Evaluation of the permutational structure of quantum gases at finite temperature

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Proposed is an alternative method for permutational sampling in quantum gases using the path integral formulation of statistical mechanics. It is shown that in principle we are able to use two operators which enable us to construct a Markov chain through a graph of the irreducible representation of the symmetric group. As an illustration of this method, a test calculation of four particles in a harmonic trap is performed.

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I. INTRODUCTION

Irrespective of their experimental realization, the theoretical existence of condensed phases of noninteracting media is indeed remarkable, and the mathematical structures with which they are imbued can lead to a variety of interesting observations. It is not difficult to show that a system of noninteracting indistinguishable particles with bosonic symmetry will undergo a second order phase transition if the spatial dimension is greater than two. For $d \leqslant 2$ it has been rigorously shown that a bosonic system will not undergo phase transition for $T > 0$ [1,2]. Theoretically, however, it was found that this is dependent on the form of the confining potential [3] confirmed by evidence of Bose-Einstein condensates (BECs) having recently been observed in quasi-two-dimensional traps [4].

The experimental observation of BECs in systems with both positive and negative *s*-wave scattering length [5–7], and the rapid expansion of novel trapping potentials in BECs such as optical and magnetic lattices [8–10] and quasi-one- and two-dimensional harmonic traps [4,11,12], has given a renewed impetus to the theoretical description of low temperature atomic gases.

Of the theoretical approaches, path integral Monte Carlo (PIMC) techniques stand as one of the most useful nonperturbative methods and is the only method able to produce exact properties of systems at finite temperature, via sampling of the thermal density matrix. One of the ubiquitous problems in all approaches to evaluating the partition function for bosonic systems is a transparent way of sampling the permutation space inherent in all problems involving indistinguishable particles. Previous approaches such as those in [13–15] advocate either the sampling of some cyclic subset of S_n, the symmetric group of order $n!$, typically up to C_4 or C_5, or approximate the interacting partition function structure to that of a noninteracting system, which is only strictly valid for systems which are weakly coupled.

In this paper we wish to make some remarks regarding the permutational structure of the partition function for bosonic particles. We present an algorithm which allows us to construct a Markov chain through permutation space for an explicit probability measure which maps between conjugacy classes of the symmetric group. It is partially inspired by the recent work regarding Markov processes on Young tableaux [16–19] and the connection between irreducible representations of the symmetric group and the analytic form of the bosonic partition function for noninteracting systems. Unlike a previous method [15], which is restricted to weakly interacting systems, we propose that this method samples the ring configuration structure at any temperature without any *a priori* knowledge of the noninteracting counterpart. This enables us to quantify ring configuration probabilities over a larger temperature scale and evaluate the relative importance of certain structures to the partition function.

The aims of this paper are (1) to give a rigorous formulation of the role of permutation cycles in the canonical ensemble partition function via a correspondence with irreducible representations of the symmetric group, and (2) to propose a practical scheme for computational implementation within PIMC. As an illustration we perform calculations on noninteracting bosons in a one-dimensional harmonic potential, the results of which are presented in Sec. IV, a system which has a very well understood theoretical basis.

This paper is organized as follows. In Sec. II we provide the theoretical outline for the path integral formulation of statistical mechanics in the canonical ensemble and derive a form of the partition function based upon the conjugacy classes of the symmetric group of n elements. In Sec. III we outline the basis for effective evaluation of the discrete permutational space by considering random growth of partitions of the symmetric group using one loop operators. We are able to stochastically sample the graph of partitions and show that this theoretically will enable us to determine loop configuration probabilities as a function of temperature.

II. PATH INTEGRAL STATISTICAL MECHANICS

The basis of the path integral formulation of statistical mechanics is the decomposition property of the many body density matrix $\rho(R,R';\beta)$, and the resulting classical configuration integral for calculating the properties of quantum systems [13,20]

$$\rho(R,R';\beta) = \int dR_1 \rho(R,R_1;\beta/2)\rho(R_1,R';\beta/2), \qquad (1)$$

where

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$$\rho(R,R';\beta) = \langle R|e^{-\beta\mathcal{H}}|R'\rangle \tag{2}$$

and $|R\rangle = |x^1, x^2, \ldots, x^N\rangle$ denotes the coordinate representation of the full N particle Hilbert space. The Hamiltonian operator $\mathcal{H}$ in general contains q-number quantities representing particle kinetic and potential terms and Eq. (2) represents that of an interacting many body quantum problem for distinguishable (Boltzmannian) particles. The partition function is given as the trace of the density matrix

$$Z = \mathrm{Tr}(\rho) = \int dR\langle R|e^{-\beta\mathcal{H}}|R\rangle = \mathrm{Tr}(e^{-\beta\mathcal{H}}), \tag{3}$$

the final line indicating that it is independent of the representation. The convolution property of the density matrix is exact and gives us a representation of the density matrix at temperature T as the convolution of two density matrices at temperature $2T$, effectively mapping low temperature problems to that of higher temperatures. Using the Trotter formula, $\exp(-\beta\mathcal{H}) = \exp(-\tau\mathcal{H})^M$, where $\tau = \beta/M$, we may perform this operation an arbitrary number of times to obtain the expression

$$Z = \prod_{i=0}^{M}\left[\int dR_i \rho(R_{i+1}, R_i; \beta/M)\right], \tag{4}$$

with the trace condition requiring that $R_{M+1} = R_0$. In the limit that M tends to infinity, $\tau \to 0$ and we obtain an expression for the partition function which is functionally dependent on the classical action. The path integral expression is

$$Z = \oint_{R(0)}^{R(\beta)=R(0)} \mathcal{D}R e^{-\beta S}, \tag{5}$$

where

$$\oint \mathcal{D}R = \lim_{M\to\infty} \prod_{i=0}^{M}\left[\int dR_i\right] \tag{6}$$

is the functional integration measure. The dynamical quantity of interest, the Euclidean action, is now rendered a c-number quantity on which the partition function is functionally dependent.

For the discrete form of the partition function given in Eq. (4), the procedure of taking the trace of a convolution of M density matrices is to represent particles as a set of M classically interacting beads interacting via a temperature dependent harmonic force, forming a closed "necklace." This is sometimes referred to as the polymer isomorphism [13]. It should be noted, however, that the interparticle potential only acts between beads of corresponding timeslices (M) [13,20]. As the number of time slices tends to infinity particles are represented as continuous closed loops. For an extensive review of path integrals in this context, the reader is referred to [13].

The formal evaluation of Eq. (5) for noninteracting particles gives the partition function to be the product of the single particle partition function, i.e.,

$$Z_N[\beta] = Z_1[\beta]^N. \tag{7}$$

When considering ensembles of indistinguishable particles one is required to permutate over particle labels. In the discretized form of the partition function we need only consider permutations over particles in the final time slice [13], i.e.,

$$\rho_B(R,R';\beta) = \frac{1}{N!}\sum_{\phi\in S_N} \rho(R,\phi R';\beta),$$

$$Z_B = \frac{1}{N!}\sum_{\phi\in S_N}\prod_{i=0}^{M-1}\left[\int dR_i \rho(R_{i+1},R_i;\beta/M)\right] \times \int dR_M \rho(R_0,\phi R_M,\beta/M). \tag{8}$$

For noninteracting systems of identical particles, the convolution property of the density matrix leads to a decomposition and the partition function becomes the product of density matrices at various temperatures. Consider a system of two particles with the Hamiltonian operator

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 \tag{9}$$

such that $[\mathcal{H}_1, \mathcal{H}_2] = 0$. In this case the Boltzmannian two-body density matrix will be $\rho(x_1x_2, x_1'x_2';\beta) = \rho(x_1, x_1';\beta)\rho(x_2, x_2';\beta)$. The partition function for the bosonic case will be

$$Z_B[\beta] = \frac{1}{2}\int dx_1 dx_2 \rho(x_1,x_1;\beta)\rho(x_2,x_2;\beta) + \frac{1}{2}\int dx_1 dx_2 \rho(x_1,x_2;\beta)\rho(x_2,x_1;\beta). \tag{10}$$

Using Eq. (1) for the second integral in Eq. (10), the partition function can be written exactly as

$$Z_B[\beta] = \frac{1}{2}[Z_1[\beta]^2 + Z_1[2\beta]], \tag{11}$$

Z_1 denoting the single particle partition function. As is frequently noted, the partition function of statistical mechanics is related to the propagator of quantum theory via rotation of time to the imaginary axis [21], and so the effect of permuting particle labels in the two particle case is to wind the trajectory twice around imaginary time

A general expression can be obtained for the N-body noninteracting partition function, involving the irreducible representations of the symmetric group. Consider the symmetric group, denoted by S_n, which is the group of all permutations on n objects, with the order being $|S_n| = n!$. The number of conjugacy classes of S_n is equal to the number-theoretic partition function $P(n)$ [22], with the property

$$\bigcup_{i=1}^{P(n)} \phi^i = S_n. \tag{12}$$

Here ϕ^i is the ith conjugacy class. The conjugacy classes can be graphically represented via the standard Young tableaux, however, for this case it is instructive to consider diagrams as shown in Fig. 1. This originates from the representation of particles in path integral statistical mechanics as

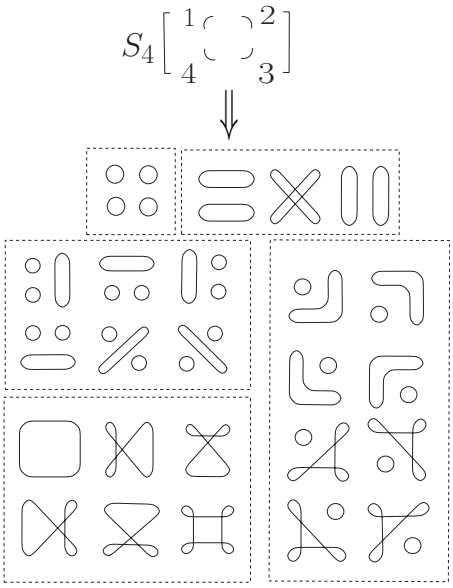

FIG. 1. Representation of the conjugacy classes of S_4.

kinetic strings. The action of elements of S_n on these strings is to attach each string starting position ($\tau=0$) with all possible final positions and integrate, giving the partition function. It should be noted that this is exactly true for the interacting as well as the noninteracting case.

Consider S_4 which contains a total of five partitions and 24 elements, which is shown in Fig. 1. From this it can be seen that elements of a particular conjugacy class are topologically equivalent. We can identify Young tableaux and partitions of n with the weakly decreasing sequence

$$\bar{\phi}^i = \{\bar{\lambda}_1^i, \bar{\lambda}_2^i, \ldots, \bar{\lambda}_\rho^i\}, \tag{13}$$

each element having the property that $\bar{\lambda}_1^i \geq \bar{\lambda}_2^i \geq \cdots \geq \bar{\lambda}_\rho^i$, or as the strongly decreasing sequence

$$\phi^i = \{(\lambda_1^i)^{k_{i,1}}, (\lambda_2^i)^{k_{i,2}}, \ldots, (\lambda_\gamma^i)^{k_{i,\gamma}}\}, \tag{14}$$

where $\bar{\lambda}_1^i > \bar{\lambda}_2^i > \cdots > \bar{\lambda}_\rho^i$. Here $k_{i,j}$ will be denoted as the multiplicity of a particular loop size. The dimension of each conjugacy class is equal to the number of Young tableaux with shape ϕ^i which is given by

$$\dim(\phi^i) = \frac{n!}{\prod_{j=1}^{\gamma} ((\lambda_j^i)^{k_{i,j}} k_{i,j}!)}. \tag{15}$$

For the purpose of this paper we need to identify two numbers $|\bar{\phi}^i| = \rho$, the number of elements in a partition, which is equal to the number of rows on the equivalent Young tableaux and $|\phi^i| = \gamma$, the number of distinct elements. For example, if we denote Φ as the set of all Young tableaux with n boxes, for the case of S_4 we have the conjugacy classes represented by the partitions

$$\begin{aligned}\Phi &= \{\{1,1,1,1\},\{2,1,1\},\{2,2\},\{3,1\},\{4\}\} \\ &= \{\{1^4\},\{2,1^2\},\{2^2\},\{3,1\},\{4\}\} \\ &= \{\phi^1, \phi^2, \phi^3, \phi^4, \phi^5\},\end{aligned} \tag{16}$$

with the dimension of each conjugacy class given as

$$\dim(\Phi) = \left\{\frac{24}{1^4 \cdot 4!}, \frac{24}{2.1^2 \cdot 2!}, \frac{24}{2^2 \cdot 2}, \frac{24}{3.1}, \frac{24}{4}\right\} = \{1,6,3,8,6\}. \tag{17}$$

With this notation, we are able to write down a general expression for the partition function of a noninteracting bosonic system of n particles, which is

$$Z_B[\beta] = \frac{1}{N!} \sum_{i=1}^{P(n)} \left(\dim(\phi^i) \prod_{j=1}^{|\phi^i|} Z_1[\lambda_j^i \beta]^{k_{i,j}} \right), \tag{18}$$

where the superscript $k_{i,j}$ denotes raising the power of the partition function to the multiplicity of this particular loop with cycle size λ_j^i. To obtain an understanding of Eq. (18), let us again consider the example of S_4 for which $P(4)=5$. Written out fully, the partition function takes the form

$$\begin{aligned}24 \times Z_B &= \prod_{j=1}^{|\phi^1|} Z_1[\lambda_j^1 \beta]^{k_{1,j}} + 6 \prod_{j=1}^{|\phi^2|} Z_1[\lambda_j^2 \beta]^{k_{2,j}} + 3 \prod_{j=1}^{|\phi^3|} Z_1[\lambda_j^3 \beta]^{k_{3,j}} \\ &\quad + 8 \prod_{j=1}^{|\phi^4|} Z_1[\lambda_j^4 \beta]^{k_{4,j}} + 6 \prod_{j=1}^{|\phi^5|} Z_1[\lambda_j^5 \beta]^{k_{5,j}} \\ &= Z_1[\beta]^4 + 6 Z_1[2\beta] Z_1[\beta]^2 + 3 Z_1[2\beta]^2 \\ &\quad + 8 Z_1[3\beta] Z_1[\beta] + 6 Z_1[4\beta].\end{aligned} \tag{19}$$

This is the exact form of the bosonic partition function for four noninteracting particles in an arbitrary external potential. The probability of randomly choosing a particular partition $\phi^i \in \Phi$ as a function of temperature is given by

$$\mu(\phi_i \in \Phi) = \frac{1}{Z_B} \dim(\phi^i) \prod_{j=1}^{|\phi_i|} Z_1[\lambda_i^j \beta]^{k_{i,j}}. \tag{20}$$

An analysis of this structure can show us the relative weight of partition structures at various temperatures. A graph of the contributions of the partitions of four particles to the partition function for noninteracting particles in a one-dimensional (1D) harmonic trap is shown in Fig. 2.

In this figure, the contributions from various elements of the permutation group are clearly evident, showing that at high temperatures the identity dominates, leading to the usual classical statistics [13,20]. Also in the $T \to 0$ limit, the partition function reduces to

$$Z_B[\beta \to \infty] = \frac{1}{N!} \sum_{i=1}^{P(n)} \dim(\phi^i), \tag{21}$$

which is exact for all noninteracting bosonic systems. For systems in which the particles interact, the evaluation of partition function elements will generally not be decomposable as a product of single particle functions [15], but the loop structure based upon the conjugacy classes of S_n will still be

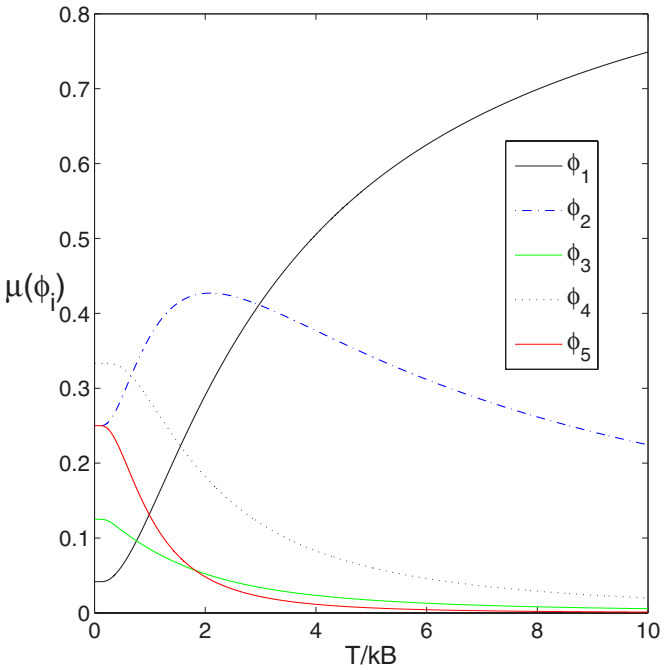

FIG. 2. (Color online) Loop structure of the four particle partition function in a 1D harmonic potential. The x axis is the temperature and the y axis the weight of the ith conjugacy class.

present. However, the range of problems for which Eq. (8) is exactly solvable for interacting systems is severely limited.

III. PIMC AND PERMUTATIONAL SAMPLING

The PIMC technique at present is the only method which renders Eq. (8) amenable to numerical solution. However, the method by which the permutational structure is accounted for either is based upon including only a subset of cyclic exchanges, usually up to C_4 or C_5, or the approximation of the exact permutational structure with that of a noninteracting system. The first method works very well in predicting properties such as the superfluid transition temperature of helium [13,23], but is equivalent to the treatment of parastatistics in bosonic systems first outlined by Green [24,25], and does not include the full permutational structure of the system. The second method works only for weakly interacting systems around the superfluid transition point as implemented in [15] via knowledge of the noninteracting partition function counterpart and is unable to give describe systems where the interactions are strong. The strong interaction regime is important especially for the case of repulsive interactions. It is specifically this regime in which the PIMC method is superior as perturbation theory becomes divergent.

In recent years mathematical methods have been developed regarding the random growth of partitions of the symmetric group, the probability measure known as the Plancherel measure and random matrices [16,19,25]. One would like to ask if this abstract mathematical method could help in the very physical application of predicting the permutational structure of BECs and superfluids at arbitrary temperatures. If we denote Φ as the set of all Young tableaux with n boxes, the probability of randomly choosing a particular partition $\phi^i \in \Phi$ as a function of temperature is given by

$$\mu(\phi_i \in \Phi) = \frac{1}{Z_B} \dim(\phi^i) Z[\phi_i;\beta] \tag{22}$$

with Z_B equal to the total interacting bosonic partition function. This is presumably the probability used in [15] to construct partitions, which was then applied to the case of a weakly interacting bose gas, however, the way they did this was not explicitly stated.

In the simplest implementation of a stochastic sampling method, one would randomly select a partition and select this with the probability given above. However, as derived by Ramanajan and Hardy, for large n the number of partitions is given by [26]

$$P(n) \simeq \frac{1}{4\sqrt{3}n} e^{\pi\sqrt{2n/3}}. \tag{23}$$

which becomes prohibitively inefficient for large n, as the rejection rate for transitions between uncorrelated partitions would be large.

We propose a set of operators which enable us to construct a Markov chain through the conjugacy classes of S_N. A similar formalism can be found in Borodin and Olshanski [17,18] in constructing partitions, identifying an operation which maps between partitions. Again consider a partition as the weakly decreasing sequence

$$\overline{\phi^i} = \{\overline{\lambda}^i_1, \overline{\lambda}^i_2, \ldots, \overline{\lambda}^i_j, \ldots, \overline{\lambda}^i_{\rho-1}, \overline{\lambda}^i_\rho\} \tag{24}$$

but with the restriction that at least one element, namely $\overline{\lambda}^i_\rho$, has the value of 1. Consider two operators a_j and $\bar{a}_j$, such that

$$a_j \phi^i = \{\lambda^i_1, \ldots, (\lambda^i_j + 1), \ldots, \lambda^i_{\rho-1}\} = \phi^k,$$

$$\bar{a}_j \phi^i = \{\lambda^i_1, \ldots, (\lambda^i_j - 1), \ldots, \lambda^i_\rho, \lambda^i_{\rho+1}\} = \phi^m, \tag{25}$$

such that

$$|a_j \bar{\phi}_i| = |\bar{\phi}_i| - 1,$$

$$|\bar{a}_j \bar{\phi}_i| = |\bar{\phi}_i| + 1. \tag{26}$$

These operators create and destroy C_1 subgroups of the conjugacy classes, in the process creating a new partition which is also a conjugacy class of the relevant permutation group. The action of these operators is to effectively move up and down a graph with $P(n)$ vertices of the partitions of S_N, leaving the sum of the elements of partitions invariant (cf. Fig. 3).

If we denote partitions which are related via a single application of a_j or $\bar{a}_j$ as neighboring partitions, we can construct a probability measure over neighboring partitions to give a formula for the transition probability under a_j and $\bar{a}_j$ as

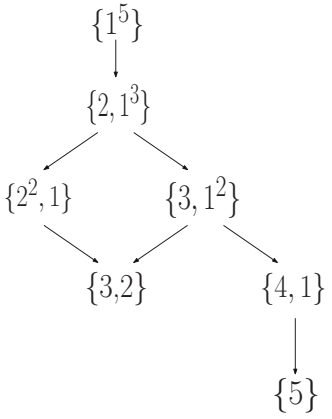

FIG. 3. Neighboring partitions of S_5 under the action of a and $\bar{a}$.

$$p^{\downarrow}(\phi_i;a_j\phi_i)=\frac{\dim(a_j\phi_i)}{\sum_j \dim(a_j\phi_i)},$$

$$p^{\uparrow}(\phi_i;\bar{a}_j\phi_i)=\frac{\dim(\bar{a}_j\phi_i)}{\sum_j \dim(\bar{a}_j\phi_i)}. \tag{27}$$

One can easily see that these transition probabilities satisfy the criterion that the sum of probabilities over neighbors is equal to one. In the construction of a Markov chain through permutation space, one could suppose that these are the correct transition probabilities to be used. Ergodicity, in the sense that the correct weight of each partition will be reproduced, is not assured via these relations. It is not, however, difficult to prove that all partitions are accessible under this scheme. If we consider the partition denoting the identity of S_N as $\{1\}_N$, then we may construct any other partition using a repeated application of a_j, that is

$$\{\lambda_1,\lambda_2,\ldots,\lambda_\rho\}=\prod_{i=1}^{\rho} a_i^{\lambda_i}\{1\}_N. \tag{28}$$

Since we are able to perform the reverse of this operation, that is reach the identity from any partition, via the use of $\bar{a}_j$, all partitions are connected. Once a partition is chosen then it can be accepted or rejected via the Metropolis scheme [27]. One hindrance to the successful application of these transition probabilities is that there does not exist any formula for the sum over neighbors which would be relatively easy to implement on a computer within a Monte Carlo code, especially for systems containing a large number of particles.

An alternative option which is relatively easy to implement would be to give all neighbors the same weight. Then one may choose a particular element of a partition to act upon with the probabilities

$$p^{\downarrow}(\phi_i;a_j\phi_i)=\frac{k_j}{|\bar{\phi}_i|-1}, \tag{29}$$

$$p^{\uparrow}(\phi_i;\bar{a}_j\phi_i)=\frac{k_j}{|\bar{\phi}_i|-k_{i,\gamma}}. \tag{30}$$

The action of $\bar{a}_j$ on a partition element is to give $\bar{a}(\lambda)\rightarrow(\lambda-1,1)$ and as such the normalization is the number of elements in a partition which are not equal to one. The action of a_j on a partition element is to give $a(\lambda,1)\rightarrow(\lambda+1)$ such that at least one element must have a value of one, and as such the normalization is the number of elements in a partition less one.

It was essentially this use of a_j exclusively by Boninsegni in [14] to construct permutation cycles for the superfluid phase of ^{4}He, containing 64 atoms. However, in this work permutation cycles were constructed at each sampling move from the identity. Again, from Eq. (28) we can see that each permutation cycle will be accessible via this scheme, however, it is not guaranteed that the correct weights will be reproduced.

IV. COMPUTATION AND DISCUSSION OF RESULTS

As a test of the proposed scheme with the analytic results given in Fig. 2, we performed a path integral Monte Carlo calculation on four bosons in a 1D harmonic trap. We used essentially the method as outlined in [13], in the primitive approximation [28].

The Trotter number was chosen such that the single particle energy was comparable to the analytic expression $\langle E\rangle=\frac{1}{2}\coth(\frac{1}{2}\beta)$, however, small enough that chosen permutations were accepted.

We implemented two schemes for permutation sampling. In the first, the results of which are summarized in Fig. 4, particle labels were randomly shuffled at each move and were accepted or rejected according to the Metropolis scheme. This was used primarily as a test for the validation of the code. In the second scheme we constructed a random walk through permutation space based upon the transition probabilities given in Eqs. (29) and (30) between partitions. At each move a partition list is created and an up or down move (a_j or $\bar{a}_j$) proposed with equal probability. In the case that a partition is at the end of a path (cf. Fig. 3), then the algorithm forces a move to the next connected vertex. In the case of a_j, once a partition element is chosen, then the nearest single loop structure is found such that the acceptance probability in the following Metropolis sampling move is maximized. The results of this method are shown in Fig. 5.

As can be seen, randomly shuffling particle labels reproduces the analytic decomposition of the partition function very well. We would, however, expect this method to become diminishingly inefficient as the particle number increased, and as the confining potential becomes significantly weaker, where the thermal wavelength of the particles will no longer be comparable to the mean particle separation, and thus would not be a viable option for a general PIMC code. Further the results of our method show that even though every partition is accessible via this algorithm, this does not guarantee that the method will reproduce the analytical result of Eq. (20).

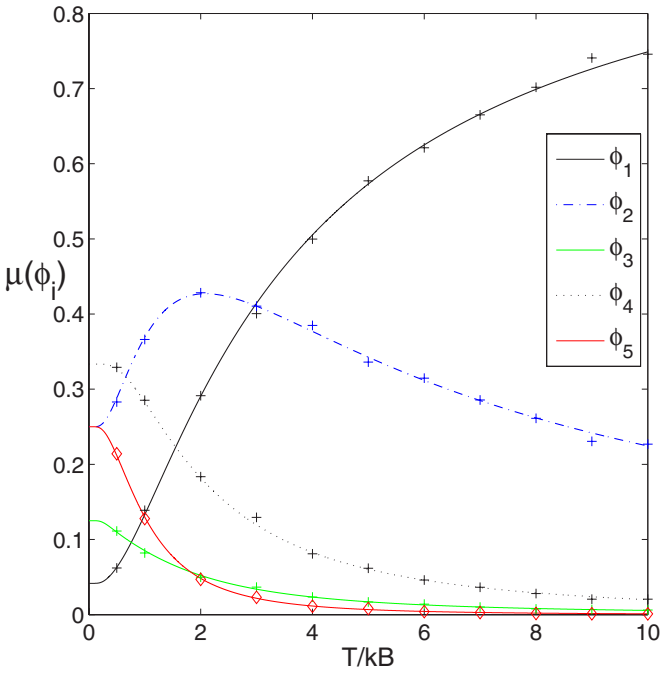

FIG. 4. (Color online) Partition structure of four bosons in a 1D harmonic trap from PIMC calculations, with partitions created via a random shuffling of particle labels. The solid line is the exact answer as given by Eq. (20).

An interesting feature of the results of the two methods of permutational sampling investigated is that, while they did not coincide with regard to the predicted permutation cycle structure, the resultant energy of the two methods was nearly identical (cf. Fig. 6).

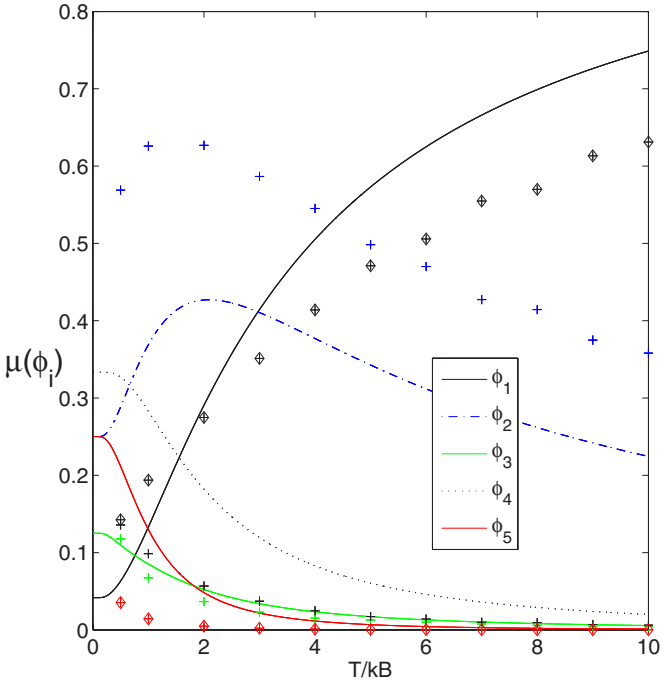

FIG. 5. (Color online). Partition structure of four bosons in a 1D harmonic trap with partitions created by the method. The solid line is the exact answer as given by Eq. (20).

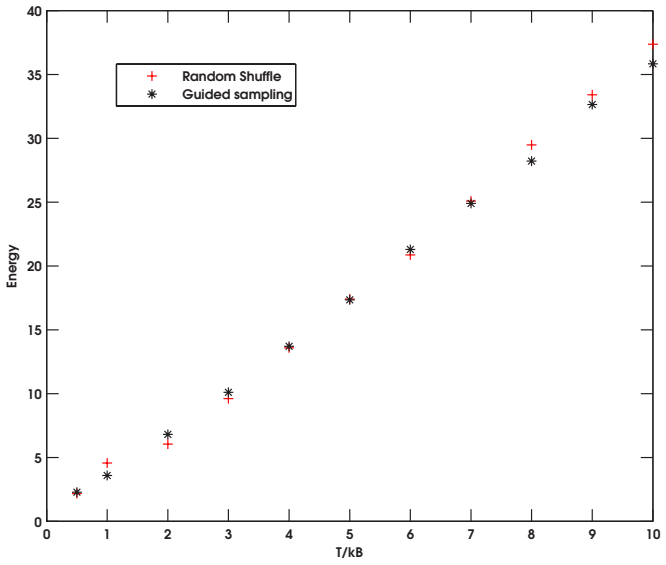

FIG. 6. (Color online) Energy as a function of temperature for four-particles bosonic particles using two different methods for sampling permutation space. The statistical errors in these calculations are beyond the resolution of this graph.

Although the method proposed was unable to reproduce the exact analytic form of Eq. (20) for this relatively basic model, we would expect that as the number of particles is increased that this would become more accurate. As the number of paths between vertices of the partition graph is increased, a walk on this graph will not be required to pass through a disproportionate number of low weight vertices. Our results show that the weight of the larger cycle lengths is underestimated, which is reflected by the fact that they lie on the end points of the graph of S_4. The larger cycle lengths contribute to quantities such as the mean winding number which derived from the mean squared winding number [23]. This method does have the advantage over other methods in that the *only* approximation is the form of the transition probabilities. After a period of equilibration, where the cycle structure is constructed from the identity, we will be able to sample the local permutational structure by using a_j and $\bar{a}_j$ without any *a priori* knowledge of cyclic structure of the partition function.

As mentioned earlier, the number of conjugacy classes of S_n has the asymptotic form

$$P(n) \simeq \frac{1}{4\sqrt{3}n} e^{\pi\sqrt{2n/3}}, \tag{31}$$

which would provide the associated computational sampling frequency as a function of particle number. However, the overhead required for the construction of partitions is minimal, with only knowledge of the current permutational structure and the proposed structure required, and thus memory requirements kept to a minimum. Further it is not necessary that the entire graph of partitions be sampled as many configurations will have only minor contributions, these depending on the temperature. After an initial period of equilibration, the process will sample the local neighborhood of the

highest weight permutations, those which will contribute the greatest to observables. Although the intrinsic $n!$ scaling involved in the sampling of permutation space has largely been overcome, it has been replaced by algorithms scaling exponentially [13–15], which is still problematic for large n. A recent proposal for a size independent algorithm has been reported by Boninsegni *et al.* in [29] which also looks promising for investigations into large systems and calculating off-diagonal elements of the density matrix.

V. CONCLUSION

To summarize, we suggest the use of one loop operators acting upon partitions for the construction of a Markov chain through permutation space. We have derived a form of the partition function for bosonic systems in the canonical ensemble based upon the irreducible representations of the symmetric group of n objects. It was shown that the partition function can be decomposed into a sum over the conjugacy classes of S_n which defines a probability measure over Young tableaux which is a function of temperature.

There have been various proposals for a more transparent method of sampling permutation space in the recent literature both for bosonic and fermionic systems [14,15,29–31], which appear to be successful in predicting properties of interacting quantum systems. However, there still does not exist an unambiguous method for the sampling of permutation space at the same level of rigor as for calculating expectation values of continuous probability measures. One may expect that a multilevel Metropolis scheme could be developed whereby the partition structure at finite temperature is reproduced exactly, giving a more accurate sampling of the partition function. Any scheme that purports to full sampling of the permutational structure of atomic gases within a path integral Monte Carlo should be able to reproduce the analytic form for the noninteracting case. A more rigorous formulation for the construction of discrete probability measures amenable to Monte Carlo methods may lead to some very interesting new observations.

An interesting mathematical question also arises which we wish not to explicitly address here, but may be a useful connection between the theory of indistinguishable many-body systems and a large body of work in probability theory and the random growth of Young tableaux. Is one able to construct a Markov chain via the use of a_j and $\bar{a}_j$ in the canonical ensemble that in the infinite time limit will give probabilities distributed according to Eq. (20)? Further, what is the limit shape of Young tableaux in the $N\to\infty$ limit as a function of temperature [16,19]? As $T\to\infty$ we expect this to be $x\theta(x+\frac{1}{2})$, where θ is the Heaviside step function, as the identity will become dominate in this limit. In the $T\to 0$ limit, where the partition function reduces to Eq. (21), the limit shape in the grand canonical ensemble has been established and as such one would expect a continuous transformation between these limit shapes, the mapping being dependant on temperature. This will be related to finding eigenvalues of random matrices as a function of temperature. We hope to investigate this further in a future paper.

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[28] This is $e^{A+B}=e^{A}e^{B}$. There are more accurate forms available based upon the proper expansion in τ, however, we wish only here to look at the permutation structure which should be relatively independent of this.

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