Complex Langevin simulation applied to a chiral model

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Complexification approaches to the sign problem

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Outline

• The sign problem

• Old & renewed approach:
  – Complex Langevin simulation

• New approach:
  – HMC simulation on Lefschetz thimble
  – No sign problem?

• Discussion and outlook
QCD partition fn & sign problem

\[ Z(T, \mu) = \text{Tr} \ e^{-\beta(H - \mu N)} = \sum_N e^{-\beta E_N} 2\cosh(\beta \mu N) \]

→ is real positive, and a function of \( \mu^2 \)

\[ Z(T, \mu) = \int dU d\psi d\bar{\psi} e^{-S} = \int dU e^{-S_B} \det D \]

→ Importance sampling works if “\( e^{-S} \det D \)” >0

→ At finite \( \mu \), \( \det D(\mu) = \det D(-\mu)^* \) is complex: \text{sign problem}

→ Attempts to overcome the problem

→ Taylor expansion at \( \mu = 0 \), Imaginary \( \mu \), Re-weighting,
→ Density of states, ...
Old & new complexification approaches to the sign problem

- Complex Langevin simulation
- Simulation on the Lefschetz thimble
Langevin dynamics

- Statistical sampling w/o explicit weight fn (the Fokker-Planck eqn is associated)
- Equilibrium state is thermal (Brown motion)

\[ \frac{dv_i(t)}{dt} = -\gamma v_i(t) + \eta_i(t) \quad \langle \eta_i(t)\eta_j(t') \rangle = 2kT \gamma \delta_{ij} \delta(t-t') \]

- friction
- noise

\[ \lim_{t \to \infty} \frac{1}{2} \langle v_i(t)v_j(t) \rangle = \frac{1}{2} \delta_{ij} kT \]
Langevin dynamics

- Statistical sampling w/o explicit weight fn (the Fokker-Planck eqn is associated)
- Equilibrium state is the quantum vacuum

\[ \frac{\partial \phi(x, \theta)}{\partial \theta} = -\frac{\delta S[\phi]}{\delta \phi(x, \theta)} + \eta(x, \theta) \quad \langle \eta(x, \theta) \eta(x', \theta') \rangle = 2\delta(x - x')\delta(\theta - \theta') \]

force noise

Parisi-Wu
Complex Langevin dynamics

- Langevin algorithm is simple
- No obvious problem with complex action $S$

\[
\frac{\partial \phi(x, \theta)}{\partial \theta} = -\frac{\delta S[\phi]}{\delta \phi(x, \theta)} + \eta(x, \theta) \quad \langle \eta(x, \theta) \eta(x', \theta') \rangle = 2\delta(x - x')\delta(\theta - \theta')
\]

- Price to pay:
  - Complex “force” $dS/d\phi$ makes $\phi$ also complex
  - True equilibration is not formally guaranteed
Results in $\phi^4$ theory

- $S$ becomes complex at finite $\mu$

\[
S = \int d^4x \left[ |\partial_\nu \phi|^2 + (m^2 - \mu^2)|\phi|^2 \right. \\
\left. + \mu (\phi^* \partial_4 \phi - \partial_4 \phi^* \phi) + \lambda |\phi|^4 \right]
\]
Results in $\phi^4$ theory

- $S$ becomes complex at finite $\mu$

\[
S = \sum_{x \in \mathbb{L}^n} \left[ -\phi_1(x) \left[ \phi_1(x + \hat{0}) \cosh(\mu) - \phi_2(x + \hat{0}) \sinh(\mu) I \right] - \phi_2(x) \left[ \phi_2(x + \hat{0}) \cosh(\mu) + \phi_1(x + \hat{0}) \sinh(\mu) I \right] - \sum_{\hat{k}} \left( \phi_1(x) \phi_1(x + \hat{k}) + \phi_2(x) \phi_2(x + \hat{k}) \right) \\
+ (D + \frac{1}{2} \kappa) (\phi_1(x) \phi_1(x) + \phi_2(x) \phi_2(x)) + \frac{1}{4} \lambda (\phi_1(x) \phi_1(x) + \phi_2(x) \phi_2(x))^2 \right]
\]
Results in $\phi^4$ theory

- Density $n$ stays zero up to $\mu = \mu_c$; Silver Blaze

Aarts et al.

Reproduced by ourselves
When Complex Langevin works?

- Longstanding problems
  - instability - only numerical?  
  - wrong equilibrium - what's the key physics?

- TrLog(D) is unique to fermion theories, whose effects are to be studied
  - Chiral Random Matrix model (see Sano's talk)
  - Nambu-Jona-Lasinio model (in progress)
  - QCD, ..., etc.
Path-integral in complexified phase space

- Complex Langevin = sampling algorithm in complexified phase space

- In complex space, one can choose the integration contour on which ImS=const!
  - Method of steepest descent - deform the path around critical points, dS/dz=0

\[
\int_{-\infty}^{\infty} dx \ e^{i\kappa x^2} = \int_{c} dz \ e^{i\kappa z^2} = e^{i\pi/4} \int_{-\infty}^{\infty} dt \ e^{-\kappa t^2}
\]
Path-integral in complexified phase space

- Illustration

\[
S = \frac{\kappa}{2} x^2 + \frac{\lambda}{4} x^4 \rightarrow \frac{\kappa}{2} z^2 + \frac{\lambda}{4} z^4 \quad \kappa \in \mathbb{C}
\]
Path-integral in complexified phase space

Illustration

\[ S = \frac{\kappa}{2} x^2 + \frac{\lambda}{4} x^4 \rightarrow \frac{\kappa}{2} z^2 + \frac{\lambda}{4} z^4 \quad \kappa \in \mathbb{C} \]
Path integral on Lefschetz thimble

- Flow eqn: \[ \frac{d}{dt} z(t) = \frac{\partial S[z]}{\partial z}, \quad \frac{d}{dt} \bar{z}(t) = \frac{\partial S[z]}{\partial \bar{z}}, \]

- Along flow: \[ d(\text{Re}S)/dt > 0 \quad d(\text{Im}S)/dt = 0 \]

- Critical pt.: \[ \frac{\partial S[z]}{\partial z} \bigg|_{z=z_\sigma} = 0. \]

- Lefschetz thimble \( \mathcal{J}_\sigma \): a union of downward flows from \( \sigma \)

- Morse theory shows: \[ \int_{\mathbb{R}^n} dx_1 \cdots dx_n g(x)e^{f(x)} = \sum n_\sigma \mathcal{J}_\sigma \]

- \( \mathcal{J}_0 \) from \( z=0 \) is a natural choice for integration contour, on which \( \text{Im}S=0!! \) - No sign problem!?
Path integral on Lefschetz thimble

- Coordinates on $J_0$
  - Thimble is $\mathbb{R}^n$ dimensional, the same as the original
  - For any point $z$ on $J_0$, there is a unique flow by $\tau$ starting at $z_0 = \epsilon^\alpha V^a(0)$ near 0: natural coordinates $(\tau, \epsilon^\alpha)$
  - We need Jacobian $\det(V(z))$, which is in general complex: residual sign problem

\[
\int d\phi e^{-S(\phi)} = \int_{J_0} dz e^{-S(z)} = \int d\xi \left| \frac{dz}{d\xi} \right| e^{-S(\xi)}
\]

- $\{V(z)\}$ needs to be parallel-transported from 0

Cristoforetti et al (Aurora Coll.)
HMC algorithm on Lefschetz thimble $J_0$

- Pick up an initial pt randomly:
  \[ z = \epsilon^\alpha V_i^\alpha(0) + \int_0^\tau dt \, \partial S[z(t)] \equiv z[\epsilon^\alpha, \tau] \]

- Use coordinates $\xi^\alpha(\epsilon^\alpha, \tau)$

\[ \dot{\xi}^\alpha = p^\alpha \]
\[ \dot{p}^\alpha = -\frac{\partial S}{\partial \xi^\alpha} = -\frac{1}{2} \left\{ \partial_i S[z] V_i^\alpha(\tau) + \bar{\partial}_i S[z] \bar{V}_i^\alpha(\tau) \right\} \exp(-|\kappa^\alpha|\tau) \]

- HMC needs ( Field conf “z” & tangent vecs “$V^\alpha$” )

- Prepare ( $z, \{V^\alpha\}$ ) at ($\epsilon^\alpha, \tau$) by solving flow eqn (parallel-transport of $V^\alpha(0)$))

- Jacobian $\det\{V\}$ should also be included

- Repeat HMC towards thermalization
First trial look at HMC on $J_0$ of $\phi 4$

- $\kappa=\lambda=1$, $\mu=0.3$, $N=4$
- The HMC code runs!

- Trajectory length=0.08, step size=0.008 (very rough)
HMC on Lefschetz thimble $J_0$ of $\phi^4$

- Time consuming: several min for one trajectory
  - Core i7 PC w/ C2070 GPU
- Residual sign problem seems numerically almost absent!
  - If exact!?, physical reasoning & proof should be possible (by Honda, Kato, Komatsu + us)
  - Unlike the Fresnel integral, $Z(\mu)$ is real positive and respects Charge Conjugation symmetry
Discussion and outlook

• Complex Langevin
  - does sampling in enlarged complexified space
  - works beautifully in some cases
  - more realistic cases with fermions, phase transitions, to be examined

• Lefschetz thimble
  - functional version of steepest descent method
  - time consuming to handle thimble geometry
  - But sign problem may be almost absent!