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

Tamás Haidekker Galambos [1,2] Csaba Tőke[1]

[1]Institute of Physics, Budapest University of Technology and Economics, Budafoki út 8., H-1111 Budapest, Hungary

[2]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

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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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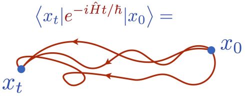
- With **node-fixing** ansatz, useful for fermions: electrons, e-p plasma, ^{3}He, etc.
- In the presence of a magnetic field, **phase-fixing** is mentioned in the literature, but rarely applied.
- How far can we get by phase fixing? Do we obtain an efficient, universal method?

Path-integrals and Monte Carlo

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



   Interference of complex amplitudes; not amenable to numerics.

2. Quantum statistical mechanics. Density matrix:

$$\langle R(0)| \, e^{-\mathcal{H}\beta} \, |R(\beta)\rangle \, , \quad \beta = \frac{1}{k_B T}, \quad R \equiv (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N).$$

   Thermodynamical properties and correlation functions follow via $\mathcal{Z}(\beta) = \int dR \, \langle R| \, e^{-\mathcal{H}\beta} \, |R\rangle \geq 0$.

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,

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

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

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

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

- $\tau \ll \beta$, higher temperature!

PIMC, approximation to high temperature density matrix

- Trotter-Suzuki (spectrum bounded from below):

$$e^{-\tau(\mathcal{T}+\mathcal{V})} = e^{-\tau\mathcal{T}} e^{-\tau\mathcal{V}} + O(\tau^2)$$

The "primitive approximation to the action."

$$\rho(R_i, R_{i+1}; \tau) = \langle R_i | e^{-\tau\mathcal{T}} e^{-\tau\mathcal{V}} | R_{i+1} \rangle = \frac{1}{(4\pi\lambda\tau)^{dN/2}} \exp\left(-\frac{(R_i - R_{i+1})^2}{4\lambda\tau}\right) e^{-\tau V(R_{i+1})}$$

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- Kinetic energy ⇒ springs between neighboring slices;
  Interaction: potential each slice;
  Partition function: closed (ring) polymer.

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- Kinetic energy ⇒ springs between neighboring slices; 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.,

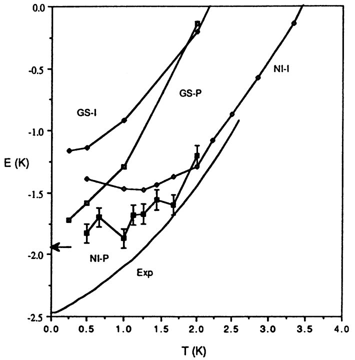
- Energy (different estimators)
- Density
- Pair-correlation function
- Specific heat
- Pressure
- Single-particle density matrix
- Momentum distribution
- Condensate fraction for bosons, ...

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.
- Estimators sum large positive and negative contributions - sign problem!
- 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

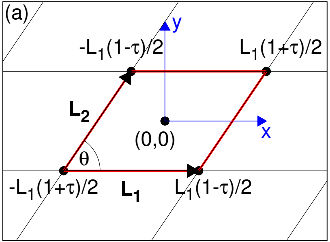
$$|\rho(R_M, R_1; \tau)||\rho(R_2, R_3; \tau)| \ldots |\rho(R_{M-1}, R_M; \tau)|,$$

  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

$$\rho^{\mathrm{PBC}}(\mathbf{r},\mathbf{r}';\beta) = \frac{1}{N_\phi}\rho^{\mathrm{open}}(\mathbf{r},\mathbf{r}';\beta)\sum_{m=0}^{N_\phi-1}\left\{\vartheta\begin{bmatrix}0\\ a_m\end{bmatrix}\left(z_1\middle|\tau_1\right)\vartheta\begin{bmatrix}0\\ 2b'_m\end{bmatrix}(z_2|\tau_2)+\right.$$

$$\left.+(-1)^k\vartheta\begin{bmatrix}0\\ a_m+\frac{1}{2}\end{bmatrix}\left(z_1\middle|\tau_1\right)\vartheta\begin{bmatrix}\frac{1}{2}\\ 2b'_m\end{bmatrix}(z_2|\tau_2)\right\},$$

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

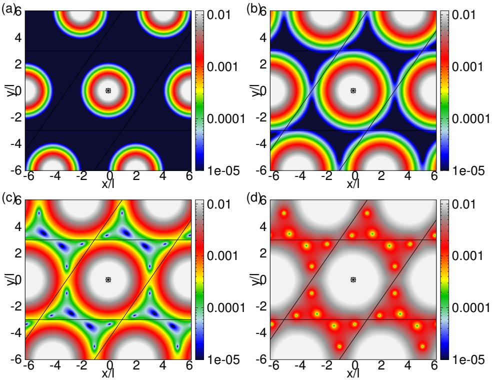
$$\vartheta\begin{bmatrix}a\\ b\end{bmatrix}(z|\tau) = \sum_n e^{i\pi\tau(n+a)^2+2i(n+a)(z+b\pi)},$$

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

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

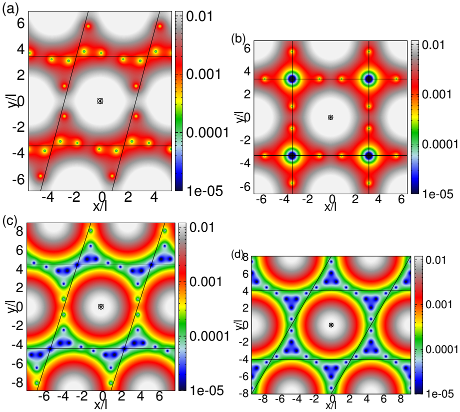
$$a_m = \frac{\phi_1}{2\pi N_\phi}+\frac{m}{N_\phi},\ b_m = -\frac{\phi_2}{2\pi}-\frac{N_\phi\Re\tau}{2},\ \text{and}\ b'_m = b_m + N_\phi a_m\Re\tau.$$

Single-particle propagation on the torus



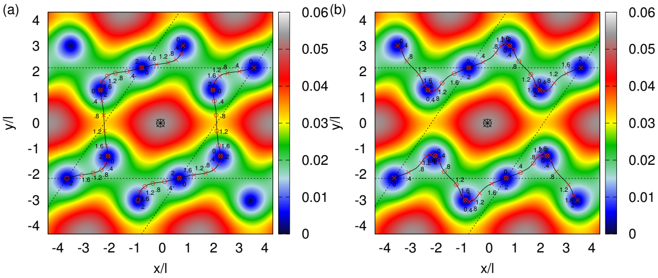
Evolution of $|\rho^{\mathrm{PBC}}(\mathbf{r}, \mathbf{r}'; \beta)|$.
We set $N_\phi = 6$, $L_2/L_1 = 1.17$, $\theta \approx 55^\circ$, $\phi_1 = \phi_2 = 0$, and $\mathbf{r}' = 0$.
The panels correspond to $\beta\hbar\omega_c = 0.3$, 0.7, 1.1, and 5, respectively.

Zeros of the density matrix on the torus



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

Zeros of the density matrix on the torus, twist



- The trajectories of the zeros as we tune (a) ϕ_1 and (b) ϕ_2 between 0 and 2π. We set $\beta\hbar\omega_c = 200$, $\mathbf{r}' = 0$, $N_\phi = 2$, $L_2/L_1 = 1.19$ and $\theta \approx 56^\circ$.
- A single particle will never spread out completely on the torus for $B \neq 0$.

II. Sampling paths, $B = 0$

- Select m, move R_m, use Metropolis rejection rule—bad idea.

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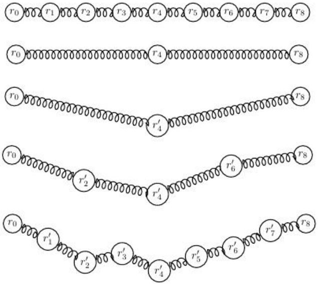
- Select m, move R_m, use Metropolis rejection rule—bad idea.
- For $B = 0$, bisection. The Levy construction for a Brownian bridge
- Valid because

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

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

$$\frac{|\rho^{\text{open}}(\mathbf{r}_{i-s}, \mathbf{r}_i; s\tau)||\rho^{\text{open}}(\mathbf{r}_i, \mathbf{r}_{i+s}; s\tau)|}{|\rho^{\text{open}}(\mathbf{r}_{i-s}, \mathbf{r}_{i+s}; 2s\tau)|}$$

  is *not* a normalized probability density.
- Under periodic boundary conditions (torus),

$$\frac{|\rho^{\text{PBC}}(\mathbf{r}_{i-s}, \mathbf{r}_i; s\tau)||\rho^{\text{PBC}}(\mathbf{r}_i, \mathbf{r}_{i+s}; s\tau)|}{|\rho^{\text{PBC}}(\mathbf{r}_{i-s}, \mathbf{r}_{i+s}; 2s\tau)|}$$

  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

$$\alpha_i = \frac{|\rho^{\mathrm{PBC}}(z_{m-1}, Z_i; \tau)||\rho^{\mathrm{PBC}}(Z_i, z_{m+1}; \tau)|}{|\rho^{\mathrm{PBC}}(z_{m-1}, z_{m+1}; 2\tau)|}.$$

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

$$\frac{|\rho^{\mathrm{PBC}}(z_{m-1}, z'_m; \tau)||\rho^{\mathrm{PBC}}(z'_m, z_{m+1}; \tau)|}{|\rho^{\mathrm{PBC}}(z_{m-1}, z_m; \tau)||\rho^{\mathrm{PBC}}(z_m, z_{m+1}; \tau)|} \frac{T(z_m|z_{m-1}, z_{m+1})}{T(z'_m|z_{m-1}, z_{m+1})}.$$

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

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

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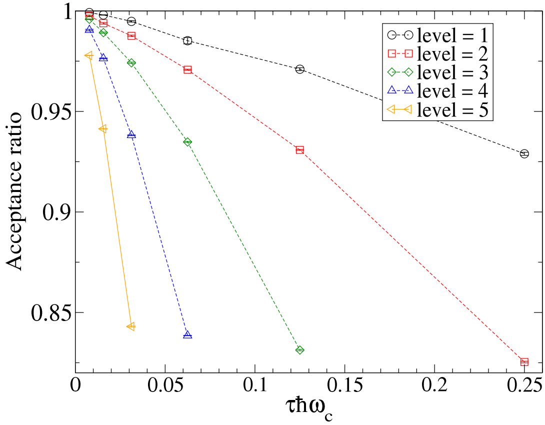
$$P_1 = \frac{T(z_{L+1}, \ldots z_{R-1} | z_L, z_R)}{T(z'_{L+1}, \ldots z'_{R-1} | z_L, z_R)}$$

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 $8 \leq M \leq 256$.

III. Rotating Yukawa bosons: the model

- Rotating gas in co-rotating frame

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

parameters ϵ and a.

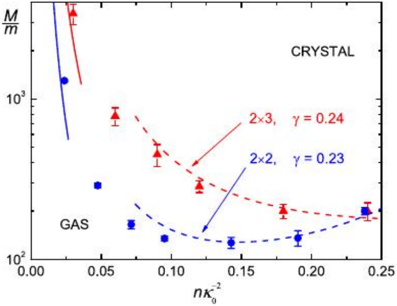
- Coriolis-force $\iff$ magnetic field; parameters connected as

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

- $K_0(r)$ 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,

$$\rho_F(R, R'; \beta) = \mathrm{Det}(\rho^{\mathrm{PBC}}(\mathbf{r}_i, \mathbf{r}'_j; \beta)).$$

- For bosons,

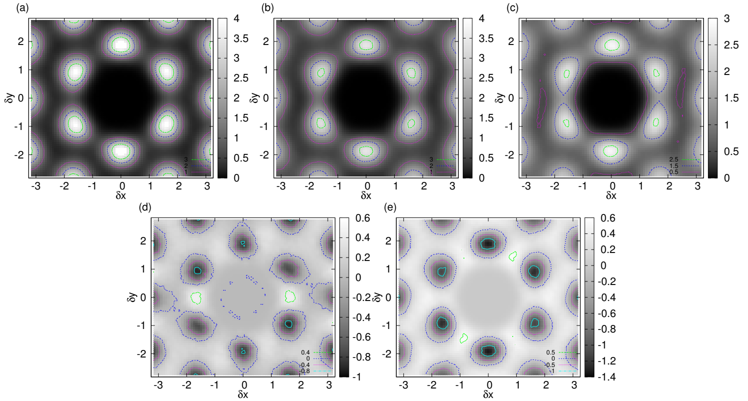
$$\rho_B(R, R'; \beta) = \mathrm{Perm}(\rho^{\mathrm{PBC}}(\mathbf{r}_i, \mathbf{r}'_j; \beta)),$$

  Perm stands for the permanent.
- For distinguishable particles,

$$\rho_D(R, R'; \beta) = \prod_{i=1}^{N} \rho^{\mathrm{PBC}}(\mathbf{r}_i, \mathbf{r}'_i; \beta).$$

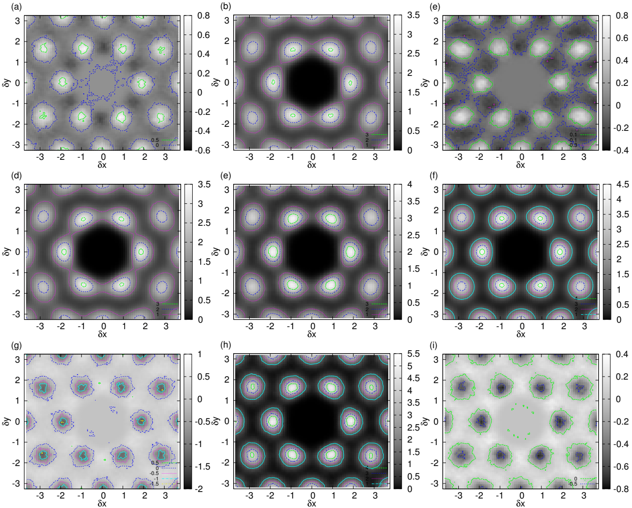
- Only **qualitative predictions** are expected.
- $B = 0$: Margo and Ceperley, PRB 48, 411; Nordborg and Blatter, PRL 79, 1925.

Pair correlation for bosons



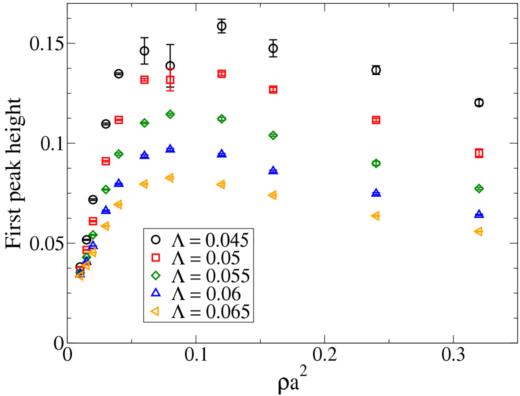
$N = 12$ bosons, $\rho a^2 = 0.02$, $N_\phi = 6$ flux quanta, and $\Lambda = 0.035$, 0.04, and 0.045. Differences $g_{\Lambda=0.04} - g_{\Lambda=0.035}$ and $g_{\Lambda=0.045} - g_{\Lambda=0.04}$. Decreasing crystalline correlation as Λ is increased.

Pair correlation for spinless fermions



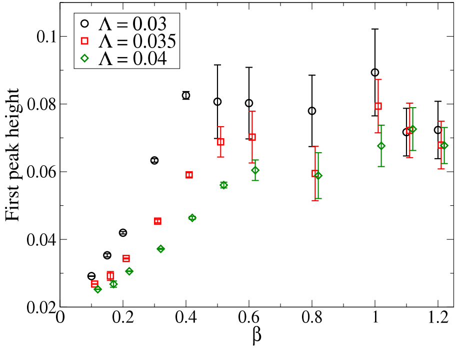
$N = 16$ fermions, $\rho a^2 = 0.02$, $N_\phi = 8$ flux quanta.
$\Lambda = 0.03$, 0.035, 0.04 ($\Uparrow$);
$\beta = 0.4$, 0.5, 0.6 ($\Rightarrow$).

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 Λ parameter values vs. density ρa^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 Λ-values with CDW at intermediate temperatures.
- At low enough temperature, CDW starts to disappear (?)

Ultimate goal: Coulomb interacting systems

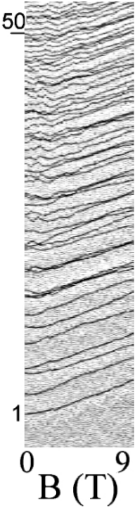
- Primitive approximation is not valid — **cumulant action** elaborated by Tamás.

  Feymann-Kac + cumulant approximation:

$$e^{-U(R,R';\tau)} = \left\langle \exp\left(-\int_0^\tau V(R(t))dt\right)\right\rangle_{\text{RW } R'\to R}$$
$$\approx \exp\left\langle -\int_0^\tau V(R(t))dt\right\rangle_{\text{RW } R'\to R}.$$

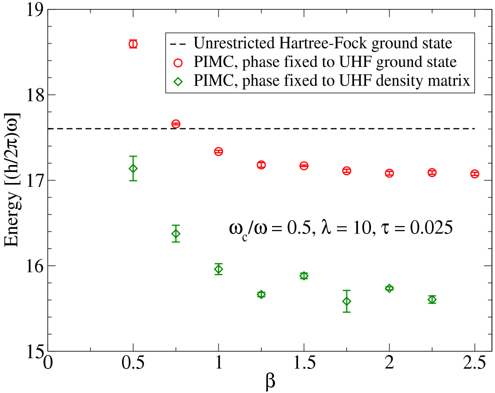
- Ignore the intricacies of the torus for a while: investigate quantum dots.

  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

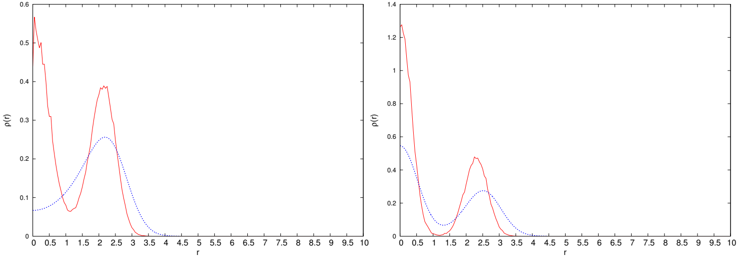


$$\omega = \sqrt{\omega_0^2 + \omega_c^2/4},$$
$$\ell = \sqrt{\hbar/m\omega},$$
$$\lambda = \frac{e^2}{4\pi\epsilon\ell}\Big/\hbar\omega.$$

$N = 3$, fully polarized, $\omega_c/\omega = 0.5$.

Phase fixed to unrestricted Hartree-Fock, either to ground state $\Psi_0^{\mathrm{UHF}}(R)\Psi^{\mathrm{UHF}*}_0(R')$, or to $\sum_n e^{-\beta\epsilon_n}\Psi_n^{\mathrm{UHF}}(R)\Psi^{\mathrm{UHF}*}_n(R')$.

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 a magnetic field is feasible
- But we still have to bring the two together..

Thank you for your attention!