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Path Integral Studies of the 2D Hubbard Model Using a New Projection Operator

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Feynman's path integral formulation of quantum mechanics, supplemented by an approximate projection operator (exact in the case of noninteracting particles), is used to study the 2D Hubbard model. The projection operator is designed to study Hamiltonians defined on a finite basis set, but extensions to continuous basis sets are suggested. The projection operator is shown to reduce the variance by a significant amount relative to straightforward Monte Carlo integration. Approximate calculations are usually within one standard deviation of exact results and virtually always within two to three standard deviations. In addition, the algorithm scales with the number of discretization points P as either P or P^2 (depending on the method of implementation), rather than the P^3 of the Hubbard–Stratonovich transformation. Accuracy to about 5%–10% in energies and spin–spin correlation functions are found using moderate amounts of computer time.

I. INTRODUCTION

The study of condensed phase, many-Fermion systems is a challenge to all numerical methods. While Feynman's path integral formulation of quantum mechanics[1] offers several important advantages over alternative techniques (such as exact inclusion of electron correlation, ability to study finite temperatures, and the use of complete sets of states), its practical application has been hindered because the density matrix can be negative, which prevents the straightforward use of Monte Carlo or related methods that rely on sampling from nonnegative weighting functions. The popular Hubbard–Stratonovich (HS) transformation[2] has made studies of small systems possible, but only by straining the limits of modern computational resources. Recently, we have developed[3] an approximate implementation of the path integral formulation that gives accurate results in a variety of systems defined on continuous basis functions. The justification for the approximation was that it "projected out" regions of phase space that did not contribute to the properties of the Fermion system. In this paper, we make this idea of excluding regions of phase space well defined by studying the 2D Hubbard model, which has a Hamiltonian that is defined on a finite set of states. By excluding a set of paths corresponding approximately to the nodes of the density matrix at different temperatures, we demonstrate that accurate results (exact for the case of noninteracting particles) with reasonably small variances can be obtained in a relatively small amount of computer time. The spirit of the projection operator is similar to that used in Green's function Monte Carlo or quantum Monte Carlo,[4–6] where the approximate location of the ground state wave function's nodes are used to reduce the variance.

II. FORMALISM

In this section, we describe our path integral approach. Consider the discretized form of the partition function for N_α spin-up Fermions and N_β spin-down Fermions with $N = N_\alpha + N_\beta$:

$$Q = \int d\tau_1 \, d\tau_2 \cdots d\tau_P \, \rho(\tau_1,\tau_2,\epsilon)\rho(\tau_2,\tau_3,\epsilon)\cdots\rho(\tau_P,\tau_1,\epsilon),$$

$$(2.1)$$

where τ_i stands for the N coordinates at imaginary time i and $\epsilon = \beta/P$, where β is the inverse temperature and P is the number of discretization points. Since any of the ρ's can be negative, the integrand cannot be interpreted as a probability and, hence, standard Monte Carlo and molecular dynamics techniques cannot be used. The integral can, however, be cast into a form that allows straightforward Monte Carlo using importance sampling

$$Q/Q' = \int d\tau_1 \, d\tau_2 \cdots d\tau_P |P(\tau_1,\tau_2,\ldots,\tau_P)|$$

$$\times \left\{ \frac{P(\tau_1,\tau_2,\ldots,\tau_P)}{|P(\tau_1,\tau_2,\ldots,\tau_P)|} \right\} \bigg/$$

$$\int d\tau_1 \, d\tau_2 \cdots d\tau_P |P(\tau_1,\tau_2,\ldots,\tau_P)|$$

$$= \left\langle \frac{P(\tau_1,\tau_2,\ldots,\tau_P)}{|P(\tau_1,\tau_2,\ldots,\tau_P)|} \right\rangle_{|P(\tau_1,\tau_2,\ldots,\tau_P)|}, \quad (2.2)$$

where

$$Q' = \int d\tau_1 \, d\tau_2 \cdots d\tau_P |P(\tau_1,\tau_2,\ldots,\tau_P)|, \quad (2.3)$$

$P(\tau_1,\tau_2,\ldots,\tau_P) \equiv \rho(\tau_1,\tau_2,\epsilon)\rho(\tau_2,\tau_3,\epsilon)\cdots\rho(\tau_P,\tau_1,\epsilon)$ and $\langle A \rangle_P$ denotes the ensemble average of A over a distribution function P. As should be clear, the Monte Carlo estimator for Q/Q' is the sum of plus and minus ones. If we denote the number of $+1$ contributions to the estimator by N_+ and the number of -1 contributions to the estimator by N_-, then

$$Q/Q' = (N_+ - N_-)/(N_+ + N_-)$$

and

$$\sigma^2 = \{(N_+ + N_-)(N_+ + N_-)$$

$$- N_+^2 - N_-^2 + 2N_+ N_- \}/$$

$$[(N_+ + N_-)^2(N_+ + N_- - 1)]$$
$$= 4N_+ N_- / \{(N_+ + N_-)^2(N_+ + N_- - 1)\}.$$

Letting $n = N_+ - N_-$ and $N_+ + N_- = N$ and assuming $N - 1 \cong N$, we find

$$\sigma/(Q/Q')$$
$$= 2\sqrt{N_+ N_- /(N_+ + N_- - 1)}/(N_+ - N_-)$$
$$= 2\sqrt{(N^2 - n^2)/4N}/n. \qquad (2.4)$$

Thus, the smaller n, the larger the relative error. Let us assume that it is possible to find a subset of the $N_+ + N_-$ paths containing $\tilde{N}$ paths $(\tilde{N} < N)$ for which $\tilde{N}_+ - \tilde{N}_- = m$ with $m \ll n$ (for noninteracting particles, we will have $m = 0$). If we do not include these $\tilde{N}$ paths in the average (through the use of a projection operator, for instance), it is straightforward to show that the relative error is now (assuming a total of N passes that successfully pass the projection test)

$$\sigma/(Q/Q')_m = 2\sqrt{(N^2 - \tilde{n}^2)/4N}/\tilde{n}, \qquad (2.5)$$

where $\tilde{n} = \{N/(N - \tilde{N})\}(n - m) > n$ as long as m is small and by $(Q/Q')_m$ we indicate that a projection operator for which $\tilde{N}_+ - \tilde{N}_- = m$ has been used; thus if $m \neq 0$, only an approximate value of Q/Q' will be obtained since we will be ignoring nonzero contributions to Q. However, our numerical results indicate that the approximate result can still be in good agreement with exact results, justifying this approach. By using this projection operator, the relative error from Eq. (2.5) is reduced since $\tilde{n} > n$. Thus, we look for a projection operator that can discard paths that make no net contribution to Q/Q'. In this paper, we work with a projection operator that is similar in spirit to the one previously used, however, several alternative operators do exist, some of which are mentioned later in this section.

We proceed in obtaining a projection operator in the following way: assume that we know the set of coordinates for which $\rho(\tau_m, \tau_n, \gamma) = 0$ for $1 \leqslant m, n \leqslant P$ and $\epsilon \leqslant \gamma \leqslant \beta$. In this case, we can write the exact form of the partition function as

$$Q = \int d\tau_1\, d\tau_2 \cdots d\tau_P \rho(\tau_1, \tau_2, \epsilon)\rho(\tau_2, \tau_3, \epsilon) \cdots \rho(\tau_P, \tau_1, \epsilon)$$
$$\times \prod_{k=2}^{P+1} \mathscr{P}[\tau_1, \tau_k, (k-1)\epsilon], \qquad (2.6)$$

where $\mathscr{P}[\tau_1, \tau_k, (k-1)\epsilon] = \begin{cases} 0 & \text{if } \rho[\tau_1, \tau_k, (k-1)\epsilon] = 0 \\ 1 & \text{otherwise} \end{cases}$

and

$$Q/Q' = \int d\tau_1\, d\tau_2 \cdots d\tau_P\, \mathscr{F}(\tau_1 | \tau_2, \dots, \tau_P)|P(\tau_1, \tau_2, \dots, \tau_P)|$$
$$\times \left\{\frac{P(\tau_1, \tau_2, \dots, \tau_P)}{|P(\tau_1, \tau_2, \dots, \tau_P)|}\right\} \bigg/ \int d\tau_1\, d\tau_2 \cdots d\tau_P$$
$$\times \mathscr{F}(\tau_1 | \tau_2, \dots, \tau_P)|P(\tau_1, \tau_2, \dots, \tau_P)|$$

$$= \left\langle \frac{P(\tau_1, \tau_2, \dots, \tau_P)}{|P(\tau_1, \tau_2, \dots, \tau_P)|} \right\rangle_{\mathscr{F}(\tau_1|\tau_2, \dots, \tau_P)|P(\tau_1, \tau_2, \dots, \tau_P)|}, \qquad (2.7)$$

where

$$\mathscr{F}(\tau_1 | \tau_2, \dots, \tau_P) \equiv \prod_{k=2}^{P+1} \mathscr{P}[\tau_1, \tau_k, (k-1)\epsilon].$$

To show this is exact, assume that for a specific τ_1 and τ_m, $\rho[\tau_1, \tau_m, (m-1)\epsilon] = 0$. In this case, the sum over all intermediate points must be zero and, hence, all paths which have these particular values of τ_1 and τ_m can be discarded in order to lower the fractional error. We note that this idea can be extended in an approximate manner to exclude configurations for which ρ is "small"; i.e., to exclude sums for which contributions to Q are negligible, leading to a nonzero value of m in the determination of $\tilde{n}$ in Eq. (2.5). For noninteracting particles, we know when ρ is 0 for all temperatures since we know its exact form. For interacting particles, we do not necessarily know where the nodes in ρ are. However, we can use two approaches to obtain accurate results. The first, which we use here and which is similar to the approach we have taken in our previous work, is to assume that if $\rho = 0$ at temperature β/P, then it is small for lower temperatures and, hence, exclude those paths from our calculations. The second approach would be to numerically find the nodes of the density matrix (or the ground state wave function) and use this information to obtain accurate energies and densities. In the next sections, we apply these ideas to the 2D Hubbard model. For our applications, we have symmetrized Eq. (2.7) by writing it as

$$Q/Q' = \int d\tau_1\, d\tau_2 \cdots d\tau_P\, \mathfrak{F}\; |P(\tau_1, \tau_2, \dots, \tau_P)|$$
$$\times \left\{\frac{P(\tau_1, \tau_2, \dots, \tau_P)}{|P(\tau_1, \tau_2, \dots, \tau_P)|}\right\} \bigg/$$
$$\int d\tau_1\, d\tau_2 \cdots d\tau_P\, \mathfrak{F}\; |P(\tau_1, \tau_2, \dots, \tau_P)| \qquad (2.8)$$

$$= \left\langle \left\{\frac{P(\tau_1, \tau_2, \dots, \tau_P)}{|P(\tau_1, \tau_2, \dots, \tau_P)|}\right\} \right\rangle_{\mathfrak{F}\; |P(\tau_1, \tau_2, \dots, \tau_P)|}, \qquad (2.9a)$$

or

$$= \left\langle \mathfrak{F}\left\{\frac{P(\tau_1, \tau_2, \dots, \tau_P)}{|P(\tau_1, \tau_2, \dots, \tau_P)|}\right\} \right\rangle_{|P(\tau_1, \tau_2, \dots, \tau_P)|} \bigg/$$
$$\langle \mathfrak{F} \rangle_{|P(\tau_1, \tau_2, \dots, \tau_P)|} \qquad (2.9b)$$

where

$$\mathfrak{F} \equiv \frac{1}{P} \sum_{i=1}^{P} \mathscr{F}(\tau_i | \tau_1, \dots, \tau_{i-1}, \tau_{i+1}, \dots, \tau_P). \qquad (2.10)$$

In the form of Eq. (2.9a), the algorithm should scale as P^2, while in the form of Eq. (2.9b), the scaling should be as P. Which form is used clearly depends on the problem at hand, for if $\mathfrak{F}$ projects out most of the regions allowed by $|P|$, then it is better to use Eq. (2.9a), while if a significant fraction of the paths allowed by $|P|$ are not discarded by $\mathfrak{F}$, then Eq. (2.9b) is the proper choice. In the calculations described in this paper, we have found Eq. (2.9b) to be satisfactory and hence expect the algorithm to scale approximately as P (these scalings should be compared to the P^3 scaling of the HS transformation[2]). In the cases of interacting particles, we do not know the exact form of $\mathfrak{F}$, rather we use the approximation described above and determine both the exact and approximate results by

$$Q/Q'_{\text{approx}} = \langle \mathfrak{F}P/|P| \rangle_{|P|}/\langle \mathfrak{F} \rangle_{|P|} \qquad (2.10a)$$

and

$$Q/Q'_{\text{exact}} = \langle P/|P| \rangle_{|P|}. \qquad (2.10b)$$

A similar strategy was performed for the calculation of the average energy and the site–site spin correlation functions. Comparison between exact and approximate results will be listed in the tables.

III. APPLICATION: THE 2D HUBBARD MODEL

The 2D Hubbard model[2] is defined on an $L \times L$ lattice by

$$\mathcal{H} = \sum_i h_i + \sum_{i<j} \mathcal{U}_{ij}, \qquad (3.1)$$

where h_i are the single particle Hamiltonians that couple nearest-neighbor sites with coupling strength $-t$, $\mathcal{U}_{ij}$ is the interaction between particles, equal to U if particles i and j have different spins and are at the same site and is zero otherwise, and (as is commonly done) periodic boundary conditions are *not* used. In our calculations, we have used $t = 1$ and $U = 0.0$, 2.0, and 4.0. $L = 3$ and we have studied the $(N_\alpha, N_\beta) = (3,2)$ and $(3,3)$ (number of holes $N_h = 5$ and 4). $\mathcal{H}$ was diagonalized in order to determine exact results and $\beta = 5.0$ a.u.; at this temperature, excited state contributions are small, but not negligible, requiring $P = 30$ for $U = 0.0$ and 2.0 and $P = 60$ for $U = 4.0$. We have chosen a simple algorithm for choosing moves for the individual particles, although in principle we could have used the ideas of Newman and Kuki[7] or Ceperley and Pollock.[8] Denote κ_i^α as the αth of the N particles at imaginary time i. A new state κ_i^α was sampled from the distribution

$$P(\kappa_i^\alpha) = |\rho(\tau_{i-1}, \tau_i, \epsilon)\rho(\tau_i, \tau_{i+1}, \epsilon)|$$

by sampling from one of the nine possible lattice sites in the manner described by Kalos and Whitlock.[9] Sampling in this manner led to adequate convergence in our calculations.

Our results are shown in Tables I and II. Between 100 000 and 275 000 passes were required to obtain the statistics shown, requiring the reasonable amounts of computer time shown in Table III. The number of passes used was chosen to achieve errors of about 5%–10%; clearly, more passes could have been made if smaller error bars were required. For the purposes of many calculations though, this level of accuracy is sufficient to extract desired answers.

TABLE I. Energies and site–site spin correlation functions. U is the Hubbard U parameter in units of $|t|$, N_h is the number of holes relative to half-filling on a 3×3 lattice, β is in atomic units, and P is the number of points into which the path is divided. E is the energy in units of $|t|$ and $n_{ij}(k)$ is the site–site correlation function for particles of type i and j (corresponding to up and down electrons) separated by k lattice sites. Exact results are from numerical diagonalizations and projected and total MC are the Monte Carlo results with and without the use of the projection operator. The numbers in parentheses represent one standard deviation.

	Exact	Projected	Total MC
$U=0$, $N_h=5$, $\beta=5.0$, $P=30$			
E	-8.4805	-8.45 (0.36)	-8.53 (1.89)
$n_{uu}(1)$	0.1877	0.190 (0.006)	0.197 (0.032)
$n_{uu}(2)$	0.4376	0.438 (0.012)	0.428 (0.062)
$n_{uu}(3)$	0.3123	0.311 (0.009)	0.307 (0.043)
$n_{uu}(4)$	0.06239	0.060 (0.002)	0.067 (0.010)
$n_{ud}(0)$	0.4531	0.461 (0.018)	0.454 (0.093)
$n_{ud}(1)$	1.2501	1.248 (0.047)	1.234 (0.251)
$n_{ud}(2)$	1.4062	1.398 (0.053)	1.411 (0.280)
$n_{ud}(3)$	0.7499	0.744 (0.028)	0.732 (0.145)
$n_{ud}(4)$	0.1407	0.148 (0.006)	0.168 (0.033)
$U=0$, $N_h=4$, $\beta=5.0$, $P=30$			
E	-9.890	-9.98 (0.52)	-10.02 (2.21)
$n_{uu}(1)$	0.6260	0.632 (0.032)	0.584 (0.137)
$n_{uu}(2)$	1.375	1.369 (0.066)	1.424 (0.289)
$n_{uu}(3)$	0.8740	0.870 (0.043)	0.875 (0.178)
$n_{uu}(4)$	0.1253	0.129 (0.007)	0.116 (0.033)
$n_{dd}(1)$	0.1877	0.191 (0.010)	0.188 (0.046)
$n_{dd}(2)$	0.4376	0.443 (0.022)	0.435 (0.094)
$n_{dd}(3)$	0.3123	0.310 (0.016)	0.322 (0.065)
$n_{dd}(4)$	0.0624	0.056 (0.004)	0.056 (0.015)
$n_{ud}(0)$	0.6719	0.669 (0.033)	0.652 (0.140)
$n_{ud}(1)$	1.813	1.825 (0.090)	1.839 (0.389)
$n_{ud}(2)$	2.094	2.096 (0.102)	2.105 (0.440)
$n_{ud}(3)$	1.187	1.178 (0.057)	1.166 (0.239)
$n_{ud}(4)$	0.2344	0.232 (0.012)	0.237 (0.050)

Upon doubling P, the timing increases by a factor of about 2.7, slightly larger than P, but significantly less than P^2, indicating our analysis of the timings to be substantially correct. In the case of $U = 0$, the projection is exact, while for $U \neq 0$, our results are approximate. Examination of the tables indicates that the projected values agree quite well with exact results, implying that the value of m discussed in Sec. II is indeed "small." In addition, it can be seen that the errors are significantly smaller when the projection is used with error bars on the order of 5%–10%, which should be accurate for examination of correlated electronic properties. The error in energies is fairly large and may inhibit the use of this approach to study the binding of holes in the high-temperature superconductors unless large amounts of computer time are utilized. However, this should be a useful method for studying other problems.

IV. CONCLUSIONS

Straightforward use of the path integral approach has been supplemented by a new type of projection operator. By discarding paths that pass through nodes of the density ma-

TABLE II. Energies and site–site spin correlation functions. U is the Hubbard U parameter in units of $|t|$, N_h is the number of holes relative to half-filling on a 3×3 lattice, β is in atomic units, and P is the number of points into which the path is divided. E is the energy in units of $|t|$ and $n_{ij}(k)$ is the site–site correlation function for particles of type i and j (corresponding to up and down electrons) separated by k lattice sites. Exact results are from numerical diagonalizations and projected and total MC are the Monte Carlo results with and without the use of the projection operator. The numbers in parentheses represent one standard deviation.

	Exact	Projected	Total MC
$U=2.0,\quad N_h=5,\quad \beta=5.0,\quad P=30$			
E	-7.8600	$-7.86\ (0.29)$	$-7.47\ (1.70)$
$n_{uu}(1)$	0.1750	0.178 (0.004)	0.163 (0.028)
$n_{uu}(2)$	0.4278	0.431 (0.010)	0.448 (0.061)
$n_{uu}(3)$	0.3255	0.319 (0.007)	0.330 (0.044)
$n_{uu}(4)$	0.07167	0.072 (0.002)	0.059 (0.011)
$n_{ud}(0)$	0.2317	0.230 (0.008)	0.227 (0.051)
$n_{ud}(1)$	1.2936	1.307 (0.042)	1.338 (0.260)
$n_{ud}(2)$	1.5833	1.558 (0.049)	1.521 (0.295)
$n_{ud}(3)$	0.7681	0.775 (0.025)	0.776 (0.151)
$n_{ud}(4)$	0.1234	0.130 (0.005)	0.139 (0.031)
$U=4.0,\quad N_h=5,\quad \beta=5.0,\quad P=60$			
E	-7.5287	$-7.49\ (0.20)$	$-7.56\ (1.05)$
$n_{uu}(1)$	0.1649	0.169 (0.003)	0.169 (0.017)
$n_{uu}(2)$	0.4182	0.423 (0.006)	0.415 (0.034)
$n_{uu}(3)$	0.3365	0.333 (0.005)	0.336 (0.026)
$n_{uu}(4)$	0.08046	0.075 (0.001)	0.077 (0.007)
$n_{ud}(0)$	0.1356	0.138 (0.003)	0.128 (0.019)
$n_{ud}(1)$	1.3029	1.301 (0.028)	1.330 (0.148)
$n_{ud}(2)$	1.6712	1.648 (0.034)	1.641 (0.180)
$n_{ud}(3)$	0.7734	0.782 (0.017)	0.772 (0.088)
$n_{ud}(4)$	0.1165	0.130 (0.003)	0.129 (0.018)
$U=2.0,\quad N_h=4,\quad \beta=5.0,\quad P=30$			
E	-8.8276	$-8.84\ (0.40)$	$-8.82\ (1.25)$
$n_{uu}(1)$	0.6157	0.609 (0.027)	0.612 (0.086)
$n_{uu}(2)$	1.355	1.358 (0.056)	1.370 (0.177)
$n_{uu}(3)$	0.8900	0.895 (0.037)	0.893 (0.114)
$n_{uu}(4)$	0.1389	0.139 (0.007)	0.125 (0.022)
$n_{dd}(1)$	0.1904	0.189 (0.009)	0.189 (0.029)
$n_{dd}(2)$	0.4375	0.444 (0.019)	0.446 (0.059)
$n_{dd}(3)$	0.3102	0.310 (0.014)	0.297 (0.040)
$n_{dd}(4)$	0.06189	0.058 (0.003)	0.068 (0.010)
$n_{ud}(0)$	0.4011	0.383 (0.017)	0.389 (0.054)
$n_{ud}(1)$	1.9411	1.971 (0.082)	1.961 (0.259)
$n_{ud}(2)$	2.1897	2.177 (0.091)	2.171 (0.286)
$n_{ud}(3)$	1.1910	1.180 (0.049)	1.183 (0.154)
$n_{ud}(4)$	0.2771	0.290 (0.012)	0.296 (0.037)
$U=4.0,\quad N_h=4,\quad \beta=5.0,\quad P=60$			
E	-8.1799	$-8.44\ (0.64)$	$-8.65\ (2.30)$
$n_{uu}(1)$	0.6167	0.629 (0.043)	0.667 (0.161)
$n_{uu}(2)$	1.3303	1.343 (0.086)	1.338 (0.309)
$n_{uu}(3)$	0.9000	0.884 (0.057)	0.871 (0.200)
$n_{uu}(4)$	0.1531	0.143 (0.011)	0.124 (0.041)
$n_{dd}(1)$	0.1924	0.186 (0.013)	0.173 (0.050)
$n_{dd}(2)$	0.4647	0.439 (0.028)	0.447 (0.105)
$n_{dd}(3)$	0.3103	0.311 (0.021)	0.318 (0.073)
$n_{dd}(4)$	0.05887	0.064 (0.006)	0.062 (0.019)
$n_{ud}(0)$	0.2404	0.243 (0.017)	0.234 (0.063)
$n_{ud}(1)$	1.9912	1.993 (0.129)	1.988 (0.467)
$n_{ud}(2)$	2.2636	2.232 (0.146)	2.240 (0.526)
$n_{ud}(3)$	1.1960	1.225 (0.078)	1.261 (0.286)
$n_{ud}(4)$	0.3088	0.306 (0.020)	0.278 (0.066)

TABLE III. Timing information for Monte Carlo runs. N_h is the number of holes in the 3×3 lattice, N is the total number of electrons, U is the Hubbard U parameter, P is the number of discretization points, passes is the number of Monte Carlo passes used to obtain error bars shown in Tables I and II, and the times are for runs on an FPS 500 computer (our FORTRAN program ran about three times slower on the FPS 500 than on the IBM 3090 located at LSU).

N_h	N	U	P	Passes	$\dfrac{\text{Time}}{1000\ \text{Passes}}$ (min)
5	4	0.0 or 2.0	30	100 000	7.4
5	4	4.0	60	275 000	20.5
4	5	0.0 or 2.0	30	100 000	10.2
4	5	4.0	60	200 000	27.0

trix at different temperatures, we have significantly decreased the errors associated with the Monte Carlo estimator. Despite using an approximate projection for cases of interacting particles, we have demonstrated that accurate results can still be obtained, encouraging pursuit of more accurate representations of the lower temperature density matrix than we have used. Further, this method scales as either P or P^2, depending on when the projection is applied. A variety of projection operators are suggested by this work, including numerical evaluation of the nodes of the density matrix or ground state wave function, or using approximate representations of the above (along the lines of quantum Monte Carlo or Green's function Monte Carlo[4–6]). In addition, we are pursuing the use of a modified form of this approximation in studies with continuous basis sets.

It is instructive to compare and contrast the approach suggested in this paper with the fixed node[4] (FN) and nodal relaxation[5] (NR) methods popular in quantum Monte Carlo and Green's function Monte Carlo. In both methods, the Schrödinger equation is solved with a diffusion process that allows births and deaths of diffusers. In the FN approximation, the nodes of the wave function are fixed and the Schrödinger equation is solved in each nodal region. The nodes act as absorbing boundaries and prevent particles from diffusing from positive to negative (and vice versa) regions. In addition to specifying the nodal structure, an importance wave function is used to reduce the variance by prohibiting unlimited growth of diffusers. In the NR method (an extension of the FN approximation which also uses an importance wave function), diffusion across approximate nodal boundaries is allowed, but unless the nodes are close to the exact nodes, the variance grows quickly. This is due to the use of a Boson wave function as an importance function which rapidly mixes a Bose contribution into the variance as the nodes are relaxed. As a result, the relatively small contributions from the Fermi wave function are overwhelmed by the relatively large Bose contributions. In the path integral approach, the nodes are approximate as in both FN and NR methods. In contrast to the FN approximation, however, there is no importance function and paths are allowed to cross nodal regions and assigned the proper weights. In addition, the path integral method samples from the Fermi distri-

bution, rather than the Bose distribution and should not suffer from the mixing of Bose contributions as does the NR method. Indeed, we have found that the error scales with the number of Monte Carlo passes N_P as $1/\sqrt{N_P}$; thus there appears to be no growth of errors as seen in the NR method. In addition, since the nodal information in the path integral method is calculated "on the fly," there is a potential time and memory savings over the other approaches. The FN and NR methods, however, do appear to attain higher accuracy (tenths of percent vs percent errors), although a detailed comparison of total computer time, length of run, etc. has not been made. However, for quantities where a few percent error is sufficient (such as correlated wave function properties), or for problems where the time scaling we achieve can allow a large number of Monte Carlo passes, the path integral approach should be very useful.

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