

# Path integral molecular dynamics for Bose-Einstein and Fermi-Dirac statistics

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We propose a promising extension of the path integral molecular dynamics method to Bose-Einstein and Fermi-Dirac statistics. The partition function for the quantum statistics was re-written in a form amenable to the molecular dynamics method with the aid of an idea of pseudopotential for the permutation of particles. Our pseudopotential is a rigorous one describing the whole effect of Bose-Einstein and Fermi-Dirac statistics. For a model calculation, we chose a system consisting of three independent particles in a one-dimensional harmonic well. The calculated total energy was in excellent agreement with the analytical result even near the ground state.

## Introduction

Liquid helium and helium cluster have received much attention from low temperature physicists and chemists. Recent progresses in experimental techniques have made it possible to implant guest atoms and molecules in the quantum medium.<sup>1)</sup> These experiments have revealed that the quantum statistics gives great effects on microscopic processes in the quantum solutions. For example, a guest molecule shows a free-rotor behavior though the molecule is solvated in the helium-4 droplet. This may be attributed to the superfluidity at molecular level. The purpose of this paper is to develop a theoretical method for investigating the interesting phenomena.

Our work is also motivated by recently proposed approximate method for extracting dynamic correlation in the quantum many-body systems. This method is designated path integral centroid molecular dynamics (CMD).<sup>2)</sup> The CMD has been applied to various distinguishable particle systems including the normal phase of the liquid <sup>4</sup>He<sup>3)</sup> and yielded encouraging results. Recent studies have shown that proper definition of the centroid variables is possible even for Bose-Einstein and Fermi-Dirac statistics. Our methodology presented in this paper can provide a computational route of the CMD calculations for the quantum statistics.

## Methodology

Standard Quantum Monte Carlo exploits the fact that the partition function of a quantum mechanical system, which can be written in terms of an imaginary time path integral, is formally equivalent to the configuration integral of a system consisting of classical ring polymers.<sup>4,5)</sup> The indistinguishability of the particles due to Bose-Einstein and Fermi-Dirac statistics was described by allowing the polymers to hook up in any possible way. Equilibrium quantum statistical properties of the many-body systems can be obtained using suitably modified classical Monte Carlo simulation techniques.<sup>4-6)</sup> In this study, the effect of the indistinguishability for  $N$  identical particles is represented exactly by the following pseudopotential of the permutation,  $V_{ps}$ <sup>7)</sup>

$$V_{ps} = \begin{cases} -\frac{1}{\beta} \sum_{s=1}^M \ln \text{perm} \tilde{\mathbf{A}}(s, s+1) & \text{(for boson)} \\ -\frac{1}{\beta} \sum_{s=1}^M \ln |\det \tilde{\mathbf{A}}(s, s+1)| & \text{(for fermion)}. \end{cases}$$

Here,  $M$  represents total number of imaginary time slices and  $\beta$  inverse temperature. The  $\text{perm} \tilde{\mathbf{A}}(s, s+1)$  and  $\det \tilde{\mathbf{A}}(s, s+1)$  are permanent and determinant of  $N \times N$  matrix  $\tilde{\mathbf{A}}(s, s+1)$ , respectively. The matrix element  $\tilde{A}_{ij}(s, s+1)$  corresponds to free-particle propagator from the position  $\mathbf{r}_i^{(s)}$  to  $\mathbf{r}_j^{(s+1)}$  divided by that from  $\mathbf{r}_i^{(s)}$  to  $\mathbf{r}_i^{(s+1)}$  where  $s$  is an imaginary time slice. Using the pseudopotential, we define the weight function applicable to molecular dynamics. Furthermore, we introduce fictitious momentum to define a set of equation of motion for generating the bosonic or fermionic distribution dynamically. Detailed description of the equation of motion and the method of the integration are presented elsewhere.<sup>7)</sup>

## Results and discussion

We show some calculated results for the system consisting of three independent non-interacting particles in a one-dimensional harmonic well. The Hamiltonian of the system is  $H = \sum_{i=1}^N \frac{p_i^2}{2} + \frac{x_i^2}{2}$  where  $N = 3$  and we use the units by which  $m = \omega = \hbar = 1$  for computational simplicity. Calculations were carried out for three system temperatures  $T = 0.5, 1.0,$  and  $2.0$ . The systems obeying Bose-Einstein and Fermi-Dirac statistics were investigated. The results of the distinguishable particle systems are also presented for comparison. The calculated total energies are shown in Fig. 1.

For this system, the total energy is obtained algebraically.<sup>5)</sup> As shown in the figure, the calculated energies agree very well with the analytical results. Even near the ground state, the calculated results reproduce well the analytical values for all the statistics. Higher ground state energy for the fermions is ascribed to the Pauli principle. Here, the system is assumed to consist of spin polarized fermions. Overall temperature dependence for three statistics is also well described by our method.

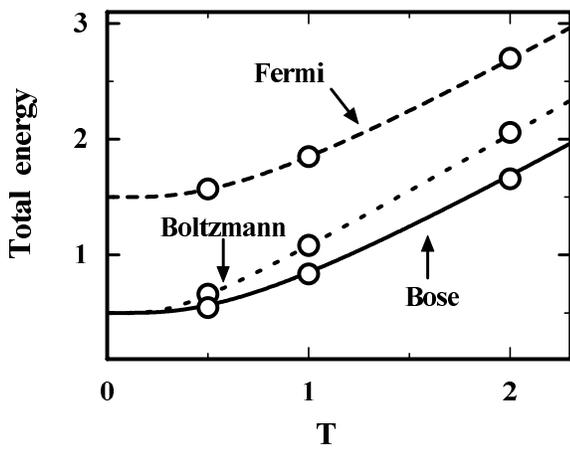


Fig. 1. Averaged total energy per particle as a function of  $T$ . Analytical results are represented by solid (Bose-Einstein), dashed (Fermi-Dirac), and dotted (Boltzmann) lines. Circles represent the results of the present path integral molecular dynamics calculations.

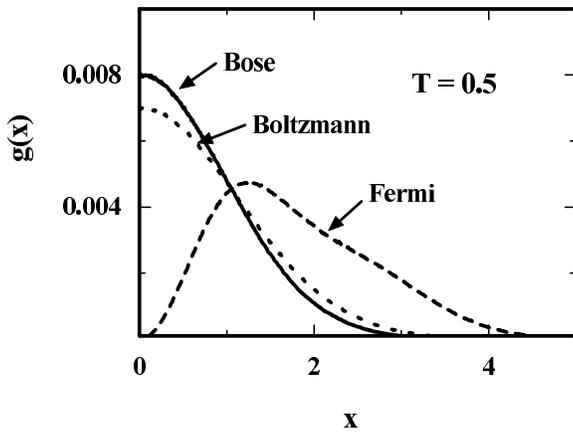


Fig. 2. Pair correlation functions at  $T = 0.5$ . Solid line is for the Bose oscillators, dashed for the Fermi oscillators, and dotted for the Boltzmann oscillators.

In Fig. 2, we show pair correlation function. This is defined by

$$g(x) = \left\langle \frac{1}{M} \frac{2}{N(N-1)} \sum_{s=1}^M \sum_{i=1}^{N-1} \sum_{j>i}^N |x_j^{(s)} - x_i^{(s)}| \right\rangle .$$

An enhanced amplitude of the bosonic correlation function compared with the Boltzmann correlation function is found around the origin. This is due to the attractive pseudopotential among the particles. With respect to the fermionic correlation function, we find a hole around the origin to satisfy Pauli exclusion principle. Here, we stress that there is no interparticle interactions in the Hamiltonian. The apparent difference among the pair correlation functions comes purely from the difference of the statistics.

### Concluding remarks

A path integral molecular dynamics method for the bosonic and fermionic systems has been developed based on the pseudopotential description of the permutation. A pilot calculation has been performed: three independent particles in a one-dimensional harmonic well. The calculated energies were in excellent agreement with the algebraic results for the both statistics, Bose-Einstein and Fermi-Dirac statistics having been successfully described by the pseudopotential of the permutation. One of the most important applications of our methodology is superfluid liquid helium. To perform the simulation with reasonable computational cost, we should improve computational algorithm of the pseudopotential. This will be presented in the near future.

### References

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