Classical and path integral Monte Carlo simulation of charged particles in traps

Alexei Filinov, Michael Bonitz, in collaboration with Vladimir Filinov, Patrick Ludwig, Jens Böning, Henning Baumgartner

Christian-Albrechts-Universitaet zu Kiel, Institut für Theoretische Physik und Astrophysik, Institute of Physics, Rostock University
Institute for High Energy Density RAS, Russia

Plasma crystal (classical particles)

Electrons in nanostructures (quantum particles)
Contents

- Introduction: Classical MC for trapped particles
- General idea of PIMC simulations
- Quantum statistics. PIMC for bosons and fermions
- Practical issues. Applications
- Examples: Many-body correlation effects of excitonic systems in semiconductors
Idea of classical thermodynamic Monte Carlo

**Goal:**
- Obtain exact thermodynamic equilibrium configuration $R$ of interacting particles at given temperature, particle number, external fields etc.

$$R = (r_1, r_2, ..., r_N) \quad \text{Coordinates of all particles (microstate)}$$

- Evaluate measurable quantities, such as energy, potential energy $V$, pressure, pair distribution function etc.

$$\langle V \rangle (\beta, N) = \frac{1}{Z} \int dR V(R) e^{-\beta V(R)}, \quad \beta = \frac{1}{k_B T},$$

- Averaging with canonical probability distribution (Boltzmann factor)

**Realization:**
- try all possible configurations ("move" particles) and choose the most probable one

- Metropolis Monte Carlo procedure (Markov process)

- compute averages from fluctuating microstates

--> See examples
Monte Carlo calculations – like in classical case - are possible since the density matrix is positive on the diagonal (true probability density)

But: for interacting systems DM $\rho$ is unknown.

--> We can sample particle's coordinates $R$ only after we find an analytical representation for the DM.
There exist several equivalent formulation of quantum mechanics:

- Schrödinger picture: time-dependent wave functions
- Heisenberg picture: time-dependent operators (matrices)
- Feynman: path integral representation
  - describes time evolution (wave function) or thermodynamic state (“imaginary time”) via density operator
  - analytical solutions only for few models
  - numerical solutions: computationally very demanding
    breakthrough in connection with Monte Carlo methods since the 1970s
Properties of the density matrix (1)

- Operator notation (thermodynamic equilibrium) \( \hat{\rho} = \exp[-\beta \hat{H}] \)

Original idea (Feynman): solution of Schrödinger equation \( \hat{U}(t) = \exp[-i \hat{H} t/\hbar] \)
via time evolution operator --> path integral representation of quantum mechanics

System Hamiltonian includes N-particle kinetic energy and potential energy operators (not commuting!)

\[
\hat{H} = \hat{K} + \hat{V} , \quad [\hat{K}, \hat{V}] \neq 0
\]

- Coordinate representation: superposition of wavefunctions weighted with probability density (with N-particle energy eigenvalues)

\[
\langle R | \hat{\rho} | R' \rangle = \rho(R, R'; \beta) = \sum_{\alpha} \phi_\alpha(R) \phi_\alpha(R') e^{-\beta E_\alpha}
\]

- Density operator known only for few cases,
Example: high temperature -> classical system with weak interaction

- Idea (Feynman): express Density operator of interacting low temperature system by known high-temperature limit --> gives rise to path integral
Properties of the density matrix (2)

• Convolution property of density matrix:
  low-temperature DM related to DM at higher temperature

\[ \rho(R, R'; \beta_1 + \beta_2) = \langle R | e^{-(\beta_1 + \beta_2) \hat{H}} | R' \rangle, \quad \beta_1 + \beta_2 = \frac{1}{k_B(T_1 + T_2)} \]

\[ \int dR_1 \langle R | e^{-\beta_1 \hat{H}} | R_1 \rangle \langle R_1 | e^{-\beta_2 \hat{H}} | R' \rangle = \int dR_1 \rho(R, R_1; \beta_1) \rho(R_1, R'; \beta_2) \]

• Generalization: use convolution property M times

\[ \langle R | \hat{\rho} | R' \rangle = \langle R | \exp[-\Delta \beta \hat{H}] \ldots \exp[-\Delta \beta \hat{H}] | R' \rangle, \quad \Delta \beta = \beta / M \]

\[ \langle R | \hat{\rho} | R' \rangle = \langle R | \exp[-\Delta \beta \hat{H}] \ldots \exp[-\Delta \beta \hat{H}] | R' \rangle, \]

\[ \rho(R, R'; \beta) = \int dR_1 dR_2 \ldots dR_{M-1} \rho(R, R_1; \Delta \beta) \rho(R_1, R_2; \Delta \beta) \ldots \rho(R_{M-2}, R_{M-1}; \Delta \beta) \rho(R_{M-1}, R'; \Delta \beta) \]

M factors connected by M-1 intermediate integrations.

Note: total dimension of integral: \((M-1) \cdot 3 \cdot N\), may be very large number
success of method relies on highly efficient Monte Carlo integration
Properties of the density matrix (3)

- Visualization of diagonal elements of density matrix:

\[ \rho(R, R; \beta) = \int dR_1 dR_2 ... dR_{M-1} \rho(R, R_1; \Delta \beta) \rho(R_1, R_2; \Delta \beta) ... \rho(R_{M-2}, R_{M-1}; \Delta \beta) \rho(R_{M-1}, R; \Delta \beta) \]

- 2 arbitrary particles (e, h) represented by set ("chain") of points ("beads")
  this chain is closed. It is called "path" (therefore: "path integral")

All intermediate points do occur,
We have to integrate over all possible intermediate points (paths)
Obtain high-temperature expression of the DM, use Trotter's theorem (1959)

\[ \hat{\rho} = e^{-\beta(\hat{T} + \hat{V})}, \quad \hat{\rho} = \lim_{M \to \infty} \left[ e^{-\Delta \beta \hat{T}} e^{-\Delta \beta \hat{V}} \right]^M \]

\[ \hat{\rho} \approx \left[ e^{-\Delta \beta \hat{T}} e^{-\Delta \beta \hat{V}} \right]^M + O(e^{-\Delta \beta^2 M[\hat{T},\hat{V}]^2}) \approx \left[ e^{-\Delta \beta \hat{T}} e^{-\Delta \beta \hat{V}} \right]^M + O(1/M) \]

Coordinate representation of the high temperature density matrix

\[ \rho(R_i, R_{i+1}; \Delta \beta) = \langle R_i | e^{-\Delta \beta \hat{T}} e^{-\Delta \beta \hat{V}} | R_{i+1} \rangle = \exp \left[ -\frac{\pi}{\lambda^2_{\Delta}} (R_{i+1} - R_i)^2 + \Delta \beta V(R_{i+1}; \Delta \beta) \right] \]

\[ \hat{T} = -\frac{\hbar^2}{2m} \Delta \quad V \text{ diagonal (local)}, \quad \text{DeBroglie wave length} \quad \lambda^2_{\Delta(e, h)} = 2\pi \hbar^2 \Delta \beta / m_{e, h} \]

Resulting Particle extension \( \sim \lambda(\beta) \)
Analytical form of the N-particle density matrix

- Density matrix has analogy to a classical system of interacting polymers (use action $S$)

$$\rho(R, R; \beta) = \int_V dR_1 dR_2 ... dR_{M-1} \exp \left[ - \sum_{i=1}^{M} S_i \right],$$

$$S_i = \frac{\pi}{\lambda^2} (R_{i+1} - R_i)^2 + \Delta \beta U(R_i)$$

"Spring" term holding polymers (paths) together

Full interaction energy of polymers (Example: electron-hole system)

$$U(R_i) = U_{ee}(R_i^e; \Delta \beta) + U_{hh}(R_i^h; \Delta \beta) + U_{eh}(R_i^e, R_i^h; \Delta \beta)$$

Classical Coulomb interaction or effective regularized potential

Averaging over many configurations yields smooth probability densities of interacting quantum systems which become exact with $M \rightarrow \infty$

Figure 1.5: (a) Snapshot of a configuration of 5 electrons in a 2D harmonic trap (XY plane) from path integral Monte Carlo simulations. The electrons 3, 4 and 5 are in the identical permutations. The pair exchange is between the electron 1 and electron 2. (b) The Y-coordinates of the electrons as a function of the time-slice number $m$. Labels show electron indices.
Example: two electrons in 2D parabolic trap

Classical particles

PIMC simulations of Jens Böning and Alexei Filinov

low density  medium density  high density

---> PIMC simulations yield probability density of correlated particles
Basic numerical issues of PIMC

- How to sample the paths.

  It is necessary to explore the whole coordinate space for each intermediate point. This is very time consuming.

  To speed up convergence: move several slices (points of path) at once

- Choose action as accurate as possible

  e.g. use effective interaction potentials which take into account two, three and higher order correlation effects. More accurate actions help to reduce the number of time slices by a factor of 10 or more.

- How to calculate physical properties.

  There are different approaches for calculating expectation values of physical observables, such as the energy, momentum distribution, etc. They are called estimators. In each particular case convergence can be improved by choosing the proper estimator.
In statistical mechanics thermodynamic averages are calculated as

\[
\langle \hat{O} \rangle(\beta) = \text{Tr} \left[ \frac{\hat{O} \hat{\rho}(\beta)}{\text{Tr} \hat{\rho}(\beta)} \right] = \frac{\int dRdR' \langle R | \hat{O} | R' \rangle \langle R' | \hat{\rho}(\beta) | R \rangle}{\int dR \langle R | \hat{\rho}(\beta) | R \rangle}
\]

\[
\langle \hat{O} \rangle(\beta) = \int dR dR' O(R, R') p(R, R') \text{sign}[\rho(R, R'; \beta)]
\]

\(p(R,R')\) normalized probability density (recover same form like in classical case)

- For diagonal operators: \(O(R, R') = O(R) \delta(R - R')\)

probability density given by

\[
p(R; \beta) = \frac{1}{Z} |\rho(R, R; \beta)|
\]

With DM obtained from high-temperature decomposition:

\[
\rho(R, R'; \beta) = \int dR_1 dR_2 ... dR_{M-1} \rho(R, R_1; \Delta \beta) \rho(R_1, R_2; \Delta \beta) ... \rho(R_{M-2}, R_{M-1}; \Delta \beta) \rho(R_{M-1}, R'; \Delta \beta)
\]
Numerical realization of PIMC (neglecting exchange)

- Sampling of configurations with probability $p$: use Metropolis method
  Configuration space consists of positions and spin projections of all $N$ particles:

  Old configuration:
  $$s = (R, R_1, R_2, \ldots, R_{M-1}; \sigma_1, \ldots, \sigma_N)$$

  New configuration:
  $$s' = (R', R'_1, R'_2, \ldots, R'_{M-1}; \sigma'_1, \ldots, \sigma'_N)$$

  Particle spin projections

  Construct sequence of uncorrelated configurations (Markov chain) $[s_1, s_2, \ldots, s_L]$

  Generated states (configurations) should have the correct probability distribution given by:

  $$p(R, \beta) = \frac{1}{Z} \rho(R, R; \beta)$$

- Realization in thermodynamic equilibrium (Metropolis): use ratio of probabilities:

  $$p_s = \frac{1}{Z} \exp[-\sum_{i=1}^{M} S_i(R_i; \Delta \beta)], \quad \quad \quad T(s, s') = \frac{p_{s'}}{p_s} = \exp[-\sum_{i=1}^{M} (S_i(s'; \Delta \beta) - S_i(s; \Delta \beta)))]$$

  $$p_{s'} = \frac{1}{Z} \exp[-\sum_{i=1}^{M} S_i(R'_i; \Delta \beta)], \quad \quad \quad T(s', s) \quad : \text{transition probability used to construct Markov chain.}$$

- Final result for physical observables in PIMC: average over all configurations

  $$\langle O \rangle = \lim_{L \to \infty} \frac{1}{L} \sum_{i=1}^{L} \frac{O(s_{i+1})/T(s_i \to s_{i+1})}{1/L \sum_{i=1}^{L} 1/T(s_i \to s_{i+1})}, \quad \quad \quad L: \text{length of Markov chain.}$$

  Averages of all quantities of interest are computed in one simulation.
(1) Specify total number of "time slices" $M$. This affects the error of the high-temperature representation. (Try different $M$, check convergence with respect to $M$)

(2) Randomly choose positions of $N$ particles.

(3) Set maximum number $L$ of Monte Carlo steps. Initialize variables for thermodynamic averages and MC step counter (set to zero).

(4) Set a "menu" of different Monte Carlo moves in the Metropolis algorithm.

(5) Choose a particle $i$ at random among $N$ particles.

(6) Proceed with the sampling of the path coordinates depending on the chosen possibility from the "menu" of Monte Carlo moves, e.g.

(a) Whole particle displacement (like for classical particle).
(b) Multilevel (bisection) deformation of particle trajectory.
[c) Choose a new permutation for given particle, realize it with the bisection algorithm.]
[d) possible additional moves]

(7) Accept or reject the move using the acceptance probability. Change the system state if the move was accepted, otherwise stay in the old configuration.

(8) Accumulate thermodynamic averages.

(9) Increase MC step counter by one. If the maximum number is not reached proceed to (5).

(10) Else: finish simulations. Output of final estimators for thermodynamic averages.
How to sample paths.

- Metropolis Monte Carlo that moves a single coordinate of the path is too slow, --> move more time slices together (multilevel method).

- but: path deformation of $N$ quantum particles not independent due to quantum statistics (particles are either fermions or bosons)

- Path deformation should simultaneously realize the $N$-particle exchange properties (symmetry/antisymmetry of $N$-particle wave function or density operator)

- Therefore: consider first extension of PIMC to bosons/fermions

We will return to path sampling later
1. Properties of the system of N electrons and holes at a finite temperature \( T \) are determined by the density operator
\[
\hat{\rho} = \exp\left[-\frac{\hat{H}}{k_B T}\right]
\]

2. Due to the Fermi/Bose statistics the total density matrix should be (anti)symmetric under arbitrary exchange of identical particles (e.g. electrons, holes, e with same spin projection etc.). We have to replace
\[
\hat{\rho} \rightarrow \hat{\rho}^{Als}
\]
for fermions/bosons.

3. Construct \( \hat{\rho}^{Als} \) : as superposition of all \( N! \) permutations of \( N \) identical particles.

Example: two types \((e,h)\) of particles of with numbers \( N_e, N_h \)

\[
\rho^{Als}(R_e, R_h, R_e, R_h; \beta) = \frac{1}{N_e! N_h!} \sum_{P_e P_h} (-1)^{P_e} (-1)^{P_h} \rho(R_e, R_h, \hat{P}_e R_e, \hat{P}_h R_h; \beta)
\]

\( P \) – parity of permutation (number of equivalent pair transpositions)

- bosons: all terms have positive sign
- fermions: alternating sign
Illustration: 2 electrons and 2 holes (fermions)

\[
\rho^A(R_e, R_h, \hat{P}_e R_e, \hat{P}_h R_h; \beta) = \frac{1}{2! 2!} \sum_{P_e P_h} (-1)^{P_e} (-1)^{P_h} \rho(R_e, R_h, \hat{P}_e R_e, \hat{P}_h R_h; \beta)
\]

System of quantum particles

Classical system of interacting “polymers”

Number of possible permutations:

\[N_e! * N_h! = 4\]
Quantum exchange. PIMC for fermions/bosons (3)

Initial configuration (a):
- Particle 1 and 2 are in identity permutations;
- 3,4,5 form a permutation of length l=3 (cycle 4-3-5)

Final configuration (b):
- Particle 2 is in identity permutation;
- Particles 1 and 4 are exchanged;
- 1,3,4,5 form a new exchange cycle of length l=4 (cycle 4-1-3-5).

Figure 1.7: (a),(c) The Y-coordinates of five electrons as a function of the time-slice number m. Labels show particle indices. Thick grey and light grey lines show the paths of the particles “1” and “4” which are exchanged by sampling new paths at time-slices m = 17 – 33 (these time-slices are in the region between two dotted lines).
How to sample paths. Bisection algorithm.

- Metropolis Monte Carlo that moves a single coordinate of the path is too slow, --> move more time slices together (multilevel method).
- Key point: sample a path using mid-points $R_{\beta/2}$.
- Guiding rule to sample mid-points $R_{t/2}$:

$$P(R_{\beta/2}) = \frac{\langle R|e^{-\beta \hat{H} \beta/2}|R_{\beta/2}\rangle \langle R_{\beta/2}|e^{-\beta \hat{H} \beta/2}|R'\rangle}{\langle R|e^{-\beta \hat{H} \beta/2}|R'\rangle} \approx \frac{1}{2 \lambda_{\beta/2}^{d/2}} \exp \left[ -\frac{2\pi}{\lambda_{\beta/2}^{2}} (R_{\beta/2}^2 - R_0^2) \right]$$

Gaussian with

$$R_0 = \frac{R + R'}{2}, \quad \sigma^2 = \frac{\hbar^2 \beta}{2m}$$

Exact for ideal systems

- Construct entire path by recursion from this formula (bisection).

- Possible improved sampling:
  use optimized mean $R_0$ and variance $\sigma$ which account for local interaction strength (nearest neighbor interaction).

$$R_0 = \frac{R + R'}{2} + \sigma \frac{\partial U(R_0)}{\partial R},$$

$$\sigma^2 = \frac{\hbar^2 \beta}{2m} + \left( \frac{\hbar^2 \beta}{m} \right)^2 \Delta U(R_0)$$
Construction of new paths
Construction of new paths

- Select time slices.

![Diagram](image)

4 $\Delta \beta$
Construction of new paths

- Select time slices.

- Select permutation from possible ones (pairs, triplets, etc.), using

\[ p(R, \hat{PR}'; 4 \Delta \beta) \]

\[ 4 \Delta \beta \]
Construction of new paths

- Select time slices.
- Select permutation from possible ones (pairs, triplets, etc.), using
  \[ p(R, \hat{PR}'; 4\Delta \beta) \]
- Sample mid-points.
Construction of new paths

- Select time slices.

- Select permutation from possible ones (pairs, triplets, etc.), using
  \[ p(R, \hat{PR}'; 4\Delta \beta) \]

- Sample mid-points.

- Bisect again, up to lowest level.
Construction of new paths

- Select time slices.
- Select permutation from possible ones (pairs, triplets, etc.), using
  \[ p(R, \hat{PR}'; 4\Delta \beta) \]
- Sample mid-points.
- Bisect again, up to lowest level.
- Accept or reject entire move.
Advantages of the bisection method

- Detailed balance property is satisfied at each level.
- We do not waste time on moves for which paths come close and the potential energy strongly increases (for repulsive interaction). Such configurations are rejected already on early steps.
- Computer time is spent more efficiently because we consider mainly configurations where the acceptance rate is high.
- Sampling of particle permutations is easy to perform in the bisection method.
Indirect excitons in an electrostatic trap

Two coupled e-h layers

$\omega_e$ $\omega_h$

Exciton

Dipole moment in L=30 nm wide QW at field $E = 20 \text{kV/cm}$

$E = 20 \text{kV/cm}$

$d = 20.4 \text{ nm} \left(6.65 a_B^{ZnSe}\right)$

Stronger dipole interaction of excitons

GaAs/AlGaAS-quantum well

$e_r = 12.58$

$m_{el} = 0.067m_0$

$m_h = 0.34m_0$

$1a_B = 9.98 \text{nm}$

$1H_a = 11.5 \text{meV}$

ZnMgSe/ZnSe-quantum well

$e_r = 8.7$

$m_{el} = 0.15m_0$

$m_{hh} = 0.86m_0$

$m_{hh} = 0.37m_0$

$1a_B = 3.07 \text{nm}$

$1H_a = 53.9 \text{meV}$

We consider the system with equal number electron-hole pair (optically excited) $N = N_e = N_h$

$$\hat{H} = \hat{H}_e + \hat{H}_h + \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{e_i e_j}{\varepsilon |\mathbf{r}_i - \mathbf{r}_j|}$$

Single particle Hamiltonian

$$\hat{H}_a = \sum_{i=1}^{N_a} \left( -\frac{\hbar^2}{2m^*_a} \nabla^2_{\mathbf{r}_i} + \frac{m^*_a}{2} \omega^2_{a} r^2_1 \right)$$

The density is controlled by the trap frequency $m_e \omega^2_e = m_h \omega^2_h$

and characterized by coupling parameter

$$\lambda = \left(\frac{e^2}{\varepsilon \varepsilon_0}\right) / \hbar \omega_e$$

At low temperature and small d, electrons and holes form bound state: exciton (boson)
Quantum crystal of Excitons in an electrostatic trap

\[ \lambda = \frac{e^2}{\varepsilon l_0}, \quad l_0 = \sqrt{\frac{\hbar}{m_r \omega}} \]

Vary trap frequency and Coupling parameter by changing field strength

Structural transitions:
Classical exciton liquid → Exciton crystal → Exciton Bose fluid

PIMC simulations of Patrick Ludwig and Alexei Filinov
Quantum crystal of Excitons in an electrostatic trap

\[ \lambda = \frac{e^2}{\varepsilon l_0}, \quad l_0 = \sqrt{\frac{\hbar}{m_r \omega}} \]

Vary trap frequency and Coupling parameter by changing field strength

Structural transitions:
Classical exciton liquid
→ Exciton crystal
→ Exciton Bose fluid

PIMC simulations of Patrick Ludwig and Alexei Filinov
1. Spin statistics: Fully spin polarized electrons and holes (to enhance quantum statistical effects in small systems)
2. Classical system: only identity permutation
3. Ideal quantum gas at T=0: equal probability of all permutations

Using a threshold value \( P_{cr} = \frac{0.8}{N_x} \), we obtain the Bose condensate fraction according to \( \alpha_B = \frac{N_B}{N_x} \)

At low temperatures it reaches 80%.
Permutation probability. Influence of particle number and interaction.

**Coulomb coupling parameter**

\[ \lambda = \left( \frac{e^2}{\epsilon l_0} \right) \frac{\hbar}{\omega_e} \]

---

**a)** \( N_x = 300 \)

Permutation probability, \( \log P(L) \)

- \( \lambda = 30 \)
- \( \lambda = 92 \)
- \( \lambda = 165 \)

**b)** \( N_x = 100 \)

Permutation probability, \( \log P(L) \)

- \( \lambda = 30 \)
- \( \lambda = 40 \)
- \( \lambda = 92 \)
- \( \lambda = 165 \)

---

**c)** \( T = 26 \text{ mK} \)

Exciton number, \( N_x \)

- \( 300 \)
- \( 100 \)
- \( 30 \)
- \( 10 \)

Condensate fraction, \( N_0 / N \)

---

**Permutation length, \( L \)**

---

**Coupling, \( \lambda \)**
Superfluidity

- Loss of viscosity below critical temperature
  - discovered in liquid He by P.L. Kapitza 1938
  - L.D. Landau: two-fluid (normal+suprafluid) model

Andronikashvili experiment

Superfluid density (fraction) from Classical/quantum moment of inertia $I$

$$\frac{\rho_s}{\rho} = 1 - \frac{I_{\text{quant}}}{I_{\text{class}}}$$

First principle result for interacting bosons from path area $A$

$\rightarrow$ Quantum Monte Carlo simulations
  (D. Ceperley, 1995)

Moment of inertia computed in PIMC from area enclosed by path $A$
Path integral Monte Carlo results for strongly correlated excitons

\[ \rho_s / \rho = \frac{e^2 / \varepsilon l_0}{\hbar \omega} \]

\[ l_0 = \sqrt{\frac{\hbar}{m_r \omega}} \]

A. Filinov, M. Bonitz, P. Ludwig, and Yu. Lozovik, phys. stat. sol. (c) 3, 2457 (2006)

ZnSe 30nm quantum well, \( E=20 \text{kV/cm} \)
General aspects of PIMC

Alternative strategies

Limitations of the simulations

Scope of applications
Thermodynamic averages. Estimators.

**Quantities of interest:** Energy, pressure (equation of state), specific heat, fluctuations, condensate or superfluid fraction, pair distribution function.....

**In principle:** all quantities follow from density matrix or partition function \( Z \)

---

**Limitations**

1. We usually calculate only ratios of integrals, e.g., free energy and entropy require special techniques.

2. The variance of some estimators can be too high.

3. Many quantities are defined as dynamical quantities, but we are limited to only imaginary time (static quantities).

---

Example: thermodynamic estimator for the internal energy

\[
E = -\frac{\partial}{\partial \beta} \ln Z_F = -\frac{1}{Z_F} \frac{\partial Z_F}{\partial \beta}
\]

\[
E = E_{kin} + \left\langle \tau \sum_{m=1}^{M} V(R^{(m)}) \rightangle
\]

\[
E_{kin} = \frac{d(M+1)N}{2\beta} - \left\langle \sum_{m=1}^{M} \frac{(M+1)m_e(R^{(m+1)} - R^{(m)})^2}{2\hbar^2\beta^2} \rightangle
\]

\[
r^{(m)} = r^{(0)} + \sum_{\tau=1}^{m} \lambda_M \xi^{(\tau)}
\]

\[
E_{pot} = \frac{m_e\omega^2}{2M} \sum_{i=1}^{N} \sum_{m=1}^{M} (r_i^{(m)} - r_0)^2 + \frac{e^2}{\epsilon M} \sum_{i<j} \sum_{m=1}^{M} \frac{1}{(r_i^{(m)} - r_j^{(m)})^2}
\]

---

One of the forms of virial estimator
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.

\[
\rho^{SA}(R, R; \beta) = \frac{1}{N!} \sum_P (\pm 1)^P \rho(R, \hat{P} R; \beta)
\]

Bose systems: all permutations contribute with the same (positive) sign
Fermions: essential cancellation of positive and negative terms (corresponding to even and odd permutations), both are close in their absolute value.

Accurate calculation of this small difference is drastically hampered with the increase of quantum degeneracy (low T, high density).
Fermion sign problem. Concepts of fermionic PIMC (2)

\[ \rho^A(R, R; \beta) = \frac{1}{N!} \sum_P (-1)^P \rho(R, \hat{P} R; \beta) \]

- Fermions: essential cancellation of positive and negative terms (corresponding to even and odd permutations), both are close in their absolute value.

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

Used approaches to overcome Fermion problem in PIMC:

(a) Fixed-node (fixed-phase) approximation.

Idea: 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.

(b) Direct PIMC.

Idea: Do not sample individual permutations in the sum. Instead: use the full expression presented in a form of an $N \times N$ 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.


(c) Multilevel-blocking PIMC.

Idea: 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 lower temperature. Further use it in the sampling probabilities of path coordinates on the next level (corresponding to the density matrix at even lower temperature). Most of the sign fluctuations are already excluded at higher levels and sampling at low levels (lower temperatures) becomes more efficient.

Application of PIMC to quantum charged particles

General fields of use

- low temperature systems (relevance of quantum effects)
- Small dimensions (system size comparable to DeBroglie wavelength $\lambda$
- high density: 2-particle distance comparable to / smaller than $\lambda$

1. Single particle in complicated potential
   e.g. disorder effects --> effective solution of Schrödinger's equation
   (ground state, $T=0$) or finite temperature extension (density matrix)

2. Two-particle interaction
   improvement of pair potential at small distances (include quantum effects)

3. Finite number of particles in traps
   atoms, ions at ultralow temperature (Bose condensates etc.)
   electrons, holes in quantum dots

4. Macroscopic quantum systems
   electrons and ions in astrophysics: planet cores, dwarf stars,
   highly excited solids (many electrons, holes in nanostructures)
How to sample paths. Bisection algorithm.

Application of PIMC to quantum charged particles (1)

- low temperature systems (relevance of quantum effects)
- Small dimensions (system size comparable to DeBroglie wavelength $\lambda$
- high density: 2-particle distance comparable to / smaller than $\lambda$

1. Single particle or bound complexes in complicated potential (e.g. disorder effects)
   --> effective solution of Schrödinger's equation (ground state, $T=0$)
   or finite temperature extension (density matrix)

**Example:1** realistic semiconductor heterostructure (quantum well) with well fluctuations

**Example:2** electrons, holes, excitons in strong external E-field
Shift of energy bands in electric field:
Change of quantum probability distribution of electrons and holes

$$\Delta E(z) = e \cdot E_z \cdot z$$
Exact Quantum pair potentials

1. Exact pair potential from exact 2-particle density matrix (numer.)

\[ U_{\text{pair}}^{ab}(r) = -k_B T \ln \rho_{ab}(r, r) \]

2. Derive analytical potential (1 fit parameter)

**Result:**
Drastic improvement of previous potentials (Kelbg, Deutsch etc.)
\[ \rightarrow \text{applicable to strong coupling including bound states} \]

Yields exact thermodynamic properties (on 2-particle level)
We have presented an introduction to first principle path integral Monte Carlo simulations (PIMC) and applications.

Virtually exact method for thermodynamics of quantum systems at any interaction strength. Limited only by fermion sign problem (min temperature).

There are many technical and simulation details: they will be discussed in the lab course on Thursday by Alexei Filinov.

Proceedings: basics of PIMC simulation of trapped particles (brief).


It includes chapters on:
- Particle in cell simulations, by H. Ruhl
- Density functional theory, by G. Bertsch
- Quantum Kinetic equations, by M. Bonitz and D. Semkat
- Classical and Path integral Monte Carlo, by A. Filinov and M. Bonitz
- Quantum MD, by A. Filinov, V. Filinov, Yu. Lozovik and M. Bonitz

http://www.theo-physik.uni-kiel.de/~bonitz