Cluster expansion of the many-body Feynman path-integral for hard spheres

Anish Bhardwaj(1) and Efstratios Manousakis(1,2)

(1) Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32306-4350, USA
(2) Department of Physics, University of Athens, Panepistimioupolis, Zografos, 157 84 Athens, Greece
E-mail: manousakis@magnet.fsu.edu

Abstract. We apply a recently developed technique, which is based on a cluster expansion of the many-body Feynman path-integral, to the case of a dense system of distinguishable particles interacting with a hard-sphere potential. We find that our quantum hypernetted-chain approximation yields accurate results for the pair distribution function as compared to path-integral Monte Carlo results even in the high density regime.

1. Introduction

Monte Carlo simulations of classical systems are very successful[1] and have rendered the application of other techniques, such as the cluster expansion[2] and the hypernetted-chain (HNC) technique[3, 4, 5, 6, 7, 8, 9], obsolete. Quantum simulations have also been successful for systems of bosons and unfrustrated quantum spin-systems and in some selected classes of fermion problems which do not suffer by the “infamous-sign” problem. There are cases, however, such as frustrated quantum spin systems and fermion problems where quantum simulations cannot yield an exact answer and, therefore, development of other methods, can be useful in complementing the excellent effort and results provided by quantum simulations. In Ref. [10] we have developed a cluster expansion of the many-body path integral. We also extended the hypernetted-chain approach as a resummation technique for quantum systems. We demonstrated the accuracy of our quantum hypernetted-chain (QHNC) method by applying it to the system of a Lennard-Jones fluid and compared the results for distinguishable particles to those obtained by path-integral Monte Carlo (PIMC) simulation. In the present paper we review the technique and we apply it to the system of hard spheres described by the following Hamiltonian

\[ \hat{H} = -\frac{1}{2} \sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j} v(r_{ij}), \]

\[ v(r) = \begin{cases} \infty & r \leq 1, \\ 0 & r > 1. \end{cases} \]

We have used units, such that the distance is measured in units of the hard-core radius \( \sigma \) and the energy is measured in units of \( \epsilon = \hbar^2/(m\sigma^2) \), where \( m \) is the particle mass.
Recent Developments in Computer Simulation Studies in Condensed Matter Physics

IOP Conf. Series: Journal of Physics: Conf. Series 1252 (2019) 012002    doi:10.1088/1742-6596/1252/1/012002

Hard-spheres as a classical statistical mechanics problem involves no energy scale and only the particle density is a parameter which controls the behavior of the pair distribution function. When the kinetic energy operator is introduced in the Hamiltonian the partition function takes the form $Z = \text{tr} e^{-\theta H}$, where $\theta = e/(k_b T)$. Thus, the quantum mechanical version of the problem is controlled by two parameters, the temperature $\lambda = 1/\theta$ and the particle density. This paper is organized as follows. In Sec. 2 we discuss the main idea behind the method. In Sec. 3 we present our results for the pair distribution function for the hard-core system and in Sec. 4 we discuss the main conclusions drawn from this study.

2. The main idea of the method

Here we discuss the basic idea behind the cluster expansion method for the quantum mechanical many-body system. We begin from the partition function for distinguishable particles. Next, we slice the temperature (imaginary-time) direction into $M$ time-slices of extent $\delta \tau$, such that $M \delta \tau = h \beta$, and we introduce the Trotter approximation in splitting the kinetic and potential energy parts. We encounter the following two diagrammatic elements. First, there is the world-line $r_i^{(k)}$, $k = 0, 1, 2, \ldots, M - 1$, of each particle $i$ connecting each particle position at each time-slice labeled by $k$ ($\tau_k = k \delta \tau$) to the next time slice $k + 1$, which is represented by a solid line and it contributes a factor given by

$$L_i(kl) = \left( \frac{m}{2\pi \tau_{kl} h} \right)^{\frac{3}{2}} e^{-\frac{m}{\hbar^2 \tau_{kl}} \left( r_i^{(k)} - r_i^{(l)} \right)^2}, \quad \tau_{kl} = |k - l| \delta \tau. \quad (3)$$

Notice that while world-lines only connect successive time slices it is important to generalize the function $L$ as above as it will become clear below. Second, at any given time-slice $k$ any pair of particles $i, j$ interacts giving rise to a Boltzmann factor, which is split as follows $e^{-\frac{\pi}{\hbar^2} v(r_{ij}^{(k)})} \equiv 1 + h_{ij}^{(k)}$. Here $h$ is a short-range function (for hard-spheres $h_{ij}^{(k)}(r < \sigma) = -1$ and $h_{ij}^{(k)}(r > \sigma) = 0$) and this allows us to expand the product of such terms as

$$\prod_{l=0}^{M-1} \prod_{i<j} (1 + h_{ij}^{(l)}) = 1 + \sum_{l=0}^{M-1} \sum_{i<j} h_{ij}^{(l)} + \ldots \quad (4)$$

We obtain various contributions to the partition function which are represented by diagrams and constitute the cluster expansion. Each point in the diagram labeled by $i, k$ represents the position of particle $i$ at time-slice $k$ and it corresponds to an integration $\int d^3 r_i^{(k)}$ over these positions and it is represented by a solid circle.

If only the unit factor, in the above expression, is retained for all interacting pairs at all time-slices we obtain the partition function of the non-interacting system. The function $h_{ij}^{(k)}$ is a short-range function and, in the case of the cluster expansion of the classical fluid corrections, which arise from including similar such terms, give rise to the van der Waals modification of the equation of state for the non-ideal classical gas. We diagrammatically represent these $h_{ij}^{(k)}$ factors by a dashed-line connecting particle $i$ and $j$. A few examples of such diagrams, for the case of two-particles, are shown in Fig. 1. There are diagrams in which a solid circle is not-connected by a dashed-line. In this case the coordinates of the particle represented by the solid circle can be integrated out and eliminated from the diagram, thus, simplifying it, which leads to world lines $L$ connecting not just successive time slices. As a result the diagram of Fig. 1(a) becomes a constant, which is equal to the classical non-interacting partition function. Also the diagram of Fig. 1(b) becomes the diagram presented in Fig. 1(c).

We can also consider the cluster expansion of the pair-distribution function $g(r)$ and we obtain diagrams like those shown in Figs. 1(d),1(e),1(f). In such diagrams there are two open
circles representing the external points 1 and 2 over which there is no integration. Solid points represent internal points over which there is an integration. We can prove that only connected diagrams contribute to $g(r)$ (see Ref. [10]).

The simpler way to proceed is to consider a density expansion. The sum of those diagrams which contain only two particles, i.e., the external particles, corresponds to the zeroth order in density $\rho$. Three-body diagrams, such as in Fig. 1(f), are diagrams which are linear in $\rho$.

The next level, in which we sum up an infinite class of diagrams, is to generalize the classical hypernetted chain (HNC) approach to our case of the quantum many-body problem. This has been done in Ref. [10] and its accuracy was demonstrated by applying it to the Lennard-Jones fluid at liquid $^4$He densities.

3. Results for hard spheres

Figure 2. The $g(r)$ for three-dimensions as obtained in zeroth and first order is compared to the exact results obtained by PIMC for $\theta = 0.2$ (a) $\rho = 0.125\sigma^{-3}$ and (b) $\rho = 0.250\sigma^{-3}$.

First, we present the results of a systematic density expansion. (a) We sum all the diagrams which are of zeroth order in the density. It is the sum of all possible two-body diagrams with any number of $h$-lines connecting their world-lines. (b) We sum all diagrams up to first order in the density. These are all the diagrams which include two or three particles. The results for the pair-distribution function $g(r)$ for these two levels of approximation are compared with
Figure 3. The $g(r)$ as obtained by solving the QHNC equations is compared to the exact results obtained by PIMC for (a) $\rho = 0.125\sigma^{-3}$ and $\theta = 0.2$, 1 and (b) $\rho = 0.250\sigma^{-3}$ and $\theta = 0.2$.

the exact results obtained by our PIMC calculations in Fig. 2. In addition, we have added the results obtained for the same density for the classical hard-sphere system. Notice that there is a significant difference between the classical MC (of classical HNC) and the results of PIMC obtained for the quantum case. Our zeroth order correctly captures the initial rise of $g(r)$. The first order yields surprisingly reasonably good results for $\rho = 0.125\sigma^{-3}$.

In Fig. 3 we present the results obtained by the self-consistent solution to the QHNC equations given in Ref. [10] for $\theta = 0.2$ and 1 and for $\rho = 0.125\sigma^{-3}$ and $\rho = 0.25\sigma^{-3}$. Notice that the results are in very good agreement with the results of PIMC simulation.

4. Conclusions
The QHNC method presented in this paper is demonstrated to yield accurate results for the pair distribution function of a quantum system of hard-spheres in the regime where quantum fluctuations have a significant contribution. We also show that while the method is expected to yield accurate results in the low-density or high-temperature limits, the calculated results using the QHNC are reasonably accurate even in the regime of relatively low temperature and high density. Our future goal is to extend this method to study other problems, such as fermionic and frustrated quantum-spin systems.

5. Acknowledgments
This work was supported in part by the U.S. National High Magnetic Field Laboratory, which is funded by NSF DMR-1157490 and the State of Florida.

References
[1] Landau D P and Binder K 2009 Cambridge University Press 3rd Ed.
[2] Mayer J E and Mayer M G 1940, J. Wiley, Chapt. 13
[3] Hiroike K 1957 J. Phys. Soc. Jpn 12 326
[4] Hiroike K 1957 J. Phys. Soc. Jpn 12 864
[5] Morita T 1958 Prog. Theor. Phys. 20 920
[6] Morita T 1959 Prog. Theor. Phys. 21 361
[7] Morita T 1960 Prog. Theor. Phys. 23 175
[8] Morita T 1960 Prog. Theor. Phys. 23 829
[9] Morita T and Hiroike K 1960 Prog. Theor. Phys. 23 1003
[10] Bhardwaj A and Manousakis E 2018 https://arxiv.org/abs/1803.11118