Path Integral Monte Carlo

a paper by Keola Wierschem

Abstract

Path Integral Monte Carlo is a powerful computational technique for describing the equilibrium states of quantum many-bodied systems. This technique applies Feynman's path integrals to the classic method of Monte Carlo, allowing the simple analysis of systems at low temperature, a realm in which quantum effects become important. This technique has been applied to the problems of helium in bulk, helium adsorbed on graphite, molecular hydrogen adsorbed on graphite, and also molecular hydrogen on alkaline-doped silver. The author is currently using PIMC methods developed by Marlon Pierce (helium on graphite) and Kwangsik Nho (molecular hydrogen on graphite) to investigate the properties of helium on a cylindrical graphite-like surface.

Introduction

Path Integral Monte Carlo is a computational method used to study equilibrium states of atoms and molecules at low temperatures. Of particular interest to physicists is the behavior of small atoms and molecules at low temperatures. These can exibit zero-point motion. Helium, in particular, is very light and interacts weakly, and becomes a superfluid at 2.17 K. Path Integral Monte Carlo has been used to study helium in bulk [1] and as a thin film on a graphite surface [2]. The computational results of these studies were in accordance with experimental observations of helium in bulk and adsorbed on graphite. The author is studying helium on a curved graphite-like surface using the PIMC method. Most of the computer code was already written for this, although it was modified for the new (curved) geometry of the substrate. In this paper I will describe how Monte Carlo works, then explain what Path Integrals are and why they are used, and finally discuss some past applications of Path Integral Monte Carlo.

Monte Carlo

Some readers may know of Monte Carlo as a numerical integration technique. In Monte Carlo integration, points within the range of integration are randomly drawn, the function being integrated is evaluated at these points, and the average of these values is the approximated integral. As the number of points randomly drawn approaches infinity, the approximated value of the integral approaches the exact value.

Monte Carlo in Statistical Mechanics

New particle positions are proposed. These new particle positions are chosen at random, in such a way to allow any particle to move to any point in configuration space within a finite number of moves. The probability of new positions are calculated in a systematic manner. A random number drawn to determine if move occurs, and the process is repeated until the system relaxes. When the system has relaxed, the energy of the system should remain approximately constant. It is important to note that Monte Carlo is an exact simulation technique. Error is due to approximations in the particle interactions, finite-size effects, and the use of pseudo-random numbers.

Sampling Technique

Start with any configuration of particles, and systematically propose new particle positions. These proposed moves are then accepted or rejected based on the energy difference in the two positions. This must satisfy detailed balance, $P(a)P(a->b) = P(b)P(b->a)$.
The probability of being at a and moving to b must be equal to the probability of being at b and moving to a. Also, the system must be able to reach all possible configurations in a finite number of iterations. An iteration occurs when a new position has been proposed and accepted/rejected for each particle in the system.

Accept or Reject?

Based on Hamiltonian of system, that is, kinetic and potential energy. Also changes with the temperature and the forces involved.

Path Integrals

Path integrals were developed by R. P. Feynman in the mid-20th century. They introduce an extra variable, "imaginary time", $\tau = \frac{1}{k_B T}$. Imaginary time is the inverse of temperature, and allows one to understand quantum interactions at low temperature in terms of the better understood classical interactions at higher temperature.

Path Integral Monte Carlo

Path integral Monte Carlo uses path integrals to reduce the temperature of interactions in standard Monte Carlo. The more paths used, the lower the temperature of the resultant system. Along each path, each atom is represented as a "bead". Thus, if I am using 10 paths to reduce the effective temperature by 10, each atom is represented as 10 beads, one at each point along the entire pathway. See figure 2. PIMC been used to study superfluidity, a quantum effect occuring at low temperatures. In fact, one of the first applications of the path integral concept was as an explanation for the superfluidity phenomenon.

Superfluidity

A superfluid has zero viscosity, or resistance to flow. Helium is the observed superfluid to date. Bulk helium becomes superfluid at about 2.17 K. PIMC can be used to search for new superfluids. Using computer simulation, one can study any number of systems with very little cost.

PIMC Applications

Ceperley and Gordillo applied the PIMC method to the case of molecular hydrogen, H_2, on the surface of silver doped with different alkali metals. What they found was evidence of hydrogen superfluidity, if the alkali metals were placed on the silver in such a way as to disrupt the formation of a comensurate solid. See figure 3.

My own work has been to investigate the phases of helium on a cylindrical, graphite-like surface. By this I mean the potential was modeled after graphite. Figures 4-7 show a system of 10 atoms after "thermalization" has occured. The radius of the cylindrical graphite-like surface is 5 Angstroms, and the z-axis employs periodic boundary conditions and is 5 Angstroms long. The atoms have aligned themselves along the z-axis, where they are relatively free to move about. Of course, with different dimensions and atom densities, the picture could easily change.

Summary

Monte Carlo is a powerful technique based on random sampling. Path integrals, when applied to MC, allow one to simulate the quantum effects of particles that occur at low temperatures.

References

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[3] M. C. Gordillo and D. M. Ceperley, Physical Review Letters 79, 3010 (1997).