

Introduction to Path Integral Monte Carlo. Part III.

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November 19, 2008

Outline

- 1 Calculation of superfluid fraction: finite and macroscopic systems
- 2 Winding number: ergodicity. Worm algorithm. Grand Canonical ensemble
- 3 Fermion sign problem
- 4 Comparison of Fermi/Bose statistics: superfluidity
- 5 Numerical issues of PIMC
 - Improved high-temperature action
 - Effective pair potential
 - Thermodynamic averages
- 6 Summary

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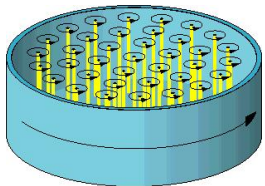
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Examples: Superfluidity

- Superfluidity: loss of viscosity of interacting bosons below critical temperature. Discovered in liquid ^4He (P.L.Kapitza, 1938).



- Rotating bucket experiment (Andronikashvili):



$T > T_{BKT}$:

Spontaneous creation of vortices by thermal excitation. Vanishing of superfluid density.

Uniform 2D system: *Superfluid - normal fluid* phase transition at critical temperature T_{BKT} (Berezinskii, Kosterlitz, Thouless):

$$k_B T_{BKT} = \rho_s \frac{\pi \hbar^2}{2m^2}$$

Computation of superfluid fraction γ_{sf}

- Two-fluid model (Landau):
Only normal fluid component of a liquid responds to slow rotation of the container walls.



Computation of superfluid fraction γ_{sf}

- Quantum mechanical moment of inertia I_{qm} deviates from classical expectation value I_{class} \rightarrow *non-classical rotational inertia (NCRI)*

$$\gamma_{sf} = 1 - \frac{I_{qm}}{I_{class}}, \quad I_{qm} = \frac{d\langle \hat{L}_z \rangle}{d\omega}, \quad I_{class} = \sum_{i=1}^N m_i r_i^2$$

Hamiltonian in the rotating frame:

$$\hat{H}_\omega = \hat{H}_0 - \omega \hat{L}_z, \quad \langle \hat{L}_z \rangle = \text{Tr}[\hat{L}_z e^{-\beta \hat{H}_\omega}], \quad \hat{L}_z = \sum_{i=1}^N (x_i p_{iy} - y_i p_{ix})$$

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- Derivative of the exponential operator

$$\frac{de^{-\beta \hat{H}_\omega}}{d\omega} = \sum_{k=1}^M e^{-(k-1)\tau \hat{H}_\omega} \frac{de^{-\tau \hat{H}_\omega}}{d\omega} e^{-(M-k)\tau \hat{H}_\omega} = \int_0^\beta dt e^{-t \hat{H}_\omega} \frac{d\hat{H}_\omega}{d\omega} dt e^{-(\beta-t)\hat{H}_\omega}$$

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$$\left. \frac{d\langle \hat{L}_z \rangle}{d\omega} \right|_{\omega \rightarrow 0} = \left\langle \int_0^\beta dt \hat{L}_z e^{-t \hat{H}_0} \hat{L}_z e^{-(\beta-t)\hat{H}_0} \right\rangle = I_{qm}$$

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- Superfluid fraction (in linear response $\omega \rightarrow 0$)

$$\gamma_{sf} = \frac{\rho_s}{\rho} = 1 - \frac{1}{I_{class}} \left\langle \int_0^\beta dt \hat{L}_z e^{-t \hat{H}_0} \hat{L}_z e^{-(\beta-t) \hat{H}_0} \right\rangle$$

Computation of superfluid fraction γ_{sf}

$$\frac{d\langle L_z \rangle}{d\omega} = \tau \text{Tr} \left[\hat{L}_z^2 e^{-M\tau\hat{H}_0} + \sum_{k=2}^M \hat{L}_z e^{-(k-1)\tau\hat{H}_0} \hat{L}_z e^{-(M-(k-1))\tau\hat{H}_0} \right]$$

Consider any term in the second sum. Angular momentum operates only on the kinetic energy part of the action and commutes with the internal potential energy. In the coordinate representation we obtain

$$\int dR dR_1 \dots dR_{M-1} (-i\hbar) \sum_{i=1}^N \left(x_i \frac{\partial}{\partial y_i} - y_i \frac{\partial}{\partial x_i} \right) \langle R | e^{-\tau\hat{H}_0} | R_1 \rangle \dots =$$

$$\int dR dR_1 \dots dR_{M-1} (-i\hbar) \sum_{i=1}^N \left(\frac{-2\pi}{\lambda_\tau^2} \right) [\mathbf{r}_{1i} \times \mathbf{r}_i]_z \langle R | e^{-\tau\hat{H}_0} | R_1 \rangle \dots$$

Area of the path segment

$$A_{1z} = \sum_{i=1}^N [\mathbf{r}_{1i} \times \mathbf{r}_i]_z, \quad A_{kz} = \sum_{i=1}^N [\mathbf{r}_{(k+1)i} \times \mathbf{r}_{ki}]_z$$

Hence, the second sum can be written as $\langle \dots \rangle = \text{Tr}[\dots \hat{\rho}] = \int dR \dots \langle R | e^{-\tau\hat{H}_0} | R_1 \rangle \dots$

$$(-i\hbar)^2 \left(\frac{-2\pi}{\lambda_\tau^2} \right)^2 \cdot \left(\langle A_{1z} \sum_{k=1}^M A_{kz} \rangle - \left(\frac{-2\pi}{\lambda_\tau^2} \right)^2 \langle A_{1z}^2 \rangle \right)$$

Computation of superfluid fraction γ_{sf}

Similar for the first term (operator \hat{L}_z operates twice on one link) we obtain

$$\hat{L}_z^2 \langle R | e^{-\tau \hat{H}_0} | R_1 \rangle = (-i\hbar)^2 \left(\frac{-2\pi}{\lambda_\tau^2} \right)^2 A_{1z}^2 \langle R | e^{-\tau \hat{H}_0} | R_1 \rangle + (-i\hbar)^2 \left(\frac{-2\pi}{\lambda_\tau^2} \right) \sum_{i=1}^N (x_i x_{1i} + y_{1i} y_i)$$

Now we Combine the first and the second term

$$I_{qm} = I_c - I_q$$

where I_c is the classical part of the response

$$I_c = \left\langle m \sum_{i=1}^N (x_i x_{1i} + y_{1i} y_i) \right\rangle$$

and the quantum part

$$I_q = \frac{m^2}{\hbar^2 \tau} \langle A_{1z} A_z \rangle, \quad A_z = \sum_{k=1}^M A_{kz}$$

In the end do symmetrization: $\langle A_{1z} A_z \rangle = \frac{1}{M} \sum_{k=1}^M \langle A_{kz} A_z \rangle = \frac{1}{M} \left\langle \sum_{k=1}^M A_{kz} A_z \right\rangle = \langle A_z^2 \rangle$.

Superfluid fraction: finite systems

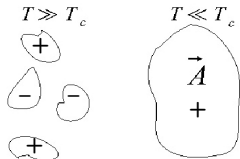
- Final result. Superfluid fraction in a finite system: particles are placed in an external field (e.g. a rotating cylinder around ω)

$$\gamma_{sf} = \frac{4m^2 \langle A_z^2 \rangle}{\hbar^2 \beta I_{\text{class}}}, \quad A_z = \frac{\mathbf{A} \cdot \boldsymbol{\omega}}{\omega}$$

[P.Sindzingre, M.Klein, D.Ceperley, Phys.Rev. Lett. **63**, 1601 (1981)]

- Area enclosed by the paths

$$\mathbf{A} = \frac{1}{2} \sum_{i=1}^N \sum_{k=0}^{M-1} \mathbf{r}_{ki} \times \mathbf{r}_{(k+1)i}$$



Superfluid fraction: finite systems

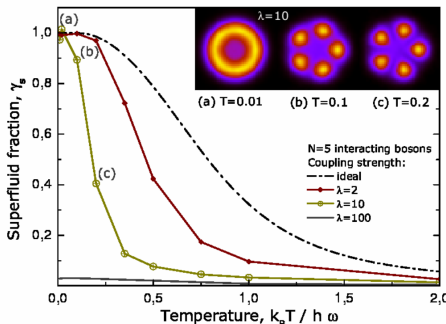
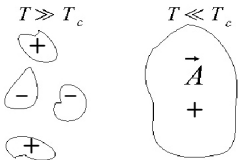
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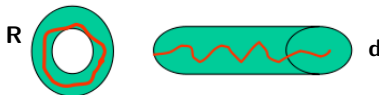
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Superfluid fraction for $N = 5$ charged bosons in a two-dimensional trap. $\lambda = (e^2/\epsilon_0\hbar\omega)/(\hbar\omega)$ is the coupling constant.

Superfluid fraction: macroscopic systems

- Instead of a filled cylinder (with N particles) we consider two cylinders with the radius R and spacing d , with $d \ll R$. Such a torus is topologically equivalent to the usual periodic boundary conditions:



$$I_{\text{class}} = mNR^2, \quad A_z = N_{\text{round}} \cdot \pi R^2 = W_z R/2$$

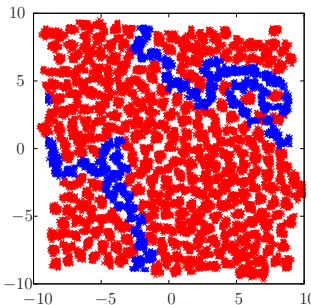
$$W_z = 2\pi R \cdot N_{\text{round}}$$

- Winding number W : total length of the paths along the torus

$$\mathbf{W} = \sum_{i=1}^N [\mathbf{r}_i(\beta) - \mathbf{r}_i(0)]$$

- Superfluid fraction:

$$\gamma_{sf} = \frac{4m^2 \langle A_z^2 \rangle}{\hbar^2 \beta I_{\text{class}}} \rightarrow \frac{m \langle W_z^2 \rangle}{\hbar^2 \beta N}$$



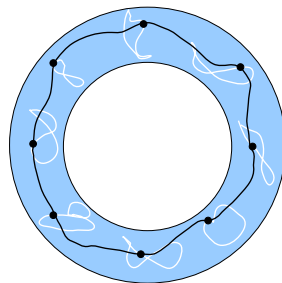
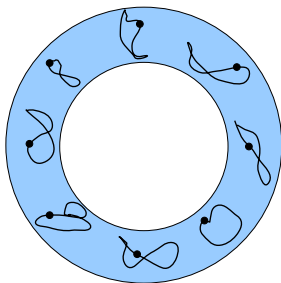
Simulation box with periodic boundary conditions

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Winding number: ergodicity

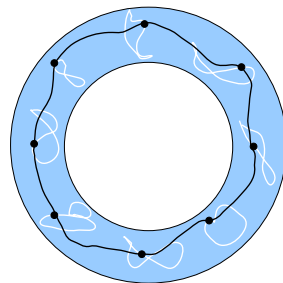
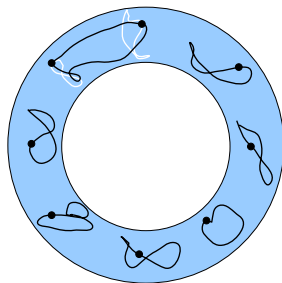
- Changing a winding number requires a global update in the permutation space.



We start from identity permutations

Winding number: ergodicity

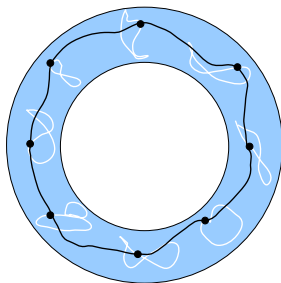
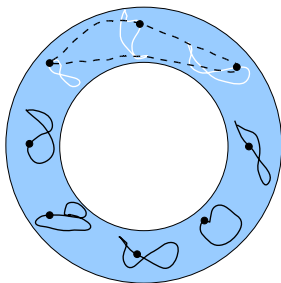
- Changing a winding number requires a global update in the permutation space.



Two particle exchanges are very probable: $\bar{r} \sim \lambda_D(T)$

Winding number: ergodicity

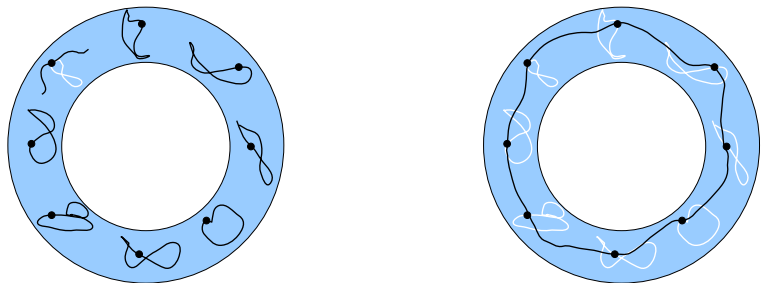
- Changing a winding number requires a global update in the permutation space.



Three particle exchanges can happen but very infrequent: $2\bar{\tau} > \lambda_D(T)$. Probability of longer permutations is **exponentially suppressed** !
 We are trapped in 2-3-particle permutation sector \Rightarrow
Zero winding numbers and zero superfluidity!

Winding number: ergodicity

- Changing a winding number requires a global update in the permutation space.



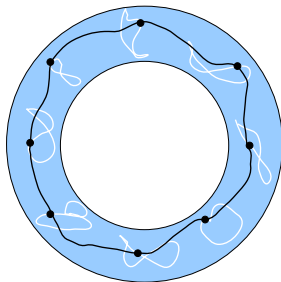
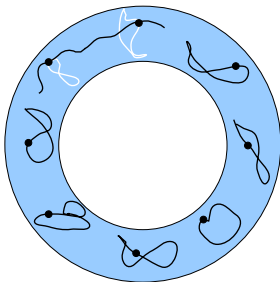
Idea: expand the configuration space to the **offdiagonal sector** \mathbf{G} and sample **offdiagonal** density matrix $\rho(R, \hat{P}R'; \beta) \Rightarrow$ *Worm algorithm*

[Prokof'ev, Svistunov and Tupitsyn (1997);

N.Prokof'ev, B.Svistunov, Boninsegni, Phys.Rev.Lett **96**, 070601 (2006)]

Winding number: ergodicity

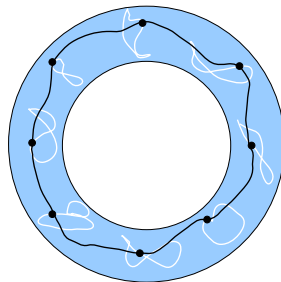
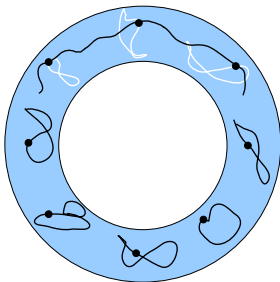
- Changing a winding number requires a global update in the permutation space.



Continue to work in the offdiagonal sector \mathbf{G} to sample two-particle exchanges

Winding number: ergodicity

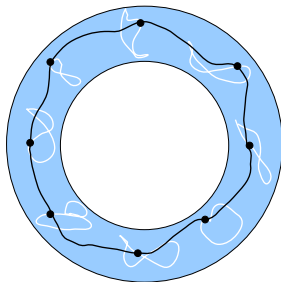
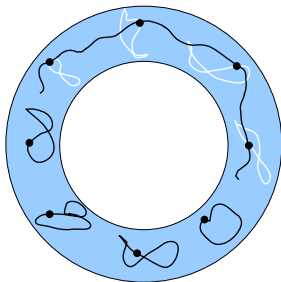
- Changing a winding number requires a global update in the permutation space.



Enjoy stable high acceptance rate for any permutation length !

Winding number: ergodicity

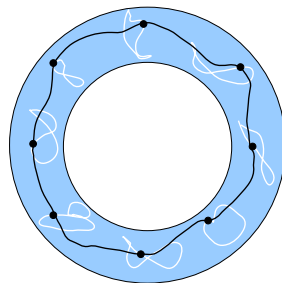
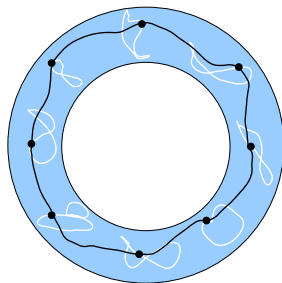
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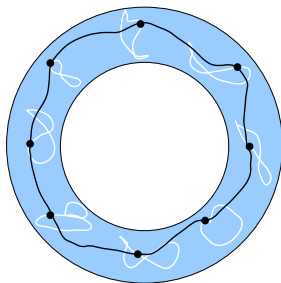
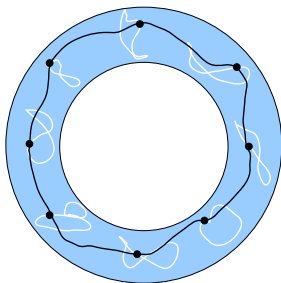
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Occasionally close the trajectory to return back in the **diagonal** sector \mathbf{Z} . Measure thermodynamic observables related to the diagonal density matrix $\rho(R, \hat{P}R; \beta)$ or partition function Z .

Winding number: ergodicity

- Changing a winding number requires a global update in the permutation space.



Conclusion:

- Accurate statistics on W requires permutation lengths $\sim N^{1/d}$.
- With typical few-particle update sampling (diagonal sector) we stay in one permutation sector \Rightarrow non-ergodic sampling of W .
- More advanced algorithms are required: Ising model – cluster algorithm; PIMC – worm algorithm (expanded conf. space \mathbf{Z} and \mathbf{G}).

Worm algorithm

Key features:

- All updates in **open-path-configurations** are performed exclusively through the end-points of the disconnected paths \Rightarrow Local sampling with high acceptance rates!
- **No global updates with exponentially low acceptance !**
- Topological classes are sampled efficiently.
- No critical slowing down in most cases.
- Open paths are related to important physics, i.e correlation functions, and are not merely an algorithm trick.
- Usual PIMC in *Canonical ensemble* can now be easily generalized to *Grand Canonical ensemble* \Rightarrow New tool for corresponding experimental systems.

Why Grand Canonical ensemble is better

$$Z_{GCE} = \sum_{N=0}^{\infty} e^{\int_0^{\beta} \mu N(\tau) d\tau} Z_{CE}(N, V, \beta)$$

Advantages of the simulations in grand canonical ensemble (GCE):

- Off-diagonal one-particle d. matrix:

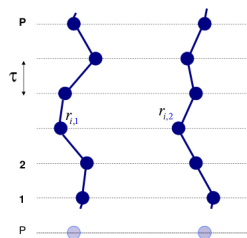
$$n(r, r', t' - t) = \langle \Psi(r', t') \Psi^\dagger(r, t) \rangle$$

- Condensate fraction:

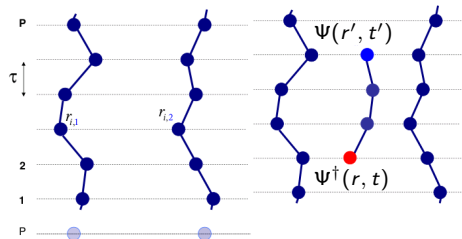
$$n(\mathbf{r}, \mathbf{r}') = N_0 \phi_0^*(\mathbf{r}) \phi_0(\mathbf{r}') + \sum_{i \neq 0} n_i \phi_i^*(\mathbf{r}) \phi_i(\mathbf{r}')$$

$$n(\mathbf{r}, \mathbf{r}')|_{|\mathbf{r}-\mathbf{r}'| \rightarrow \infty} \rightarrow N_0$$

Canonical (CE)



Grand Canonical (GCE)



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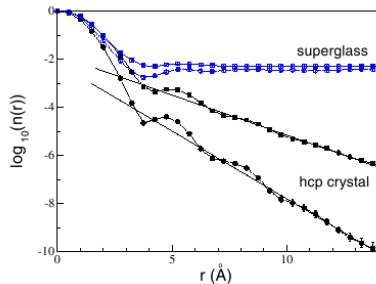
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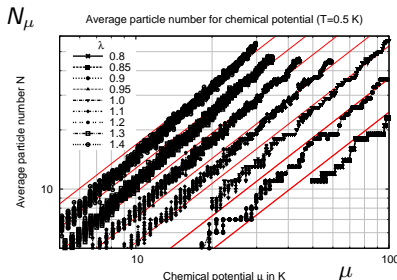
Prokof'ev, Svistunov, Boninsegni, PRE 74, 036701 (2007)

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Advantages of the simulations in grand canonical ensemble (GCE):

- μ is an input parameter and $\langle N \rangle_{\mu}$ is a simple diagonal property.
- Compressibility, $kVT = \langle (N - \langle N \rangle)^2 \rangle_{\mu}$.

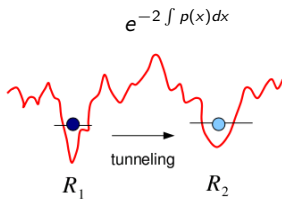


μ -dependence of the particle number N in 2D He^4 clusters in a parabolic trap $\omega \sim 1/\lambda^2$.

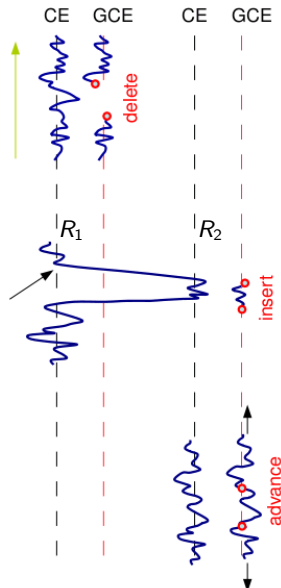
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Advantages of the simulations in grand canonical ensemble (GCE):



- Solve ergodicity issue for disorder problems
- Allows for efficient sampling of exponentially rare event



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Sign problem

Let us consider a standard Monte Carlo problem:

- Integration over space of states ν . Each configuration has a weight factor:
 $W_\nu > 0, \quad e^{-E_\nu/T}$
- Expectation values:

$$\langle A \rangle = \frac{\sum_\nu A_\nu W_\nu}{\sum W_\nu}$$

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- Frequently for quantum mechanical systems W_ν is not-positive definite function. Then

$$\langle A \rangle = \frac{\sum_\nu A_\nu \text{sign}(W_\nu) \cdot |W_\nu|}{\sum_\nu \text{sign}(W_\nu) \cdot |W_\nu|}$$

- Now we can proceed with the standart MC using $|W_\nu|$ as a sampling probability

$$\langle A \rangle = \frac{\sum_{\nu'} A_{\nu'} \text{sign}(W_{\nu'})}{\sum_{\nu'} \text{sign}(W_{\nu'})} = \frac{\langle A \cdot \text{sign} \rangle}{\langle \text{sign} \rangle}$$

Sign problem

- The trouble comes in cases: $\langle \text{sign} \rangle \rightarrow 0$.

Both $\langle A \cdot \text{sign} \rangle$ and $\langle \text{sign} \rangle$ have finite errorbars which fluctuate

$$\langle A \rangle + \delta A = \frac{\langle A \cdot \text{sign} \rangle + \delta_{AS}}{\langle \text{sign} \rangle + \delta_S} \approx \frac{\langle A \cdot \text{sign} \rangle}{\langle \text{sign} \rangle} \left(1 + \frac{\delta_{AS}}{\langle A \cdot \text{sign} \rangle} + \frac{\delta_S}{\langle \text{sign} \rangle} \right)$$

or

$$\frac{\delta A}{\langle A \rangle} \approx \frac{\delta_{AS}}{\langle A \cdot \text{sign} \rangle \rightarrow 0} + \frac{\delta_S}{\langle \text{sign} \rangle \rightarrow 0}$$

Sign problem

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or

$$\frac{\delta A}{\langle A \rangle} \approx \frac{\delta_{AS}}{\langle A \cdot \text{sign} \rangle \rightarrow 0} + \frac{\delta_S}{\langle \text{sign} \rangle \rightarrow 0}$$

- There is no generic solution of the sign-problem.

This prevents MC methods from studies:

- interacting fermions
- magnetic systems
- real time dynamics, etc.

But the sign-problem can be reduced or eliminated by a proper choice of the basis set. Example:

$$\hat{H}\Psi_\nu = E_\nu\Psi_\nu, \quad \Psi\text{-eigenfunctions}$$

$$Z = \sum_\nu e^{-\beta E_\nu} \quad \text{- all terms are positive}$$

Fermion sign problem in PIMC

- Metropolis algorithm gives the same distribution of permutations for both Fermi and Bose systems. The reason is that for sampling permutations we use the modulus of the off-diagonal density matrix

$$\begin{aligned} \rho^{S/A}(R, R; \beta) &= \frac{1}{N!} \sum_P (\pm 1)^P \rho(R, \hat{P}R; \beta) = \\ &= \frac{1}{N!} \sum_P (\pm 1)^P \int dR_1 \dots dR_{M-1} \rho(R, R_1; \beta) \dots \rho(R_{M-1}, \hat{P}R; \beta) \end{aligned}$$

Bosons: all permutations contribute with the same (positive) sign

Fermions: positive and negative terms (corresponding to even and odd permutations) are close in their absolute value and cancel each other.

- Accurate calculation of this small difference is drastically hampered with the increase of quantum degeneracy (low T, high density).

Fermion problem: partial solutions for Quantum MC

1 *Fixed-node (fixed-phase) approximation*

Use restricted (reduced) area of PIMC integration which contains only even permutations. Most of the area with the cancellation of even and odd permutations are excluded using an approximate trial ansatz for the N-particle fermion density matrix. Requires knowledge of nodes of DM.

References: D.M.Ceperley, *Fermion Nodes*, J. Stat. Phys. 63, 1237 (1991); D.M.Ceperley, *Path Integral Calculations of Normal Liquid ^3He* , Phys. Rev. Lett. 69, 331 (1992).

Fermion problem: partial solutions for Quantum MC

2 *Direct PIMC*

Do not sample individual permutations in the sum. Instead use the full expression presented in a form of an determinant. In this case the absolute value of the determinant is used in the sampling probabilities. Its value becomes close to zero in the regions of equal contributions of even and odd permutations and Monte Carlo sampling successfully avoids such regions.

References: V.S.Filinov, M.Bonitz, W.Ebeling, and V.E.Fortov, *Thermodynamics of hot dense H-plasmas: Path integral Monte Carlo simulations and analytical approximations*, Plasma Physics and Controlled Fusion 43, 743 (2001).

Fermion problem: partial solutions for Quantum MC

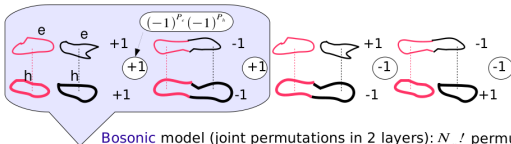
3 *Multilevel-blocking PIMC*

Trace the cancellations of permutations by grouping the path coordinates into blocks (levels). Use numerical integration to get good estimation of the fermion density matrix at high temperature. Further use it in the sampling probabilities of path coordinates on the next level (corresponding to the density matrix at lower temperature). Most of the sign fluctuations are already excluded at higher levels and sampling at low levels (lower temperatures) becomes more efficient.

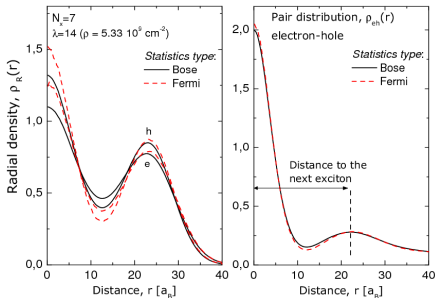
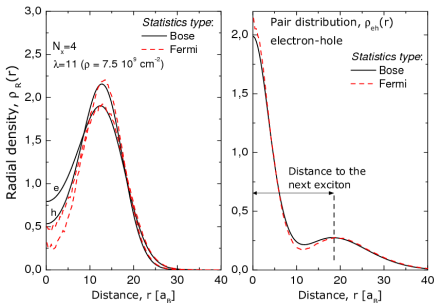
References: R.Egger, W.Hausler, C.H.Mak, and H.Grabert, *Crossover from Fermi Liquid to Wigner Molecule Behavior in Quantum Dots*, Phys. Rev. Lett. 82, 3320 (1999).

Comparison of Fermi/Bose statistics for excitons

Exact treatment of excitons as composite particles consisting of two fermions:
 $N_e!N_h!$ permutations, total density matrix is antisymmetric.

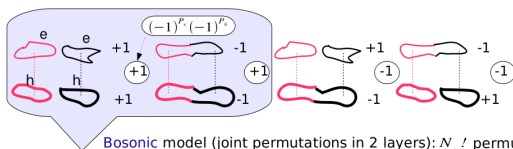


Total density matrix is symmetrical! Reduced number of permutations!



Comparison of Fermi/Bose statistics for excitons

Exact treatment of excitons as composite particles consisting of two fermions:
 $N_e!N_h!$ permutations, total density matrix is antisymmetric.



Bosonic model (joint permutations in 2 layers): $N_x!$ permutations
 Total density matrix is symmetrical! Reduced number of permutations!

- Exact fermionic calculations clearly show the effect of Fermi repulsion on the radial distributions.
- This favors localization of individual particles and reduces the density in between the central particle and the shell.
- Although the effect is small it has a large effect on the superfluid fraction.

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Comparison of Fermi/Bose statistics: superfluidity

Simulation: Spin polarized electron-hole bilayer (two coupled ZnSe quantum wells).

External confinement: parabolic trap.

Parameters: $T = 312\text{mK}$, $d = 20.1\text{nm}$.

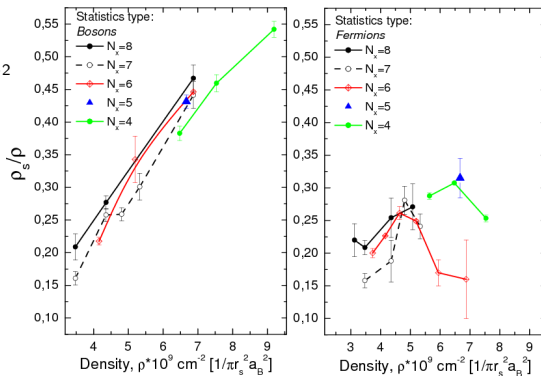
A.Filinov, M.Bonitz, P.Ludwig, and Yu.E.Lofovnik, phys. stat. sol. (c) 3, No. 7, 2457 (2006)

Applicability of bosonic model:

Critical density: $\rho^* \approx 5 \cdot 10^9 \text{cm}^{-2}$

$\rho \leq \rho^*$: both models agree.

$\rho > \rho^*$: fermionic calculations indicate drop in the superfluid fraction.



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Improved high-temperature action

- We need to improve the simple factorization formula for unbound potentials, e.g. $V(r) = -1/r$

$$\rho(\mathbf{R}, \mathbf{R}', \tau) \approx \prod_{i=1}^N \rho_F(\mathbf{r}_i, \mathbf{r}'_i, \tau) \cdot \exp \left[-\tau \prod_{j < k} V(\mathbf{r}_{jk}) \right]$$

⇒ not be normalized (due to singularity).

- Alternative: take into account two-body correlations “exactly”

$$\rho(\mathbf{R}, \mathbf{R}'; \tau) \approx \prod_{i=1}^N \rho_F(\mathbf{r}_i, \mathbf{r}'_i; \tau) \times \prod_{j < k} \frac{\rho^{[2]}(\mathbf{r}_j, \mathbf{r}_k, \mathbf{r}'_j, \mathbf{r}'_k; \tau)}{\rho_F(\mathbf{r}_i, \mathbf{r}'_i; \tau) \rho_F(\mathbf{r}_k, \mathbf{r}'_k; \tau)} + O(\rho^{[3]}),$$

Three-body and higher order terms become negligible by decreasing $\tau = \beta/M$.

Two-body density matrix

- Effective pair potential U^{pair}

$$\frac{\rho^{[2]}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}'_1, \mathbf{r}'_2; \tau)}{\rho_F(\mathbf{r}_1, \mathbf{r}'_1; \tau)\rho_F(\mathbf{r}_2, \mathbf{r}'_2; \tau)} = e^{-\tau U_{12}^{pair}}$$

$U^{pair}(\mathbf{r}_1 - \mathbf{r}_2, \mathbf{r}'_1 - \mathbf{r}'_2; \tau)$ is temperature-dependent and finite at $\mathbf{r}_{12} = 0$.

- Two-body density matrix $\rho^{[2]}$ can be obtained by solving two-particle problem.
- Replace singular potentials with bounded effective potentials defined as

$$\rho(\mathbf{r}_{12}, \mathbf{r}'_{12}; \tau) = \rho_F(\mathbf{r}_{12}, \mathbf{r}'_{12}; \beta) \exp \left[-\tau U^{pair}(\mathbf{r}_{12}, \mathbf{r}'_{12}; \tau) \right]$$

Advantages of effective potentials

Exact treatment of pair correlations allows:

- drastically reduce number of factorization factors \Rightarrow
- reduce dimension of integrals \Rightarrow
- simplification of path integral sampling.

Approaches to computation of the pair density matrix:

- 1 Cumulant approximation (Feynman-Kacs)
[R.Feynman and A.R.Hibbs *Quantum Mechanics and Path Integral*]
- 2 Solution of two-particle Bloch equation (matrix squaring technique)
[Klemm and Storer (1974), D.Ceperley]
- 3 Perturbation or semi-classical approximation
[Kelbg, Ebeling, Deutsch, Feynman, Kleinert (1963-1995)]

Two-body density matrix: eigenstates and Feynman-Kacs

- Sum over eigenstates of the Hamiltonian

$$\rho(\mathbf{r}, \mathbf{r}', \tau) = \sum_i e^{-\tau E_i} \Psi_i^*(\mathbf{r}) \Psi_i(\mathbf{r}')$$

Can be used if all eigenstates are known analytically, e.g. for Coulomb potential (Pollock Comm. Phys. 52, 49 (1988)).

- Feynman-Kac formula: $\rho(\mathbf{r}, \mathbf{r}'; \tau) =$

$$= \int_{\mathbf{r}(0)=\mathbf{r}}^{\mathbf{r}(\tau)=\mathbf{r}'} D\mathbf{r}(t) \exp \left[- \int_0^\tau \left(m\dot{\mathbf{r}}^2(t)/2 + V_{12}(\mathbf{r}(t)) \right) dt \right] = \left\langle e^{-\int_0^\tau V_{12}(\mathbf{r}(t)) dt} \right\rangle_{\rho_F}$$

The average can be calculated by Monte Carlo sampling of all Gaussian random walks from \mathbf{r} to \mathbf{r}' .

Two-body density matrix: matrix squaring

- Matrix squaring technique: Factorization into a center-of-mass, relative coordinates, $\rho(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}'_i, \mathbf{r}'_j; \tau) = \rho_{\text{cm}}(\mathbf{R}, \mathbf{R}'; \tau)\rho(\mathbf{r}, \mathbf{r}'; \tau)$, and expansion in partial waves:

$$\rho^{2D}(\mathbf{r}, \mathbf{r}'; \tau) = \frac{1}{2\pi\sqrt{r r'}} \sum_{l=-\infty}^{+\infty} \rho_l(r, r'; \tau) e^{i l \Theta},$$

$$\rho^{3D}(\mathbf{r}, \mathbf{r}'; \tau) = \frac{1}{4\pi r r'} \sum_{l=0}^{+\infty} (2l+1) \rho_l(r, r'; \tau) P_l(\cos \Theta)$$

- Convolution equation: k -iterations raise the temperature by 2^k : $\tau/2^k \rightarrow \tau$

$$\int_0^\infty dr'' \rho_l(r, r''; \frac{\tau}{2^{m+1}}) \rho_l(r'', r'; \frac{\tau}{2^{m+1}}) = \rho_l(r, r'; \frac{\tau}{2^m}), \quad m = k-1, \dots, 0$$

- Semi-classical approximation: the start for the matrix-squaring iterations

$$\rho_l(r, r'; \tau/2^k) = \exp\left(-\frac{\tau/2^k}{|r-r'|} \int_r^{r'} V(x) dx\right)$$

Two-body density matrix: perturbative solution

- First order perturbation solution for the two-particle Bloch equation:

$$\frac{\partial}{\partial \tau} \rho(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}'_i, \mathbf{r}'_j; \tau) = -\hat{H} \rho(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}'_i, \mathbf{r}'_j; \tau)$$

$$\rho_{ij} = \frac{(m_i m_j)^{3/2}}{(2\pi\hbar\tau)^3} \exp\left[-\frac{m_i}{2\hbar^2\tau}(\mathbf{r}_i - \mathbf{r}'_i)^2\right] \exp\left[-\frac{m_j}{2\hbar^2\tau}(\mathbf{r}_j - \mathbf{r}'_j)^2\right] \exp[-\tau\Phi^{ij}],$$

- Solution for Coulomb interaction:

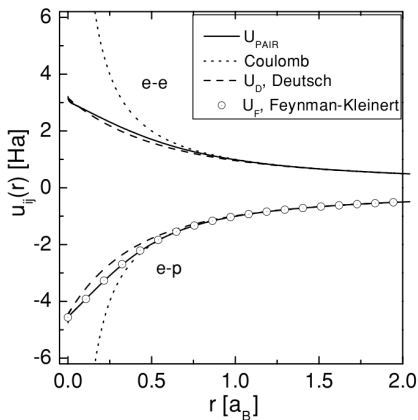
$$\Phi^{ij}(\mathbf{r}_{ij}, \mathbf{r}'_{ij}; \tau) \equiv e_i e_j \int_0^1 \frac{d\alpha}{d_{ij}(\alpha)} \operatorname{erf}\left(\frac{d_{ij}(\alpha)/\lambda_{ij}}{2\sqrt{\alpha(1-\alpha)}}\right),$$

where $d_{ij}(\alpha) = |\alpha\mathbf{r}_{ij} + (1-\alpha)\mathbf{r}'_{ij}|$, $\operatorname{erf}(x)$ is the error function, $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x dt e^{-t^2}$, and $\lambda_{ij}^2 = \frac{\hbar^2\tau}{2\mu_{ij}}$ with $\mu_{ij}^{-1} = m_i^{-1} + m_j^{-1}$.

- The diagonal element ($\mathbf{r}'_{ij} = \mathbf{r}_{ij}$) is called the Kelbg potential (DKP)

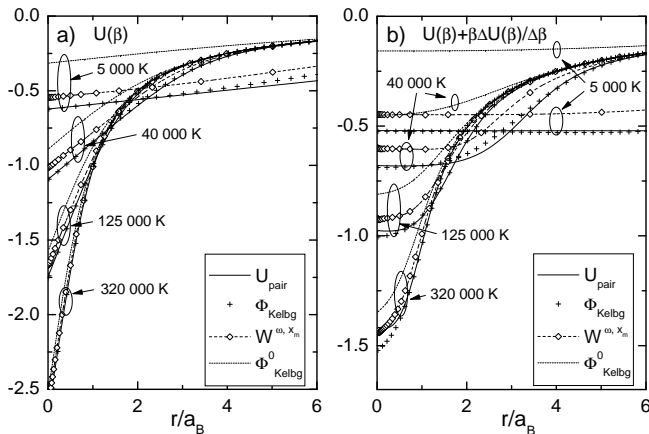
$$\Phi(r_{ij}, \tau) = \frac{q_i q_j}{r_{ij}} \left[1 - e^{-\frac{r_{ij}^2}{\lambda_{ij}^2}} + \sqrt{\pi} \frac{r_{ij}}{\lambda_{ij} \gamma_{ij}} \left(1 - \operatorname{erf}\left[\gamma_{ij} \frac{r_{ij}}{\lambda_{ij}}\right] \right) \right].$$

Effective pair potential



Solid lines: electron–electron (e–e) and electron–proton (e–p) potential U_{pair} at $T = 10^6$ K. Dotted lines: Coulomb interaction; dashed lines: Deutsch potential; open circles: U_F variational perturbative potential (Feynman and Kleinert). Distances are in $a_B = \hbar^2/m_e e^2$ and potentials are in $Ha = e^2/a_B$ units.

Effective pair potential: temperature dependence



[Filinov, Golubnychiy, Bonitz, Ebeling, Dufty, PRE **70**, 046411 (2004)]

(a): Effective electron-proton potential (in units of Ha): the DKP $\Phi^0(\mathbf{r}; \beta)$, the improved DKP $\Phi(\mathbf{r}; \beta)$, variational potential W_1^{Ω, x_m} , pair potential U_p corresponding to the “exact” density matrix. Temperatures 5000, 40000, 125000 and 320000 K.

(b): Contribution to the potential energy: $f(\beta) = U(\beta) + \beta \frac{\partial U(\beta)}{\partial \beta}$, $E_p = \text{Tr}[f(\beta)\hat{\rho}]/Z$.

Estimators for thermodynamic averages

Quantities of interest: energy, pressure (equation of state), specific heat, structure factor, pair distribution functions, condensate or superfluid fraction, etc.

All quantities can be obtained by averaging with the thermal density matrix or as derivatives of the partition function Z .

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Examples: **Total energy**

$$E = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{1}{Z} \int dR \frac{\partial \rho(R, R; \beta)}{\partial \beta},$$

$$\rho(R, R; \beta) = \int dR_1 \dots dR_{M-1} (e^{-S_{kin} - S_V}) / \lambda_\tau^{dMN}$$

$$E = \frac{dMN}{2\beta} - \left\langle \frac{1}{\beta} \sum_{i=0}^{M-1} \frac{\pi}{\lambda_\tau^2} (R_i - R_{i+1})^2 \right\rangle + \left\langle \frac{1}{M} \sum_{i=0}^{M-1} \frac{d}{d\tau} (\tau U(R_i, \tau)) \right\rangle.$$

Kinetic energy and pressure

$$E_{kin} = \frac{m}{\beta Z} \frac{\partial Z}{\partial m}, \quad P = -\frac{\partial F}{\partial V} = \frac{1}{3V} \left\langle 2E_{kin} - \sum_{i<j} \mathbf{r}_{ij} \frac{d(\tau U(R_i, \tau))}{d\mathbf{r}_{ij}} \right\rangle$$

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Use virial estimators. Introduce temperature-dependent measure

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Use virial estimators. Introduce temperature-dependent measure

$$R_i(\tau) = R_0 + \lambda_\tau \sum_{m=1}^i \xi_m, \quad i = 1, \dots, M-1. \Rightarrow$$

$$S_{kin} = \sum_{i=0}^{M-1} \frac{\pi}{\lambda_\tau^2} (R_i - R_{i+1})^2 = \sum_{i=0}^{M-1} \pi \xi_{i+1}^2 \neq f(\beta),$$

$$\rho(R, R; \beta) = \int \frac{dR_1 \dots dR_{M-1}}{\lambda_\tau^{dMN}} (..) = \int \frac{d\xi_1 \dots d\xi_{M-1}}{\lambda_\tau^{dMN}} \lambda_\tau^{d(M-1)N} (..) \sim \frac{1}{\lambda_\tau^{dN}}$$

$$E = \frac{dN}{2\beta} + \left\langle \sum_i U(R_i(\tau)) + \beta \frac{\partial U(R_i(\tau))}{\partial R_i(\tau)} \frac{\partial R_i(\tau)}{\partial \beta} \right\rangle$$

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Use virial estimators. Introduce temperature-dependent measure
- 3 Take care for other sources of errors: systematic (Trotter formula), statistical (autocorrelation times) and finite-size (scaling with system size).

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Summary

- PIMC allows for first-principle simulations of interacting quantum particles.
- Many-body correlations can be treated at any accuracy.
- Problems remain to be solved:
 - Fermion sign problem
 - Limitations to several hundred particles due to large computational demands
 - Efficient simulations of spin and magnetic effects

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