Path-integral Monte Carlo simulation of systems in a magnetic field

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Outline of the talk

- Motivation
- Review of the Path-integral Monte Carlo (PIMC)
- The problem: PIMC in the absence of time-reversal symmetry
- Results:
  1. The free density matrix on the torus in a magnetic field
  2. The modification of sampling
  3. Case study: rotating Yukawa gases
- Outlook: towards Coulomb systems
Motivation

Fractional quantum Hall effect, also rotating BEC: proliferation of theories, but few real tests

- Experiments give partial information: gaps, transitions driven by Zeeman energy or valley splitting, perhaps fractional charge
- Numerical checks:
  1. Exact diagonalization: unbiased, limited for small systems
  2. DMRG with similar size limitations
  3. Monte Carlo evaluation of trial wave functions (VMC, DMC)

Goal: add a new method to the repertoire
The path-integral Monte Carlo method

- Path-integral Monte Carlo (PIMC): performing an imaginary-time path integral by MC sampling (Metropolis-Hastings algorithm).
- Must interpret path amplitudes as probability densities.
- Very effective for interacting Bose systems: liquid $^4$He, Ne, H$_2$, votrices in superconductors, excitons, cold atoms, etc.
- With **node-fixing** ansatz, useful for fermions: electrons, e-p plasma, $^3$He, etc.
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- With node-fixing ansatz, useful for fermions: electrons, e-p plasma, $^3$He, etc.
- In the presence of a magnetic field, phase-fixing is mentioned in the literature, but rarely applied.
- How far can we get by phase fixing? Do we obtain an efficient, universal method?
Path-integrals and Monte Carlo

1. Feynmann: probability amplitudes by summing all classical paths that connect the initial state to a final state:

\[ \langle x_t | e^{-i\hat{H}t} | x_0 \rangle = \]

Interference of complex amplitudes; not amenable to numerics.

2. Quantum statistical mechanics. Density matrix:

\[ \langle R(0) | e^{-\hat{H}\beta} | R(\beta) \rangle, \quad \beta = \frac{1}{k_B T}, \quad R \equiv (r_1, r_2, \ldots, r_N). \]

Thermodynamical properties and correlation functions follow via

\[ Z(\beta) = \int dR \langle R | e^{-\hat{H}\beta} | R \rangle \geq 0. \]
Path-integral Monte Carlo, details

- Density matrix (Euclidean, imaginary-time propagator):
  \[ \rho(R, R'; \beta) = \sum_n e^{-\beta \epsilon_n} \psi_n(R) \psi_n^*(R') . \]

Apply the convolution identity interatively,

\[ \rho(R, R'; \beta_1 + \beta_2) = \int dR'' \rho(R, R''; \beta_1) \rho(R'', R'; \beta_2) \]

\[ \rho(R, R'; \beta) = \int dR_1 \cdots dR_{M-1} \rho(R, R_1; \tau) \cdots \rho(R_{M-1}, R'; \tau) . \]

Close path by \( R = R' \equiv R_M \), integrate over \( R_M \),

\[ Z(\beta) = \int dR_1 \cdots dR_M \rho(R_M, R_1; \tau) \cdots \rho(R_{M-1}, R_M; \tau) . \]

- \( \tau \ll \beta \), higher temperature!
PIMC, approximation to high temperature density matrix

Trotter-Suzuki (spectrum bounded from below):

\[ e^{-\tau(T+V)} = e^{-\tau T} e^{-\tau V} + O(\tau^2) \]

The “primitive approximation to the action.”

\[ \rho(R_i, R_{i+1}; \tau) = \langle R_i | e^{-\tau T} e^{-\tau V} | R_{i+1} \rangle = \]

\[ \frac{1}{(4\pi \lambda \tau)^{dN/2}} \exp \left( - \frac{(R_i - R_{i+1})^2}{4\lambda \tau} \right) e^{-\tau V(R_{i+1})} \]
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- Kinetic energy ⇒ springs between neighboring slices;
  Interaction: potential each slice;
  Partition function: closed (ring) polymer.
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  Interaction: potential each slice;
  Partition function: closed (ring) polymer.

- Higher approximations necessary for hard potentials (Coulomb, Lennard-Jones, interatomic). Kinetic and potential contributions no longer separate.
Path-integral Monte Carlo, estimators

Sample the paths, and collect estimators for its derivatives, e.g.,

- Energy (different estimators)
- Density
- Pair-correlation function
- Specific heat
- Pressure
- Single-particle density matrix
- Momentum distribution
- Condensate fraction for bosons, ...
Path-integral Monte Carlo, node fixing

- For fermions, $\rho(R_m, R_{m-1}; \tau)$ can also be negative; the product of $N$ density matrices cannot be a probability density.

- Estimators sum large positive and negative contributions - sign problem!
Path-integral Monte Carlo, node fixing

- For fermions, $\rho(R_m, R_{m-1}; \tau)$ can also be negative; the product of $N$ density matrices cannot be a probability density.

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- Node fixing: sample $|\rho(R_M, R_1; \tau)| \ldots |\rho(R_{M-1}, R_M; \tau)|$, but restrict random walk to the inside of a nodal pocket of some assumed $\rho_T(R, R'; \beta)$.

- The method becomes variational.

- Energy of the normal state of $^3$He. Ceperley, PRL 69, 331
Path-integral Monte Carlo, phase fixing

- In an external magnetic field, $\rho(R_m, R_{m-1}; \tau)$ is complex; same problem.
- Phase fixing: sample

$$|\rho(R_M, R_1; \tau)||\rho(R_2, R_3; \tau)| \ldots |\rho(R_{M-1}, R_M; \tau)|,$$

But use the phase of some assumed

$$\rho_T(R, R'; \beta) = |\rho_T(R, R'; \beta)| e^{i\phi_T(R, R'; \beta)}.$$ This produces an effective potential

$$V_{\text{eff}} = \lambda \left( \nabla_R \phi_T(R, R', \tau) - \frac{e}{\hbar} A(R) \right)^2.$$

- Exists only as a repeated comment in the literature.
I. The torus in an external magnetic field

- Must be pierced by integer number of flux quanta

\[ N_\phi = \frac{|\mathbf{L}_1 \times \mathbf{L}_2|}{2\pi \ell^2} = \frac{L_1 L_2 \sin \theta}{2\pi \ell^2}, \]

so that magnetic translations by \( \mathbf{L}_1 \) and \( \mathbf{L}_2 \) commute.

- Twisted periodic boundary conditions:

\[ t(\mathbf{L}_{1,2})\psi(\mathbf{r}) = e^{i\phi_{1,2}} \psi(\mathbf{r}). \]
Density matrix (Euclidean propagator) on the torus

\[
\rho^{\text{PBC}}(\mathbf{r}, \mathbf{r}'; \beta) = \frac{1}{N_\phi} \rho^{\text{open}}(\mathbf{r}, \mathbf{r}'; \beta) \sum_{m=0}^{N_\phi-1} \left\{ \vartheta \begin{bmatrix} 0 \\ a_m \end{bmatrix} \left( z_1 | \tau_1 \right) \vartheta \begin{bmatrix} 0 \\ 2b_m' \end{bmatrix} \left( z_2 | \tau_2 \right) + \right.
\]
\[
\phantom{=} + \left. \left( -1 \right)^k \vartheta \begin{bmatrix} 0 \\ a_m + \frac{1}{2} \end{bmatrix} \left( z_1 | \tau_1 \right) \vartheta \begin{bmatrix} \frac{1}{2} \\ 2b_m' \end{bmatrix} \left( z_2 | \tau_2 \right) \right\},
\]

\[
\rho^{\text{open}}(\mathbf{r}, \mathbf{r}'; \beta) = \frac{1}{2\pi \ell^2} \frac{\sqrt{u}}{1-u} \exp \left( -\frac{1+u}{1-u} \frac{|\mathbf{r}-\mathbf{r}'|^2}{4\ell^2} + \frac{i(x'-x)(y+y')}{2\ell^2} \right), \quad u = e^{-\beta \hbar \omega_c},
\]

\[
\vartheta \begin{bmatrix} a \\ b \end{bmatrix} \left( z | \tau \right) = \sum_n e^{i\pi \tau (n+a)^2 + 2i(n+a)(z+b\pi)},
\]

\[
\tau_1 = \frac{i}{\pi} \left( \frac{L_1}{2\ell N_\phi} \right)^2 \frac{1+u}{1-u}, \quad z_1 = \frac{L_1}{4\ell^2 N_\phi} \left( y + y' + i(x' - x) \frac{1+u}{1-u} \right),
\]

\[
\tau_2 = i\pi \left( \frac{2\ell N_\phi}{L_1} \right)^2 \frac{1+u}{1-u}, \quad z_2 = \frac{N_\phi \pi}{L_1} \left( x + x' + i(y - y') \frac{1+u}{1-u} \right),
\]

\[
a_m = \frac{\phi_1}{2\pi N_\phi} + \frac{m}{N_\phi}, \quad b_m = -\frac{\phi_2}{2\pi} - \frac{N_\phi \Re \tau}{2}, \quad \text{and} \quad b_m' = b_m + N_\phi a_m \Re \tau.
\]
Single-particle propagation on the torus

Evolution of $|\rho^{\text{PBC}}(\mathbf{r}, \mathbf{r}'; \beta)|$.

We set $N_{\phi} = 6$, $L_2/L_1 = 1.17$, $\theta \approx 55^\circ$, $\phi_1 = \phi_2 = 0$, and $\mathbf{r}' = 0$. The panels correspond to $\beta \hbar \omega_c = 0.3, 0.7, 1.1, \text{ and } 5$, respectively.
Zeros of the density matrix on the torus

Zeros for $\beta \hbar \omega_c = 200$, $\phi_1 = \phi_2 = 0$ and $r' = 0$. (a) generic, $N_\phi = 6$, $L_2/L_1 = 1.13$ and $\theta \approx 75^\circ$; (b) square, $N_\phi = 7$; (c) generic, $N_\phi = 11$, $L_2/L_1 = 1.19$ and $\theta \approx 72^\circ$; (d) hexagonal, $N_\phi = 12$. 

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Zeros of the density matrix on the torus, twist

- The trajectories of the zeros as we tune (a) $\phi_1$ and (b) $\phi_2$ between 0 and $2\pi$. We set $\beta \hbar \omega_c = 200$, $r' = 0$, $N_{\phi} = 2$, $L_2/L_1 = 1.19$ and $\theta \approx 56^\circ$.

- A single particle will never spread out completely on the torus for $B \neq 0$. 

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II. Sampling paths, $B = 0$

- Select $m$, move $R_m$, use Metropolis rejection rule—bad idea.
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- Select $m$, move $R_m$, use Metropolis rejection rule—bad idea.
- For $B = 0$, bisection. The Levy construction for a Brownian bridge
- Valid because

$$p(R_i) = \frac{\rho_0(R_{i-s}, R_i; s\tau) \rho_0(R_i, R_{i+s}; s\tau)}{\rho_0(R_{i-s}, R_{i+s}; 2s\tau)};$$

is a Gaussian, variance $s\tau$. Easy to sample, do it recursively.

- Acceptance ratio = 1 for free particles.
- Generalization for PBC possible.

- Apply $e^{-U}$ either at the last level or intermediate levels.
Sampling paths, $B \neq 0$

- If $B \neq 0$, we sample by $|\rho(R, R'; \tau)|$, but

$$
\frac{|\rho^{\text{open}}(r_{i-s}, r_i; s\tau)||\rho^{\text{open}}(r_i, r_{i+s}; s\tau)|}{|\rho^{\text{open}}(r_{i-s}, r_{i+s}; 2s\tau)|}
$$

is not a normalized probability density.

- Under periodic boundary conditions (torus),

$$
\frac{|\rho^{\text{PBC}}(r_{i-s}, r_i; s\tau)||\rho^{\text{PBC}}(r_i, r_{i+s}; s\tau)|}{|\rho^{\text{PBC}}(r_{i-s}, r_{i+s}; 2s\tau)|}
$$

is not Gaussian, difficult to sample.

- Even free particles are difficult to sample.
Sampling paths for periodic BC, $B \neq 0$, single slice

- *a priori* sampling PDF $T(z'_m|z_{m-1}, z_{m+1})$: four Gaussians at
  \[
  Z_0 = \frac{z_{m-1} + z_{m+1}}{2}, \quad Z_1 = \frac{z_{m-1} + z_{m+1} + L_1}{2},
  \]
  \[
  Z_2 = \frac{z_{m-1} + z_{m+1} + L_1\tau}{2}, \quad Z_3 = \frac{z_{m-1} + z_{m+1} + L_1(1 + \tau)}{2}.
  \]

- The height of the peaks is proportional to
  \[
  \alpha_i = \frac{|\rho_{\text{PBC}}(z_{m-1}, Z_i; \tau)||\rho_{\text{PBC}}(Z_i, z_{m+1}; \tau)|}{|\rho_{\text{PBC}}(z_{m-1}, z_{m+1}; 2\tau)|}.
  \]

- Choose peak $i$ with probability $p_i = \alpha_i / (\sum_{j=0}^3 \alpha_j)$. Sample Gaussian with variance $\frac{1-u}{1+u} \rho^2 < \lambda\tau$ with $u = e^{-\hbar\omega_c\tau}$.

- Acceptance probability
  \[
  \frac{|\rho_{\text{PBC}}(z_{m-1}, z'_m; \tau)||\rho_{\text{PBC}}(z'_m, z_{m+1}; \tau)|}{|\rho_{\text{PBC}}(z_{m-1}, z_{m+1}; \tau)||\rho_{\text{PBC}}(z_{m}, z_{m+1}; \tau)|} \frac{T(z_m|z_{m-1}, z_{m+1})}{T(z'_m|z_{m-1}, z_{m+1})}.
  \]
Sampling paths for periodic BC, $B \neq 0$, multi-slice

1. Rebuild path between slice $L$ and $R = L + 2^l$ recursively
   - Sample $R_{(R+L)/2}$ from four Gaussians, variance $\frac{1-u_1}{1+u_1} \ell^2$, where $u_1 = e^{-\hbar \omega_c \tau_1}$ and $\tau_1 = 2^{l-1} \tau$.
   - Sample $R_{L+2^{l-2}}$ and $R_{R-2^{l-2}}$ from four Gaussians, variance $\frac{1-u_2}{1+u_2} \ell^2$, where $u_2 = e^{-\hbar \omega_c \tau_2}$ and $\tau_1 = 2^{l-2} \tau$.
   - Etc.
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   - Etc.

2. During this construction, store

$$P_1 = \frac{T(z_{L+1}, \ldots, z_{R-1}|z_L, z_R)}{T(z'_{L+1}, \ldots, z'_{R-1}|z_L, z_R)}$$
Sampling paths for periodic BC, $B \neq 0$, multi-slice

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   - Etc.

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$$P_1 = \frac{T(z_{L+1}, \ldots z_{R-1} | z_L, z_R)}{T(z'_{L+1}, \ldots z'_{R-1} | z_L, z_R)}$$

3. Finally, calculate

$$P_2 = \frac{\prod_{m=L+1}^R |\rho(z'_{m-1}, z'_m; \tau)|}{\prod_{m=L+1}^R |\rho(z_{m-1}, z_m; \tau)|}$$

4. Accept new path with probability $A = P_1 P_2 \times$ ratio of $e^{-\tau V_{\text{eff}}}$.
Sampling paths for periodic BC, $B \neq 0$, multi-slice

Acceptance ratio for a single particle, rectangular torus, $N_{\phi} = 2$ flux quanta, $\beta \hbar \omega_c = 2$, and $8 \leq M \leq 256$. 

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III. Rotating Yukawa bosons: the model

- Rotating gas in co-rotating frame

\[ \mathcal{H} = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \left( \nabla_i - \frac{im}{\hbar} \Omega \times r \right)^2 + \epsilon \sum_{i<j} K_0 \left( \frac{r_{ij}}{a} \right), \]

parameters \( \epsilon \) and \( a \).

- Coriolis-force \( \Longleftrightarrow \) magnetic field; parameters connected as

\[ \omega_c = 2\Omega \quad \text{and} \quad \ell = \sqrt{\frac{\hbar}{2m\Omega}}. \]

- \( K_0 (r) \) modified Bessel: short-range, soft-core interaction. Log singularity at \( r \to 0 \), exponential decay as \( r \to \infty \).

- \( \beta^* = \beta \hbar \omega_c, \quad \rho^* = \rho a^2, \quad \Lambda = \sqrt{\frac{\hbar^2}{2ma^2 \epsilon}}, \quad \kappa = \frac{a}{\ell} = a \sqrt{\frac{2m\Omega}{\hbar}}. \]
Case study: Yukawa bosons in cold atomic systems

Petrov et al. PRL 99, 130407: Fermi/Fermi mixture of very different masses $M$ and $m$ in 2D trap: Bose bound states with $K_0(r)$ interaction, apart from a nonuniversal short range

Phase boundary (blue): reentrance at constant $M/m$ possible
(Similar interaction for Abrikosov vortices in Type-II SC.)
Case study: phase fixing

- For fermions,

\[ \rho_F(R, R'; \beta) = \text{Det}(\rho^{\text{PBC}}(r_i, r_j'; \beta)) \]

- For bosons,

\[ \rho_B(R, R'; \beta) = \text{Perm}(\rho^{\text{PBC}}(r_i, r_j'; \beta)) \]

Perm stands for the permanent.

- For distinguishable particles,

\[ \rho_D(R, R'; \beta) = \prod_{i=1}^{N} \rho^{\text{PBC}}(r_i, r'_i; \beta) \]

- Only **qualitative predictions** are expected.

- \( B = 0 \): Margo and Ceperley, PRB 48, 411; Nordborg and Blatter, PRL 79, 1925.
Pair correlation for bosons

$N = 12$ bosons, $\rho a^2 = 0.02$, $N_\phi = 6$ flux quanta, and $\Lambda = 0.035$, 0.04, and 0.045. Differences $g_{\Lambda=0.04} - g_{\Lambda=0.035}$ and $g_{\Lambda=0.045} - g_{\Lambda=0.04}$. Decreasing crystalline correlation as $\Lambda$ is increased.
Pair correlation for spinless fermions

\[ N = 16 \]
\[ \rho a^2 = 0.02, \]
\[ N_\phi = 8 \text{ flux quanta.} \]
\[ \Lambda = 0.03, \]
\[ 0.035, 0.04 (\uparrow); \]
\[ \beta = 0.4, 0.5, \]
\[ 0.6 (\Rightarrow). \]
Density dependence, spinless fermions

The first peak of the pair-correlation function for \( N = 12 \) fermions at \( \beta^* = 0.5, N_{\phi} = 6 \), for various \( \Lambda \) parameter values vs. density \( \rho a^2 \).

Crystalline order exists only for a limited range of densities.
CDW vs. quantum Hall liquid, spinless fermions

The first peak of the pair-correlation function for $N = 16$ fermions at $N_\phi = 8$, $\rho a^2 = 0.02$, as a function of the inverse temperature, for $\Lambda$-values with CDW at intermediate temperatures.

At low enough temperature, CDW starts to disappear (?)
Ultimate goal: Coulomb interacting systems

- Primitive approximation is not valid — **cumulant action** elaborated by Tamás.

Feymann-Kac + cumulant approximation:

\[
e^{-U(R,R';\tau)} = \left\langle \exp\left(-\int_{0}^{\tau} V(R(t))\,dt\right) \right\rangle_{\text{RW } R' \rightarrow R}
\]

\[
\approx \exp\left\langle -\int_{0}^{\tau} V(R(t))\,dt \right\rangle_{\text{RW } R' \rightarrow R}.
\]

- Ignore the intricacies of the torus for a while: investigate quantum dots.

  Zhitenev et al., PRL 79, 2308 →

- Shell structure for small coupling, rotating electron molecules for large coupling (Landman et al., Rep. Prog. Phys. 70, 2067)
Quantum dots: phase fixing to UHF

\[ \omega = \sqrt{\omega_0^2 + \omega_c^2/4}, \]
\[ \ell = \sqrt{\hbar/m\omega}, \]
\[ \lambda = \frac{e^2}{4\pi\epsilon\ell}/\hbar\omega. \]

\[ N = 3, \text{ fully polarized, } \omega_c/\omega = 0.5. \]

Phase fixed to unrestricted Hartree-Fock, either to ground state \( \psi_{0}^{\text{UHF}}(R)\psi_{0}^{\text{UHF}*}(R') \), or to \( \sum_n e^{-\beta\epsilon_n} \psi_n^{\text{UHF}}(R)\psi_n^{\text{UHF}*}(R') \).
Quantum dots: phase fixing to UHF ground state

Radial density distribution for $N = 6$ (left) and $N = 7$ (right). $\omega_c/\omega = 0.8$, $\lambda = 6$, fully polarized.
For $N = 6$, the 6-ring predicted by UHF is unstable to (5,1) configuration. For $N = 7$, only quantitative improvement.
- PIMC in magnetic field under (twisted) periodic boundary condition is feasible
- Using Coulomb interaction is in a magnetic field is feasible
- But we still have to bring the two together..
Thank you for your attention!