Is the Feynman path integral complex enough?

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[with A. Alexandru, P. Bedaque, N. Warrington, G. Ridgway]
Motivations

first-principles studies of strongly interacting systems
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Motivations: out-of-equilibrium, transport

Heavy ion collisions: Quark gluon plasma is a liquid!
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Quark gluon plasma is a liquid. What is the viscosity, conductivity …?
Motivations

first-principles studies of strongly interacting systems

![Phase diagram of (hole-doped) cuprates mapped out in terms of the temperature and doping evolution of the in-plane resistivity $\rho_{ab}(T)$. The solid lines are the phase boundaries between the normal state and the superconducting or antiferromagnetic ground state. The dashed lines indicate (ill-defined) crossovers in $\rho_{ab}(T)$ behavior, each of which may occur in association with a fundamental change in the nature of the electronic states. Optimal doping indicates by the vertical dotted line corresponding to the pinnacle of the superconducting dome and the areas to](image-url)
Quantum Chromo Dynamics (QCD)

We know how quarks and gluons interact

Why not just compute the phase diagram, viscosity, equation of state, etc…?
Quantum fluctuations

we are interested in expectation values

equations:

\[ \langle n \rangle \Leftrightarrow \text{equation of state} \]

\[ \langle J(t)J(0) \rangle \Leftrightarrow \text{conductivity} \]

\[ \langle T^{ab}(t)T^{cd}(0) \rangle \Leftrightarrow \text{viscosity} \]
of contributions, one from each path in the region. The contribution from a single path is postulated to be an exponential whose (imaginary) phase is the classical action (in units of $\hbar$) for the path in question. The total contribution from all paths reaching $x, t$ from the past is the

$$e^{iS[x(t)\}}$$
of contributions, one from each path in the region. The contribution from a single field is postulated to be an exponential whose (imaginary) phase is the classical action (in units of \(\hbar\)) for the field in question. The total contribution from all paths reaching \(x, t\) from the past is the

\[
\langle \mathcal{O} \rangle = \int [d\phi] e^{iS[\phi]} \mathcal{O}[\phi]
\]

all fields

\[
\text{domain of PI: space of all fields}
\]
of contributions, one from each path in the region. The contribution from a single field is postulated to be an exponential whose real part is the classical action (in units of \(\hbar\)) for the field in question. The total contribution from all paths with imaginary time is the

Main features:

• Discrete space-time
• Imaginary time

\[ e^{-i\hat{H}t} \rightarrow e^{-\hat{H}\tau} \]

thermal physics!
A crash course on Lattice Field Theory

Main features:

- Discrete space-time
- Imaginary time
  \[ e^{-i\hat{H}t} \rightarrow e^{-\hat{H}\tau} \]
  thermal physics!

\[ \langle \mathcal{O} \rangle = \int d\phi_1 \ldots d\phi_N e^{-S[\phi]} \mathcal{O}[\phi] = \text{Tr}[e^{-\hat{H}/T\hat{\mathcal{O}}}] \]

finite positive

- importance of the field configuration \( \phi \): \( e^{-S[\phi]} \)
Importance sampling ("Monte-Carlo" method)

importance of the field configuration $\phi$: $e^{-S[\phi]}

\[ \langle \mathcal{O} \rangle \approx \frac{1}{N} \sum_{a=1}^{N} \mathcal{O}[\phi_a] \]

pick out the important (small action) configurations

path integral $\sim$ statistical average with $P(\phi) \propto e^{-S[\phi]}
Lattice QCD

lattice

importance sampling (Monte-Carlo)
The sign problem

In a variety of problems of interest $S$ is *complex*

$$e^{-S[\phi]}$$ is not a probability distribution

- Most theories with finite density
- Hubbard model away from half filling
- Dynamical problems (*transport, out-of-equilibrium physics*. . .)
- QCD with nonzero $\theta$ angle
The sign problem

\[
\int_{-\infty}^{\infty} e^{-(x+4i)^2} \, dx = 2\sqrt{\pi}
\]
The sign problem

importance $\propto e^{-S_R[\phi]}$ "reweighting"

$$\langle \mathcal{O} \rangle = \frac{\langle e^{-iS_I[\phi]} \rangle_{S_R}}{\langle e^{-iS_I[\phi]} \rangle_{S_R}}$$

$$\langle e^{-iS_I[\phi]} \rangle_{S_R} \propto e^{-\text{volume}/T}$$ need exponentially large resources

finite density out-of-equilibrium
The sign problem
Ways around the sign problem

- Imaginary chemical potential
- Taylor series in $\mu$
- Dual variables
- Fermion bags
- Complex Langevin
- Canonical partition function
A complex way around the sign problem

\[ \int_{-\infty}^{\infty} e^{-(x+42i)^2} \, dx = 2\sqrt{\pi} \]
A complex way around sign problem

\[ \int_{C} e^{-(z+4i)^2} \, dz = 2\sqrt{\pi} \]
A complex way around the sign problem

\[ \int_{\mathcal{C}} e^{-(z+42i)^2} \, dz = 2\sqrt{\pi} \]
The main idea: deform the QFT path integral domain to a better one in complex field space where the sign problem is mild.

Review article: “Complex paths around the sign problem” [Alexandru, GB, Bedaque, Warrington] coming soon…

[also work by Cristoforetti, Di Renzo et al, Fujii et al., Tanizaki et al.,… ]

Mathematical origins: Picard-Lefschetz theory [Pham, Fedoryuk, Witten, ….]
Good deformations

- path integral on $\mathcal{M} =$ path integral on $\mathbb{R}^N$ ("allowed")
- sign problem on $\mathcal{M} \ll$ sign problem on $\mathbb{R}^N$ ("good")
Good deformations

follow an equation of motion, "holomorphic gradient flow"

\[
\frac{d\phi(\tau)}{d\tau} = \frac{\partial S[\phi]}{\partial \phi}
\]

- path integral on \( \mathcal{M} = \) path integral on \( \mathbb{R}^N \) ("allowed")
- sign problem on \( \mathcal{M} \ll \) sign problem on \( \mathbb{R}^N \) ("good")
**Strategy**

- **deformation**
- **discretization**
- **importance sampling**

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**Dynamics**

**Finite density**

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Real time dynamics

\[ \langle \mathcal{O}(t)\mathcal{O}(0) \rangle = \frac{1}{Z} \int [d\phi] e^{\frac{i}{\hbar}S[\phi]} \mathcal{O}(t)\mathcal{O}(0) \]

transport (viscosity, conductivity),
out-of-equilibrium physics…

\[ e^{\frac{i}{\hbar}S[\phi]} \] leads to quantum interference

…and the ultimate sign problem

\[ \langle e^{-iS[\phi]} \rangle_{SR} = 0 \]
Real time dynamics - $1+1d$ QFT

interacting Bose gas: $\mathcal{L} = \frac{1}{2}(\partial \phi)^2 - \frac{1}{2}m^2\phi^2 - \frac{\lambda}{4!}\phi^4$

free theory $\lambda=0$

\[ C_p(t) = \langle \phi(t, p)\phi(0, p) \rangle_\beta \]

[Alexandru, GB, Bedaque, Ridgway, Vartak, Warrington, PRL 117081602, PRD 95 114501]
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weak coupling \( \lambda = 0.1 \)

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[Alexandru, GB, Bedaque, Ridgway, Vartak, Warrington, PRL 117081602, PRD 95 114501]
[see also follow-up by Mou, Saffin, Tranberg, ‘18]
Real time dynamics - Hybrid Monte Carlo

Case Study: 0+1 d anharmonic oscillator

$$\mathcal{L} = \frac{1}{2} \dot{\phi}^2 - \frac{1}{2} m^2 \phi^2 - \frac{\lambda}{4!} \phi^4$$

in progress

[also (finite density) Fujii, Honda, Kato, Kikukawa, Komatsu, Sano, JHEP 10 (2013) 147 01]
Real time dynamics - Hybrid Monte Carlo

Case Study: 0+1 d anharmonic oscillator

\[ \mathcal{L} = \frac{1}{2} \dot{\phi}^2 - \frac{1}{2} m^2 \phi^2 - \frac{\lambda}{4!} \phi^4 \]

\[ N_t = 24, \quad N_\beta = 4, \quad \lambda = 24 \]

in progress
chain of interacting fermions

\[ S = \int d^2x \bar{\psi}^a \left( \gamma^\mu \partial_\mu + m + \mu \gamma^0 \right) \psi^a + \frac{g^2}{2N_f} (\psi^a \gamma^\mu \psi^a)(\psi^b \gamma^\mu \psi^b) \]

\[ \rightarrow \frac{N_f}{2g^2} \int d^2x A^\mu A_\mu + \text{tr log}(\phi + A + \mu \gamma_0 + m) \]

• a prototype of QCD
  asymptotically free, sign problem at finite density

• a 2d cousin of the Hubbard model

[Alexandru, GB, Bedaque, Ridgway, Warrington, Phys. Rev. D95, 014502 ]
Many body physics - 2d Thirring model

sign problem

equation of state

[Alexandru, GB, Bedaque, Ridgway, Warrington, Phys. Rev. D95, 014502 ]
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**Sign problem**

**Equation of state**

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Many body physics - 2d Thirring model

Equation of state: low temperature limit

particularly bad sign problem:  \[ \langle e^{-iS_I[\phi]} \rangle_{S_R} \propto e^{-\text{volume}/T} \]

[Alexandru, GB, Bedaque, Ridgway, Warrington, Phys. Rev. D95, 014502 ]
Many body physics - 2d Thirring model

Equation of state

continuum limit

thermodynamic limit

[Alexandru, GB, Bedaque, Ridgway, Warrington, Phys. Rev. D95, 014502 ]
Gauge theories - 2d QED

QED with 3 "quarks" with charges $q=2,-1,-1$

$$S = \sum_{a=1}^{3} \int d^2 x \left[ F^2 + \bar{\psi}^a \left( \gamma^\mu (\partial_\mu - g q_a A_\mu) + m - \mu \gamma^0 \right) \psi^a \right]$$

sign problem
equation of state
Gauge theories - heavy dense QCD

- In the limit $m_q \to \infty$ effective theory of Polyakov loops
- Still has a sign problem for $\mu \neq 0$ but easier to simulate
- Exploratory study on a few-site lattice with $\mathcal{M} \sim \sum \text{``Lefschetz thimbles''}$ (fixed points of flow+fluctuations)

[Zambello, Di Renzo, Phys. Rev. D95, 014502]
Many body physics - Hubbard model

2d Hubbard model away from half filling on a Honeycomb lattice

fixed point of flow = saddle point of $S[\phi]$

conventional MC

average sign

deformation ~ $\sum$ “thimbles”

<table>
<thead>
<tr>
<th>Method</th>
<th>$\langle \cos \text{Im} S \rangle$</th>
<th>$\langle \cos \text{arg} J \rangle$</th>
<th>$\langle \Sigma_G \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BSS-QMC</td>
<td>0.2363±0.0032</td>
<td></td>
<td>0.2363±0.0032</td>
</tr>
<tr>
<td>HMC, $\alpha=1.0$</td>
<td>0.9627±0.0038</td>
<td>0.427±0.014</td>
<td>0.351±0.015</td>
</tr>
<tr>
<td>HMC, $\alpha=0.8$</td>
<td>0.797±0.022</td>
<td>0.915±0.008</td>
<td>0.644±0.028</td>
</tr>
</tbody>
</table>

[Ulybyshev, Winterowd, Zafeiropoulos PRD 101 (1), 014508]
Other deformations: "Learnifolds"

Machine learning, training set: points on $\mathcal{M}$

output: $\mathcal{L} \simeq \mathcal{M}$

[Alexandru, Bedaque, Lamm, Lawrence *Phys.Rev.D* 96 (2017) 9, 094505]
Sign optimized manifolds

within a family of manifolds $\mathcal{M}_\lambda$ minimize the sign problem

maximize the average phase: $\langle e^{-iS_i} \rangle_\lambda = \frac{\int_{\mathcal{M}_\lambda} d[\phi] e^{-S}}{\int_{\mathcal{M}_\lambda} d[\phi] e^{-S_R}}$

[Mori et al. ‘17-‘19, Alexandru et al. ‘18, Bursa et al. ‘18, Kashiwa et al. ‘19, Detmold et al. ‘20]
temperature
10
12
K

chemical potential
\sim 310 \text{ MeV}

heavy ion coll.
early universe
quark gluon plasma
hadron gas

you are here

neutron stars

critical point

flow

QFT: real time dynamics, finite density

pseudo-fermions, estimators

simulated annealing

machine learning, path optimization

Hybrid Monte Carlo

other deformations, ansätze

accept/reject

Metropolis step w/ $p_1$

Metropolis step w/ $p_n$

other deformations, ansätze