mathcal{A}, m_{q})\phi_{m}}$$
bosons
(commuting)
$$-need \quad x_{n} = M_{nm}^{-1}\phi_{m}$$

$$-solve \quad M_{nm}x_{m} = \phi_{n}$$

Computational resources for Lattice QCD





Cori@NERSC

Intel Xeon Phi processor Knights Landing 9300 compute nodes #5, top500, 2016 peak: 29 Petaflops =29 x 10¹⁵ 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)

Computational resources for Lattice QCD



Cori@NERSC

Intel Xeon Phi processor Knights Landing

9300 compute nodes #5, top500, 2016 peak: 29 Petaflops =29 x 10^{15} Flops





1980/81:

first lattice calculation of an equation of state for gluon matter in Bielefeld

Thermodynamics of strong-interaction matter

reminder:

Euclidean path integrals and thermodynamics (in quantum mechanics)

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

 $\psi_n(x,t) \equiv \langle x|U(t,0)|\psi_n\rangle$
 $= e^{-iE_nt/\hbar}\langle x|\psi_n\rangle$

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

$$egin{aligned} ilde{Z}(t) &= \int dx \, G(x,t;x,0) = \int dx \langle x | \mathrm{e}^{-itH/\hbar} | x
angle \ &= \int dx \sum_n \mathrm{e}^{-rac{i}{\hbar} E_n t} \psi_n(x) \psi_n^*(x) = \sum_n \mathrm{e}^{-rac{i}{\hbar} E_n t} = & \mathrm{Tr} \; \mathrm{e}^{-itH/\hbar} \ & ilde{Z}(it) = Z(eta) \; ext{ with } t = -i\hbar/T \; , \; eta = 1/T \end{aligned}$$

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

a the lattice: $N_{\sigma}^3 \times N_{\tau}$ lattice spacing: atemperature: $T = 1/N_{\tau}a$ $1/T = N_{\tau} a$ bulk thermodynamics: $rac{p}{T^4} = rac{1}{VT^3} \ln Z$ $---- V^{1/3} = N_{\odot} a$ $\frac{\epsilon}{T^4} = -\frac{1}{VT^4} \frac{\partial \ln Z}{\partial T^{-1}}$ partition function: $Z(V,T,\mu) = \int \mathcal{D} \mathcal{A} \mathcal{D} \psi \mathcal{D} ar{\psi} \; \mathrm{e}^{-S_E}$ n_B 1 $\partial \ln Z$ $\overline{T^3} = \overline{VT^3} \, \overline{\partial \mu_B / T}$ $\chi_B = 1 \quad \partial^2 \ln Z$ $\frac{1}{T^2} = \frac{1}{VT^3} \frac{1}{\partial(\mu_B/T)^2}$

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



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

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

trace anomaly (sometimes called interaction measure):

$$\begin{split} \frac{\epsilon - 3p}{T^4} &= T \frac{\mathrm{d}}{\mathrm{d}T} \left(\frac{p}{T^4} \right) = \left(a \frac{\mathrm{d}\beta}{\mathrm{d}a} \right)_{LCP} \frac{\partial p/T^4}{\partial \beta} \\ &= \left(\frac{\epsilon - 3p}{T^4} \right)_{gluon} + \left(\frac{\epsilon - 3p}{T^4} \right)_{fermion} + \left(\frac{\epsilon - 3p}{T^4} \right)_{\hat{m}_s/\hat{m}_l} \end{split}$$
pressure (reconstructed):
$$\left. \left. \frac{p}{T^4} \right|_{\beta_0}^{\beta} &= \int_{T_0}^T \mathrm{d}T \; \frac{1}{T} \left(\frac{\epsilon - 3p}{T^4} \right) \right.$$

lines of constant physics (LCP):

need T-scale $aT=1/N_{ au}$ and its relation to the gauge coupling $a\equiv a(eta)$

LCP: for given β 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)

$$\begin{array}{l} \text{trace anomaly:} \quad \frac{\epsilon - 3p}{T^4} = T \frac{\mathrm{d}}{\mathrm{d}T} \left(\frac{p}{T^4}\right) \equiv a \left(\frac{N_{\tau}}{N_{\sigma}}\right)^3 \frac{\mathrm{d}\ln Z(T,V)}{\mathrm{d}a} \qquad T \equiv \frac{1}{N_{\tau}a} \\ \\ \quad \frac{\epsilon - 3p}{T^4} \equiv \frac{\Theta_G^{\mu\mu}(T)}{T^4} + \frac{\Theta_F^{\mu\mu}(T)}{T^4} \qquad & \langle \dots \rangle_{0(\tau)} \\ \\ \quad \expectation \text{ values} \\ \\ \quad \frac{\Theta_G^{\mu\mu}(T)}{T^4} = R_\beta \left[\langle s_G \rangle_0 - \langle s_G \rangle_\tau \right] N_{\tau}^4 \qquad & \text{temperature} \\ \\ \\ \quad \frac{\Theta_F^{\mu\mu}(T)}{T^4} = -R_\beta R_m \left[2m_l \left(\langle \bar{\psi}\psi \rangle_{l,0} - \langle \bar{\psi}\psi \rangle_{l,\tau} \right) \right] N_{\tau}^4 \end{array}$$

$$egin{aligned} rac{\Theta_F^{\prime\prime}\left(T
ight)}{T^4} &= -R_eta R_m [2m_l\left(\langlear\psi\psi
angle_{l,0}-\langlear\psi\psi
angle_{l, au}
ight. + m_s\left(\langlear\psi\psi
angle_{s,0}-\langlear\psi\psi
angle_{s, au}
ight)]N_ au^4 \end{aligned}$$

beta-functions:

 $egin{aligned} R_eta(eta) &= rac{r_1}{a} \left(rac{\mathrm{d}(r_1/a)}{\mathrm{d}eta}
ight)^{-1} \ R_m(eta) &= rac{1}{m_s(eta)} rac{\mathrm{d}m_s(eta)}{\mathrm{d}eta} \end{aligned}$

scale setting:
$$r_1$$
-scale: $r^2 \frac{dV_{\bar{q}q}}{dr}\Big|_{r_1} = 1$
 $r_1 = 0.3106 \text{ fm}$

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

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

- extract r_1/a



Heavy Quark potential



– calculate a hadron mass $m_H a$

B)

– 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



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Crossover transition parameters

PDG: Particle Data Group hadron spectrum



Crossover transition parameters



Crossover transition parameters



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