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Development, justification, and use of a projection operator in path integral calculations in continuous space

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A projection operator, similar to one previously used by us for problems with a finite set of basis functions, is suggested for use with continuous basis sets. This projection operator requires knowledge of the nodes of the density matrix at all temperatures. We show that a class of nodes, determined from the noninteracting density matrix and present at high temperatures in the interacting system are preserved to first order in the interaction at low temperatures. While we cannot show that the nodes are present at intermediate temperatures, we suspect they do exist and, as a test of this conjecture, we perform a calculation of two electrons confined in a harmonic well, using the projection operator. We find that accurate results are obtained at a range of temperatures, suggesting that our conjecture is indeed correct. We find that the error limits determined using the projection operator are 1–2 times smaller than those obtained with straightforward Monte Carlo integration (corresponding to a reduction in time of 1–4 in obtaining a desired level of accuracy).

I. INTRODUCTION

Feynman's path integral formulation of quantum mechanics has been useful in studying a variety of condensed phase quantum systems.[1,2] It has the advantage of automatically including correlation, of allowing the use of a complete set of states, and allowing studies at nonzero temperatures. Until recently, however, the application of this technique to many-fermion systems defined on a continuous basis set has been limited by the large statistical errors generated by straightforward Monte Carlo techniques (the infamous "sign" problem). We have developed an approximate implementation of the path integral technique[3] which has been shown to give accurate results in a variety of systems. In an effort to understand the nature of the approximation's success, we recently studied the 2D Hubbard model,[4] using a new projection operator technique. There, we showed that, if the nodes of the density matrix are known at all temperatures, the variance can be reduced in an exact calculation. In that paper, we demonstrated this for noninteracting particles on the 2D lattice, where we know the precise location of the nodes. In addition, we used the nodes of the noninteracting system in an interacting system and showed that accurate results could be obtained even though the nodes were not exact. Our justification in that paper was that the nodes of the noninteracting system (which are the same as the interacting system at high temperature) were a good approximation to the interacting system. In this paper, we consider the first order perturbation correction to the fermion density matrix defined in continuous space and show that a class of the nodes of the free particle density matrix, while nonzero in the interacting case, make negligible contributions to the density matrix at both high and low temperatures. For intermediate temperatures, we suggest conditions under which the density matrix will be negligible. As a test of this projection operator's ability to go beyond just first order in the interaction and to investigate our expectation that the nodes

are preserved at intermediate temperatures, we study a simple model system, two electrons confined in a harmonic well. We find that using this projection technique leads to smaller statistical errors by a factors ranging from 1–2 (or, alternatively, reducing the time required to obtain a given set of error limits by a factor of 1–4).

II. REVIEW OF PREVIOUS FORMULATION

In this section, we describe how knowledge of the nodes of the density matrix can be used to reduce the variance in a path integral calculation. Consider the following integral:

$$\rho(\mathbf{r}^N, \mathbf{q}^N, 2\beta) = \int d\mathbf{z}^N \rho(\mathbf{r}^N, \mathbf{z}^N, \beta)\rho(\mathbf{z}^N, \mathbf{q}^N, \beta), \qquad (2.1)$$

where ρ is the Fermi density matrix for N quantum particles and assume that $\rho(\mathbf{r}^N, \mathbf{q}^N, 2\beta) = 0$. Imagine attempting to evaluate this integral via Monte Carlo by setting

$$\rho'(\mathbf{r}^N, \mathbf{q}^N, 2\beta) = \int d\mathbf{z}^N |\rho(\mathbf{r}^N, \mathbf{z}^N, \beta)\rho(\mathbf{z}^N, \mathbf{q}^N, \beta)| \qquad (2.2a)$$

and using

$$\rho(\mathbf{r}^N, \mathbf{q}^N, 2\beta)/\rho'$$
$$= [\int d\mathbf{z}^N |\rho(\mathbf{r}^N, \mathbf{z}^N, \beta)\rho(\mathbf{z}^N, \mathbf{q}^N, \beta)| \rho(\mathbf{r}^N, \mathbf{z}^N, \beta)$$
$$\times \rho(\mathbf{z}^N, \mathbf{q}^N, \beta)/|\rho(\mathbf{r}^N, \mathbf{z}^N, \beta)\rho(\mathbf{z}^N, \mathbf{q}^N, \beta)|]/$$

$$\int d\mathbf{z}^N |\rho(\mathbf{r}^N, \mathbf{z}^N, \beta)\rho(\mathbf{z}^N, \mathbf{q}^N, \beta)|$$

$$\equiv \langle \rho(\mathbf{r}^N, \mathbf{z}^N, \beta)\rho(\mathbf{z}^N, \mathbf{q}^N, \beta)/|\rho(\mathbf{r}^N, \mathbf{z}^N, \beta)\rho(\mathbf{z}^N, \mathbf{q}^N, \beta)| \rangle_{|\rho|}, \qquad (2.2b)$$

where the $\mathbf{z}^N$ are sampled from the absolute value of the product of the Fermi weights. The quantity that is being averaged is simply a sum of an equal number of positive and negative ones, while the variance is determined from the sum of positive ones. If we were to use $\rho(\mathbf{r}^N, \mathbf{q}^N, 2\beta)$ in a further

calculation, it would add nothing to the average, but would add to the variance. Thus the variance of a calculation that used $\rho(\mathbf{r}^N,\mathbf{q}^N,2\beta)$ could be reduced by simply projecting out any path for which $\rho(\mathbf{r}^N,\mathbf{q}^N,2\beta) = 0$. This is the scheme we used in the 2D Hubbard model[4] and it requires knowledge of the nodes of the density matrix at all temperatures. We note that in continuous space, very few paths actually have $\rho(\mathbf{r}^N,\mathbf{q}^N,2\beta) = 0$, but there may be many paths for which $\rho(\mathbf{r}^N,\mathbf{q}^N,2\beta)$ is small. If we discretize the path integral into temperature segments $\beta/P \equiv \epsilon$, the normal high temperature approximation leads to errors in the partition function of order ϵ. If we discard all paths for which $\rho(\mathbf{r}^N,\mathbf{q}^N,\tau) \propto \epsilon$, $\epsilon \leqslant \tau \leqslant \beta$, we will add negligible additional error to the partition function but can significantly reduce the variance. Thus we write the partition function for N quantum particles as

$$Q(\beta) = \int d\mathbf{r}_1^N\, d\mathbf{r}_2^N \cdots d\mathbf{r}_P^N \left\{ \prod_{j=1}^P \rho(\mathbf{r}_j^N, \mathbf{r}_{j+1}^N, \beta/P) \right\}$$
$$\times \left\{ \frac{1}{P} \sum_{j=1}^P \mathfrak{P}(\mathbf{r}_j^N) \right\} + \mathcal{O}(\epsilon), \qquad (2.3)$$

where

$$\mathfrak{P}(\mathbf{r}_j^N) = \prod_{i=1}^P \mathfrak{p}(\mathbf{r}_j^N, \mathbf{r}_i^N, \tau) \qquad (2.4)$$

and

$$\mathfrak{p}(\mathbf{r}^N,\mathbf{q}^N,\tau) = \begin{cases} 0 & \text{if } \rho(\mathbf{r}^N,\mathbf{q}^N,\tau) \propto \beta/P \\ 1 & \text{otherwise} \end{cases} \qquad (2.5)$$

and τ is the difference in imaginary times of indices i and j. This is an exact formulation in the limit $\epsilon \to 0$ and can be implemented if the nodes of ρ are known. In practice, we have found that we can sample from the absolute value of the Fermi density matrix and average the projection operator times any quantity we desire. The next part of this paper will be devoted, then, to determining conditions under which the nodes of the density matrix can be predicted from the nodes of the noninteracting density matrix.

III. NONINTERACTING DENSITY MATRIX

In this section, we discuss the conditions for the existence of a particular set of nodes of the free particle density matrix. Consider the free particle density matrix for N like-spin fermions,[1]

$$\rho(\mathbf{r}^N\mathbf{q}^N,\beta) = \sum_{\mathscr{P}} (-1)^{\mathscr{P}} \bar\rho(\mathbf{r}^N\mathbf{q}_{\mathscr{P}}^N,\beta)$$

$$= \sum_{\mathscr{P}} (-1)^{\mathscr{P}} \left\{ \frac{1}{2\pi\beta} \right\}^{3N/2}$$

$$\times \exp\left\{ -\frac{\sum_{i=1}^N (\mathbf{r}_i - \mathbf{q}_{i,\mathscr{P}})^2}{2\beta} \right\}, \qquad (3.1)$$

where we have set $\hbar = 1$ and $m = 1$, $\beta = 1/kT$, $\mathscr{P}$ refers to a particular permutation, $\mathbf{r}^N$ and $\mathbf{q}^N$ refer to the initial and final points in the path, and $\bar\rho$ is the Boltzmann statistics density matrix. If it is possible to find $\{\mathbf{r}^N,\mathbf{q}^N\}$ for which ρ is 0 for all values of β, this is one of the paths we excluded in our work on the 2D Hubbard model. In Appendix A, we show that

this will occur if the $N!$ permutations in Eq. (3.1) can be divided into $N!/2$ pairs of exponentials, each pair consisting of a positive and a negative permutation, and with the argument of the exponentials being equal. If the pairs of arguments differ by less than ϵ, the inverse temperature increment used to discretize the path integral, then the error in the low temperature partition function will be of order ϵ, which is the same error as introduced by the "short time" propagator. Such "temperature independent" nodes were used in our previous work to exclude paths in both the interacting and noninteracting 2D Hubbard model. In this paper, we shall examine such collections of $\{\mathbf{r}^N,\mathbf{q}^N\}$ in the interacting system. For the interacting system, we know that the small β approximation has the form $\rho(\beta)_{\text{interacting}} = \rho(\beta)_{\text{noninteracting}} \cdot f(\mathbf{r}^N,\mathbf{q}^N,\beta) + \mathcal{O}(\beta^2)$, with the function f being independent of the permutation. Therefore $\rho_{\text{interacting}}$ has nodes at the same locations as $\rho_{\text{noninteracting}}$ at high temperatures (including the class of nodes described above). In this paper, we will examine these nodes at all temperatures to first order in the interaction.

IV. FIRST ORDER CORRECTION

In this section, we discuss the first order correction to the noninteracting problem. Consider the first order correction to a Boltzmann statistics density matrix,[1]

$$\bar\rho^{(1)}(\mathbf{r}^N\mathbf{q}_{\mathscr{P}}^N,\beta) = -\int_0^\beta d\tau \int d\mathbf{z}^N \bar\rho_0(\mathbf{r}^N\mathbf{z}^N,\tau)$$
$$\times V(\mathbf{z})\bar\rho_0(\mathbf{z}^N\mathbf{q}_{\mathscr{P}}^N,\beta-\tau), \qquad (4.1)$$

where $\mathbf{r}^N \equiv (\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N)$, $\mathscr{P}$ refers to a particular permutation, and $V(\mathbf{z})$ is the perturbation. Physically, the structure of Eq. (4.1) suggests that $\rho^{(1)}$ should be small if ρ_0 is zero. This can be seen in the following way. If Eq. (4.1) could be written for all β as

$$\bar\rho^{(1)}(\mathbf{r}^N\mathbf{q}_{\mathscr{P}}^N,\beta) = \bar\rho_0(\mathbf{r}^N\mathbf{q}_{\mathscr{P}}^N,\beta) \, f(\mathbf{r}^N,\mathbf{q}^N,\beta), \qquad (4.2)$$

where f is independent of the permutation, $\rho^{(1)}$ would have the same nodes as ρ_0. It is clear that Eq. (4.1) cannot be written in such a way due to the perturbation. However, if we consider the integral over τ, though, we can see why $\bar\rho^{(1)}$ might be expected approximately to satisfy Eq. (4.2). For small τ, $\bar\rho_0(\mathbf{r}^N\mathbf{z}^N\tau)$ will be zero unless $\mathbf{z}_i = \mathbf{r}_i$ for all $i = 1,N$ and, hence the integral over $\mathbf{z}^N$ will be essentially independent of $\mathbf{q}^N$. The same argument will be true for τ close to β, with $\mathbf{r}^N$ and $\mathbf{q}^N$ swapped. For values of τ on the order of $\beta/2$, the $\bar\rho_0$ terms will allow values of $\mathbf{z}^N$ that differ significantly from either $\mathbf{r}^N$ or $\mathbf{q}^N$. In this case, we might expect the integral over $\mathbf{z}^N$ to be only weakly dependent on $\mathbf{r}^N$ and $\mathbf{q}^N$ and hence Eq. (4.2) once again satisfied. Thus we have reason to believe that the first order correction to ρ_0, when evaluated at the nodes of ρ_0, will be small and can be ignored in the calculation of properties of the interacting system. In the next section, we develop Eq. (4.1) and show that in three cases, our expectations are indeed met at low and high temperatures.

We can write V as a sum of one- and two-body interactions,

$$V(\mathbf{r}^N) = \sum_{i=1}^{N} \sum_{\alpha=1}^{N_\alpha} u(\mathbf{r}_i - \mathbf{R}_\alpha) + \sum_{i<j} v(\mathbf{r}_i - \mathbf{r}_j), \quad (4.3)$$

where the $\mathbf{R}_\alpha$ represent N_α sites with which the individual fermions interact. In the rest of this paper, we shall assume that u and v are spherically symmetric, as this encompasses many interesting Hamiltonians. Since the first order correction is linear in V, we can consider each term in the sums in Eq. (4.1) separately. We first work on the one-body term.

V. ONE-BODY TERM

The typical term in the correction due to a single one-body interaction is

$$-\int_0^\beta d\tau \int d\mathbf{z}^N \tilde{\rho}(\mathbf{r}^N \mathbf{z}^N, \tau) \, u(\mathbf{z}_1 - \mathbf{R}_\alpha) \, \tilde{\rho}(\mathbf{z}^N \mathbf{q}^N, \beta - \tau). \quad (5.1)$$

It is straightforward to show that this can be written

$$-\tilde{\rho}_0 (\mathbf{r}^N \mathbf{q}^N, \beta) \, \beta \int_0^1 dx \, (\alpha/\pi)^{3/2} \int dy \, u(y)$$
$$\times \exp[-\alpha(y-D)^2], \quad (5.2)$$

where $\alpha = [2\beta x(1-x)]^{-1}$, $D = r_1 + x(q_1 - r_1) - R_\alpha$ $\equiv R_0 + x(Q_0 - R_0)$ with $R_0 \equiv r_1 - R_\alpha$ and $Q_0 \equiv q_1 - R_{\alpha'}$ and $y \equiv |\mathbf{y}|$. We shall consider three forms for $u(y)$: (1) $u(y) = Q/y$, where Q can be positive or negative,

(2) $u(y)$ has some arbitrary, but short-ranged form such as might occur in a pseudopotential calculation, and (3) $u(y) = \omega^2 y^2/2$. For the first two cases, we assume that $u(y)$ is non-negligible only for $y \leqslant R_c$ (some critical length). This will be true even for the Coulomb interaction as can be noticed by performing numerical integration of the 1D Schrödinger equation for hydrogenlike atoms, where there is some distance beyond which integration is not necessary. It is useful to write the integral over x as

$$\int_0^1 dx = \lim_{\gamma \to 0} \int_\gamma^{1-\gamma} dx, \quad (5.3)$$

where γ is a small number.

A. Case 1

We can simplify Eq. (5.2) for $u(y) = Q/y$ to find

$$-\tilde{\rho}_0 \beta Q \int_0^1 dx \frac{\Phi[\alpha^{1/2} D]}{D}. \quad (5.4)$$

We expand error function in a Taylor series expansion and obtain

$$\lim_{\gamma \to 0} -\tilde{\rho}_0 \beta Q \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(2n+1)(2\beta)^{n+1/2}} \mathscr{I}(\gamma, D, n), \quad (5.5)$$

where

$$\mathscr{I}(\gamma, D, n) = \int_\gamma^{1-\gamma} \frac{dx}{(x-x^2)^{n+1/2}} \left[R_0^2 + 2R_0 \cdot (Q_0 - R_0)x + (Q_0 - R_0)^2 x^2 \right]^n$$

$$= \int_\gamma^{1-\gamma} \frac{dx}{(x-x^2)^{n+1/2}} \sum_{n_1=0}^{n} \sum_{n_2=0}^{n} \sum_{n_3=0}^{n} R_0^{2n_1} [2R_0 \cdot (Q_0 - R_0)]^{n_2} (Q_0 - R_0)^{2n_3}$$

$$\times \frac{n!}{n_1! n_2! n_3!} \delta_{n_1+n_2+n_3, n} J_{n+1/2}^{n_2+2n_3}, \quad (5.6)$$

where the sums over n_1, n_2, n_3 (with the corresponding factorials and δ function) are just the multinomial expansion for D^n and

$$J_{n+1/2}^m = \int_\gamma^{1-\gamma} dx \frac{x^m}{(x-x^2)^{n+1/2}}. \quad (5.7)$$

In Appendix B, we show that

$$J_{n+1/2}^m \gamma^{n-1/2} = (2+2\delta_{m,0})/(2n-1) + \Sigma_{i=1}^n \gamma^i c_i$$
$$= (2+2\delta_{m,0}) \text{ for } \gamma \text{ small}$$

and c_i is a finite number.
Thus

$$\tilde{\rho}^{(1)} = \lim_{\gamma \to 0} -\tilde{\rho}_0 \beta Q \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(2n+1)(2\beta)^{n+1/2}}$$

$$\times \left[\frac{2(R_0^{2n} + Q_0^{2n})}{(2n-1)\gamma^{n-1/2}} \right.$$

$$+ R_0^{2n} \sum_{i=1}^{n} \mathscr{f}_i(2R_0 \cdot Q_0/R_0^2, \, Q_0/R_0) \gamma^{-n+1/2+i} \bigg], \quad (5.8)$$

where $\mathscr{f}_m$ is some function of order unity and we have arranged the sum over i assuming that $R_0 > Q_0$ (our conclusions are independent of this assumption). As γ goes to zero, the leading order term of $\gamma^{-(n-1/2)}$ will be

$$\frac{(-1)^n}{n!(2n+1)(2\beta)^{n+1/2}} \frac{2(R_0^{2n} + Q_0^{2n})}{(2n-1)\gamma^{n-1/2}}$$

and the corrections are proportional to powers of R_0^2/β, which can be deduced by collecting all terms in the sum over n of order $\gamma^{-n'+1/2}$ which will have contributions from all $n > n'$. Such terms are of order $(R_0^2/\beta)^{n-n'}$. We have assumed that R_0 is bounded above by some critical value R_c. Hence as β is made very large, we can ignore the corrections and write the first order perturbation correction to $\tilde{\rho}$ from this term in the interaction as a sum over permutations $\mathscr{P}$ of

$$\tilde{\rho}^{(1)}(\mathbf{r}^N \mathbf{q}_{\mathscr{P}}^N, \beta) = -\tilde{\rho}_{0,\mathscr{P}} BQ \sum_{i=1}^{N_\alpha} \lim_{\gamma \to 0} \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(2n+1)(2\beta)^{n+1/2}} \cdot \frac{2(R_i^{2n} + Q_{i,\mathscr{P}}^{2n})}{(2n-1)\gamma^{n+1/2}}$$

$$= -\tilde{\rho}_0(\mathbf{r}^N \mathbf{q}_{\mathscr{P}}^N, \beta)\beta Q \sum_{i=1}^{N_\alpha} \int_0^1 dx \frac{\Phi[\alpha^{1/2} 2R_i]}{R_i} + \int_0^1 dx \frac{\Phi[\alpha^{1/2} Q_{i,\mathscr{P}}]}{2Q_{i,\mathscr{P}}} \qquad (5.10)$$

$$= \tilde{\rho}_0(\mathbf{r}^N \mathbf{q}_{\mathscr{P}}^N, \beta) f(\mathbf{r}^N, \mathbf{q}^N) \qquad (5.11)$$

correct for β large compared to R_0^2. Since the only dependence on the permutation is in the noninteracting term, the nodes will be at the same place as in the noninteracting system, which is the desired result. For $\beta \ll R_0^2$,

$$\frac{\mathbf{R}_0 \cdot \mathbf{Q}_0}{R_0^2} = 1 + \mathscr{O}(\beta/R_0^2) \quad \text{and}$$

$$Q_0/R_0 = 1 + \mathscr{O}(\beta/R_0^2) \qquad (5.12)$$

and Eq. (5.8) will depend only on R_0 (or Q_0) to order β/R_0^2, and, hence, Eq. (4.2) will be satisfied. Therefore Eq. (4.2) is satisfied at both high and low temperatures. At the present time, we are unable to confirm that Eq. (4.2) is satisfied for intermediate temperatures. However, as partial confirmation of our expectation that Eq. (4.2) should also be satisfied at intermediate temperatures, we will offer a numerical calculation that demonstrates the accuracy of this approximation at several temperatures and we will discuss in a later section some reasons why Eq. (4.2) should be satisfied at intermediate temperatures.

B. Case 2

We can perform the angular integration in Eq. (4.1) to find

$$-\tilde{\rho}_0 \beta \int_0^1 dx (\alpha/\pi)^{1/2} D^{-1} \int_0^{R_c} dz \, zu(z)$$

$$\times \{\exp[-\alpha(z-D)^2] - \exp[-\alpha(z+D)^2]\}. \qquad (5.13)$$

Expanding the exponentials and rearranging leads to

$$\tilde{\rho}_0 \beta \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \sum_{\substack{k=0 \\ k \text{ odd}}}^{n} \binom{n}{k} 2 \mathscr{U}_{k+1}(R_c)$$

$$\times \int_0^1 dx \frac{D^{2n-k-1}}{[2\beta x(1-x)]^{n+1/2}}, \qquad (5.14)$$

where $\mathscr{U}_{k+1}(R_c) \equiv \int_0^{R_c} dz \, z^{k+1} u(z)$, which will typically be proportional to R_c^{k+2}. The integral over x is of the same form as Eq. (5.6) and, thus can be written to lowest order in γ as

$$2(1 + \delta_{2n-k-1,0}) \frac{[R_0^{2n-k-1} + Q_0^{2n-k-1}]}{[(2n-1)\gamma^{n-1/2}(2\beta)^{n+1/2}]}, \qquad$$

with a correction of order

$$R_0^{2n-k-1} \mathscr{f}_k(\mathbf{R}_0 \cdot \mathbf{Q}_0/R_0^2, Q_0/R_0)/(\beta^{n+1/2} \gamma^{n-3/2})$$

leading to

$$\tilde{\rho}_0 \beta \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \sum_{\substack{k=0 \\ k \text{ odd}}}^{n} \binom{n}{k} 4(1 + \delta_{2n-k-1,0}) \mathscr{U}_{k+1}(R_c)$$

$$\times \int_0^1 dx \frac{(R_0^{2n-k-1} + Q_0^{2n-k-1})}{[2\beta x(1-x)]^{n+1/2}}, \qquad (5.15)$$

with additional terms of order,

$$R_0^{2n-k-1} \frac{\mathscr{f}_k(\mathbf{R}_0 \cdot \mathbf{Q}_0/R_0^2, Q_0/R_0) \mathscr{U}_{k+1}(R_c)}{[\beta R_0^{2n-2-k'-1} \mathscr{U}_{k'-1}(R_c)]},$$

$$\propto R_0^{k'-k+2} \left[\frac{\mathscr{U}_{k+1}}{\mathscr{U}_{k'+1}} \right] \beta,$$

$$\propto [R_0/R_c]^{k'-k} R_0^2/\beta. \qquad (5.16)$$

Thus the additional terms are small in the same way as in the Coulomb interaction and the first order correction to ρ has the desired form [Eq. (4.2)].

C. Case 3

For the harmonic oscillator, $u(y) = \omega^2 y^2/2$ and Eq. (4.1) can be integrated straightforwardly, without expanding the exponential, to find

$$-\tilde{\rho}_0 \beta \frac{\omega^2}{2} \int_0^1 dx \, [D^2 + 3/(2\alpha)].$$

The only term involving both R_0 and Q_0 is $-\tilde{\rho}_0 \beta \, \mathbf{R}_0 \cdot \mathbf{Q}_0/3$. When summed over all the particles, the dot product is the same for the two permutations with the same $\tilde{\rho}_0$ and, hence the first order correction for the harmonic oscillator is exactly zero for the harmonic oscillator (in fact, it is zero to all orders for the noninteracting particles confined to a harmonic well, as can be seen by direct inspection of the exact density matrix for the harmonic oscillator[1]).

Thus the single particle interactions considered here both satisfy the desired relation and lead to nodes that do not move to order ϵ at both low and high temperatures. We now consider the two-particle interactions of the Coulomb form.

VI. TWO-PARTICLE INTERACTION

We now focus on the two-body interaction $v(r_i - r_j)$. For the purposes of this work, we consider only the repulsive Coulomb interaction because we are most interested in studies of electrons. The typical term in the two-body correction to the density matrix is

$$-\int_0^\beta d\tau \int d\mathbf{z}^N \tilde{\rho}_0(\mathbf{r}^N \mathbf{z}^N, \tau) \tilde{\rho}_0(\mathbf{z}^N \mathbf{q}^N, \beta - \tau)/|\mathbf{z}_1 - \mathbf{z}_2|. \qquad (6.1)$$

It is straightforward to show that this is equal to

No₂ singlet
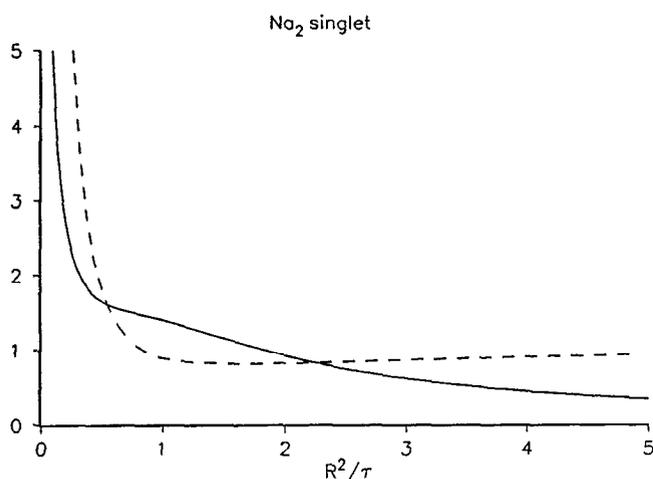
FIG. 1. A plot of $2\mathbf{R_0 \cdot Q_0}/R_0^2$ and $(Q_0/R_0)^2$ vs R_0^2/τ for the singlet state of the sodium dimer as determined in a Monte Carlo simulation. τ corresponds to the imaginary time difference between $\mathbf{R_0}$ and $\mathbf{Q_0}$. The solid line represents $2\mathbf{R_0 \cdot Q_0}/R_0^2$, while the dashed line represent $(Q_0/R_0)^2$.

$$-\tilde{\rho}_0\beta\int_0^1 dx(\alpha/2\pi)^{3/2}\int\frac{d\mathbf{y}}{y}e^{-\alpha(\mathbf{y}+\mathbf{D}_{12})^2}, \qquad (6.2)$$

where $\mathbf{D}_{12}=(\mathbf{r}_1+\mathbf{r}_2)+x(\mathbf{q}_1+\mathbf{q}_2)$. This has the same form as the single particle interaction and, hence this term will have the same type of correction as the previous terms.

Thus, to first order in one- and two-particle interactions, the density matrix has nodes at the same location as the noninteracting system at both high and low temperatures. We are not, at this time, able to show that intermediate temperatures also obey this relation, although we suspect this to be the case. In the next section, we offer some qualitative reasons why intermediate temperatures should also obey Eq. (4.2).

VII. INTERMEDIATE TEMPERATURES

From Eq. (5.8), the corrections to the density matrix that do not cancel when summing over permutations involve $2\mathbf{R_0 \cdot Q_0}/R_0^2$ and $(Q_0/R_0)^2$. If these two quantities were equal to unity, the sum over permutations would cancel even when at an intermediate temperature. These intermediate temperatures are defined by $\beta\cong R_0^2\cong Q_0^2$ [if R_0 and Q_0 are

not close, then $Q_0\ll R_0$ and corrections will depend only on R_0 to order (Q_0/R_0) and the nodal locations will be preserved]. In the present case, $|\mathbf{R_0}-\mathbf{Q_0}|^2\cong R_0^2\cong Q_0^2\cong\beta$, the triangle formed by the vectors $\mathbf{R_0}-\mathbf{Q_0}$, $\mathbf{R_0}$, $\mathbf{Q_0}$ will be approximately equilateral and the dot product $\mathbf{R_0 \cdot Q_0}\cong R_0 Q_0\cos(60°)\cong R_0 Q_0/2$ and the corrections

$$\mathcal{f}_m(2\mathbf{R_0 \cdot Q_0}/R_0^2,\ Q_0/R_0)\cong\mathcal{f}_m(1,1) \qquad (7.1)$$

and will be approximately independent of $\mathbf{Q_0}$. Thus these corrections should cancel to a large extent when summed over the permutations. As a test of what "typical" values of $2\mathbf{R_0 \cdot Q_0}/R_0^2$ and Q_0/R_0 are, we have evaluated these for the singlet state (the singlet was studied in order to allow exact calculations to be performed) of several small sodium clusters studied in our previous work. Our results are similar for $^1\mathrm{Na}^-$, $^1\mathrm{Na}_2$, $^1\mathrm{Na}_3^+$, and we show the results for $^1\mathrm{Na}_2$ in Fig. 1. As can be seen, for $\beta/R_0^2\cong 1$, $2\mathbf{R_0 \cdot Q_0}/R_0^2$ and Q_0/R_0 are close to 1, so we believe that the corrections to the intermediate temperature density matrix can indeed be small, even though we cannot demonstrate this analytically at the present time.

We have attempted to confirm this expectation using a numerical calculation, where we can evaluate the energy of a model system at a variety of temperatures in order to study the accuracy of the intermediate temperature case and to demonstrate the results for low temperatures. A model system that we have found to be useful is the Kestner–Sinanoḡlu potential[5] and, in the next section, we study this system at several temperatures.

VIII. CALCULATIONS

The Kestner–Sinanoḡlu Hamiltonian[5] has the form

$$\mathcal{H}=-1/2(\nabla_1^2+\nabla_2^2)+\omega^2(r_1^2+r_2^2)/2$$
$$+1/|\mathbf{r}_1-\mathbf{r}_2|, \qquad (8.1)$$

where we have used atomic units. This Hamiltonian mimics two electrons bound to an atom and is useful as a model because it is separable, allowing the calculation of the exact energies and correlated wave functions. The harmonic frequency can be chosen to mimic an atom with charge Z, we have chosen $Z=1$ and, hence mimic H^-. Our calculations used the formulation described briefly in Sec. III and in our paper on the 2D Hubbard model. The results are given in Table I and demonstrate that the projection operator can

TABLE I. Energies vs reciprocal temperature for the Kestner–Sinanoḡlu Hamiltonian. E_{exact} are the exact energies, E_{PIMC} are the energies obtained using straightforward Monte Carlo integration and $E_{\mathrm{PIMC, proj}}$ are the energies obtained using our projection operator. All energies and β are in atomic units and the numbers in parentheses represent one standard deviation. P is the number of points used to discretize the path integral and N_p si the number of Monte Carlo passes used in determining the average values.

β	P	N_p	E_{exact}	E_{PIMC}	$E_{\mathrm{PIMC,proj}}$
3.0	15	100 000	3.183	3.192(.031)	3.191(.031)
4.0	20	100 000	2.898	2.912(.054)	2.911(.053)
5.0	25	100 000	2.773	2.775(.076)	2.770(.074)
10.0	50	400 000	2.653	2.643(.159)	2.637(.124) ,
20.0	100	400 000	2.647	2.726(1.705)	2.648(.919)

indeed give accurate results at both low, high, and intermediate temperatures, suggesting that, the nodes of the noninteracting system make negligible contributions to the interacting system properties not just a low and high temperatures to first order in the interaction (as we have shown in this paper), but at all temperatures to higher order in the interactions.

IX. CONCLUSION

We have shown that the first order perturbation correction to the noninteracting density matrix has nodes at approximately the same locations as the noninteracting density matrix at low and high temperatures, at least for the class of nodes described in this paper. We suspect that this may be a more general property of the density matrix, but at the present are unable to prove this speculation. In order to investigate this speculation, we have performed numerical calculations on the Kestner–Sinanoğlu Hamiltonian and have demonstrated agreement with exact results can be obtained by using a projection operator based on the nodes of the noninteracting density matrix. Future work will investigate higher orders of perturbation and alternative proofs of the intermediate temperature regime.

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APPENDIX A

In this Appendix, we discuss the properties of the noninteracting density matrix for N like-spin fermions. At any temperature τ, we know the exact form of the density matrix is

$$\rho(\mathbf{r}^N, \mathbf{q}^N, \tau) = (2\pi\tau)^{-3N/2} \sum_{\mathscr{P}} (-1)^{\mathscr{P}}$$

$$\times \exp\left\{ -\frac{\Sigma_k (\mathbf{r}_k - \mathbf{q}_{k,\mathscr{P}})^2}{2\tau} \right\}. \quad (A1)$$

We seek conditions under which $\rho(\tau) \propto \epsilon \equiv \beta/P$ at all values of τ given that β is the desired temperature of the partition function and P is the number of points used to discretize the path integral. If we expand the exponential, we find

$$\rho(\mathbf{r}^N, \mathbf{q}^N, \tau) \propto \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(2\tau)^n}$$

$$\times \left\{ \sum_{\mathscr{P}} (-1)^{\mathscr{P}} \left[\sum_k (\mathbf{r}_k - \mathbf{q}_{k,\mathscr{P}})^2 \right]^n \right\}. \quad (A2)$$

The only way for ρ to be 0 at all values of τ is for all terms inside the curly brackets in Eq. (A2) to be zero. In order for this to be true, we *must* have the sums over $\mathscr{P}$ be paired into $N!/2$ pairs of equal numbers, but with opposite permutation weights. Otherwise, changing τ would cause the sum over permutations to take on a non-negligible value. In addition, if each of the pairs of permutations differ by less than ϵ, ρ will be proportional to ϵ at all temperatures.

APPENDIX B

We consider the integral

$$J_{n+1/2}^m = \int_\gamma^{1-\gamma} dx \frac{x^m}{(x-x^2)^{n+1/2}} \quad \text{for } m \leqslant 2n, \ n \geqslant 1. \quad (B1)$$

From Gradshteyn and Ryzhik,[6] we find, letting $\Gamma \equiv x - x^2$

$$m = 2n \quad J_{n+1/2}^m = \frac{x^{2n-1}}{(2n-1)\Gamma^{n-1/2}}\Big|_\gamma^{1-\gamma}$$
$$+ J_{n+1/2}^{m-1}/2 - J_{n-1/2}^{m-2}, \quad (B2a)$$

$$0 < m < 2n \quad J_{n+1/2}^m = \frac{x^{m-1}}{(2n-m)\Gamma^{n-1/2}}\Big|_\gamma^{1-\gamma}$$
$$+ \frac{(2n+1-2m)}{2(2n-m)} J_{n+1/2}^{m-1}, \quad (B2b)$$

$$m = 0 \quad J_{n+1/2}^m = -\frac{2(1-2x)}{(2n-1)\Gamma^{n-1/2}}\Big|_\gamma^{1-\gamma}$$
$$+ \frac{8(n-1)}{(2n-1)} J_{n-1/2}^0. \quad (B2c)$$

Using the fact that $\Gamma(x=1-\gamma) = \Gamma(x=\gamma)$, we find, to lowest order in γ

$$J_{n+1/2}^0 = 4/[(2n-1)\gamma^{n-1/2}], \quad (B3a)$$

$$J_{n+1/2}^1 = J_{n+1/2}^0/2 = 2/[(2n-1)\gamma^{n-1/2}]. \quad (B3b)$$

For $1 < m < 2n$, we have

$$J_{n+1/2}^m = \frac{1}{(2n-m)\gamma^{n-1/2}} + \frac{(2n+1-2m)}{2(2n-m)} J_{n+1/2}^{m-1}.$$

If we assume that $J_{n+1/2}^{m-1} = 2/[(2n-1)\gamma^{n-1/2}]$, we find that

$$J_{n+1/2}^m = \gamma^{1/2-n}\left\{ \frac{1}{2n-m} + \frac{2n+1-2m}{(2n-m)(2n-1)} \right\}$$
$$= 2/[(2n-1)\gamma^{n-1/2}]. \quad (B5)$$

Finally, for $n = 2m$, we have

$$J_{n+1/2}^m = \gamma^{1/2-n}\left\{ \frac{1}{2n-1} + \frac{1}{2n-1} \right\}$$
$$= 2/[(2n-1)\gamma^{n-1/2}]. \quad (B6)$$

The errors to terms of order $\gamma^{1/2-n}$ are of order $\gamma^{3/2-n}$ and hence become small relative to the other terms with the same value of n as γ goes to zero.

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