Gaussian Quantum Monte Carlo Methods for Fermions and Bosons

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We introduce a new class of quantum Monte Carlo methods, based on a Gaussian quantum operator representation of fermionic states. The methods enable first-principles dynamical or equilibrium calculations in many-body Fermi systems, and, combined with the existing Gaussian representation for bosons, provide a unified method of simulating Bose-Fermi systems. As an application relevant to the Fermi sign problem, we calculate finite-temperature properties of the two dimensional Hubbard model and the dynamics in a simple model of coherent molecular dissociation.

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Calculating the quantum many-body physics of interacting Fermi systems is one of the great challenges in modern theoretical physics. This issue appears in physical problems at all energy scales, from ultracold atomic physics to high-energy lattice QCD. In even the simplest cases, first-principles calculations are inhibited by the complexity of the fermionic wave function, manifest notoriously in the Fermi sign problem. In previous quantum Monte Carlo (QMC) techniques, the sign problem appears as trajectories with negative weights, which contribute to a large sampling error [1]. QMC methods are also complicated by the calculation of large determinants.

In this Letter, we introduce a new QMC method for simulating many-body fermion systems, based on a Gaussian phase-space representation. As an application to condensed matter, we study the well-known Hubbard model. Although it is the simplest model of interacting fermions on a lattice, it is rich in physics and may even describe high-temperature superconductivity [2]. We show that for the Hubbard model the Gaussian representation leads to imaginary-time equations with no negative probabilities or weights. We demonstrate that this removes the well-known Fermi sign problem [1–3], by first-principles numerical simulation without fixed-node [4] or variational approximations.

Phase-space methods [5] provide a way to simulate quantum many-body systems both dynamically and at finite temperature, and have proved useful in bosonic cases. These methods sample the time evolution of a positive distribution on an overcomplete basis set, which is usually the set of coherent states. However, whereas coherent state representations are well defined in the bosonic case, the only known coherent state techniques for fermions involve Grassmann algebra [6], which has an enormous computational complexity.

Here we introduce a phase-space method that overcomes the problem of Grassmann complexity, using a Gaussian expansion for fermions. The operator basis is constructed from pairs of Fermi operators. Because these pairs obey commutation relations, a natural solution of the Grassmann problem is achieved. Furthermore, the resulting equations obviate the need to evaluate large determinants. The elimination of anticommutators means that the technique is far more efficient than previous QMC and stochastic fermion methods [7,8]. We give examples in cases of experimental relevance involving the dynamical problem of Pauli blocking in molecular dissociation, and finite-temperature correlations of fermions in an optical lattice, where the results agree with those of other exact methods. We also perform larger simulations of the 2D Hubbard model in cases where severe sign problems were found previously.

Our starting point is a general expansion of the system density operator:

$$\hat{\rho}(t) = \int P(\vec{\lambda}, t)\hat{\Lambda}(\vec{\lambda})d\vec{\lambda}, \tag{1}$$

where $P(\vec{\lambda}, t)$ is a probability distribution, $\hat{\Lambda}$ is a suitable basis for the class of density matrices being considered, and $d\vec{\lambda}$ is the integration measure for the corresponding generalized phase-space coordinate $\vec{\lambda}$. The operators $\hat{\Lambda}$ are non-Hermitian and form a complete basis for the density operator.

To achieve a unified representation, we define a combined operator basis $\hat{\Lambda} \equiv \Omega\hat{\Lambda}_b\hat{\Lambda}_f$, where $\hat{\Lambda}_b$ and $\hat{\Lambda}_f$ are Gaussian forms over M_b bosonic modes and M fermionic modes, respectively. The (generally) complex number Ω is an additional weighting factor. The properties of the bosonic Gaussian representation are given in [9]. Here we summarize the relevant properties of the fermionic Gaussian form; proofs are given elsewhere [10].

For a system that can be decomposed into M single-particle modes, we define $\hat{\boldsymbol{a}}$ as a column vector of the M annihilation operators, and $\hat{\boldsymbol{a}}^\dagger$ as the corresponding row vector of M creation operators, whose anticommutation relations $[\hat{a}_k, \hat{a}_j^\dagger]_+ = \delta_{kj}$. We also introduce an extended $2M$ vector of all the operators: $\underline{\hat{a}} = (\hat{\boldsymbol{a}}^T, \hat{\boldsymbol{a}}^\dagger)^T$, with the adjoint defined as $\underline{\hat{a}}^\dagger = (\hat{\boldsymbol{a}}^\dagger, \hat{\boldsymbol{a}}^T)$. A general, normally ordered Gaussian operator can then be written,

$$\hat{\Lambda}_f = \mathrm{Pf}[\underline{\underline{\sigma}}_A] : \exp[\underline{\hat{a}}^\dagger(\underline{\underline{I}} - \underline{\underline{\sigma}}^{-1}/2)\underline{\hat{a}}]:, \tag{2}$$

which, because it is constructed from pairs of operators, contains no Grassmann variables. The normalization, chosen to ensure that $\mathrm{Tr}\hat{\Lambda}_f = 1$, consists of the Pfaffian of an antisymmetric form $\underline{\underline{\sigma}}_A$ of the covariance [11].

Normal ordering, denoted by $:\cdots:$, is defined as in the bosonic case, with all annihilation operators to the right of the creation operators, except that each pairwise reordering involved induces a sign change, e.g., $:\hat{a}_i\hat{a}_j^\dagger: = -\hat{a}_j^\dagger\hat{a}_i$. We define *antinormal* ordering similarly, and denote it via curly braces: $\{\hat{a}_j^\dagger\hat{a}_i\} = -\hat{a}_i\hat{a}_j^\dagger$. More generally, we can define nested orderings, in which the outer ordering does not reorder the inner one. For example, $\{:\hat{\Lambda}\hat{a}_j^\dagger:\hat{a}_i\} = -\hat{a}_i\hat{a}_j^\dagger\hat{\Lambda}$, where we assume that the kernel $\hat{\Lambda}$ always remains normally ordered.

The generalized covariance $\underline{\underline{\sigma}}$ and constant matrix $\underline{\underline{I}}$ are $2M \times 2M$ matrices, which we can write as

$$\underline{\underline{\sigma}} = \begin{bmatrix} \mathbf{n}^T - \mathbf{I} & \mathbf{m} \\ \mathbf{m}^+ & \mathbf{I} - \mathbf{n} \end{bmatrix}, \qquad \underline{\underline{I}} = \begin{bmatrix} -\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}, \tag{3}$$

where the number correlation $\mathbf{n}$ is a complex $M \times M$ matrix, the squeezing correlations $\mathbf{m}, \mathbf{m}^+$ are two independent antisymmetric complex $M \times M$ matrices, and $\mathbf{I}$ is the M-mode identity matrix.

The phase space of the fermionic representation is $\vec{\lambda} = (\Omega, \mathbf{n}, \mathbf{m}, \mathbf{m}^+)$, which has a dimension of $1 + p = 1 + M(2M - 1)$. For a combined Bose-Fermi system, there will be an additional $M_b(2M_b + 3)$ bosonic dimensions.

Under the Gaussian representation, physical quantities (operator expectation values) appear as moments of the (weighted) distribution ΩP, denoted as $\langle\cdots\rangle_P$. For quadratic products,

$$\langle\hat{a}_i\hat{a}_j\rangle = \langle m_{ij}\rangle_P, \quad \langle\hat{a}_i^\dagger\hat{a}_j^\dagger\rangle = \langle m_{ij}^+\rangle_P, \quad \langle\hat{a}_i^\dagger\hat{a}_j\rangle = \langle n_{ij}\rangle_P. \tag{4}$$

For higher order products, the corresponding moments can be determined by evaluation of the appropriate (Grassmann) Gaussian integral. There is no way to calculate the expectation value of single ladder operators or any product that is of odd order. However, in physical Hamiltonians, Fermi operators appear only in pairs, and so such "odd" states will not be generated in the course of the evolution. For physical states, the Gaussian basis provides an (over)complete representation.

An equilibrium state at temperature $T = 1/\tau$ (in units where $k_B = 1$) can be cast into an inverse-temperature differential equation for the unnormalized density operator, whereas dynamical evolution will be governed by a real-time master equation ($\hbar = 1$):

$$\frac{d\hat{\rho}}{d\tau} = -\frac{1}{2}[\hat{H}, \hat{\rho}]_+; \qquad \frac{d\hat{\rho}}{dt} = -i[\hat{H}, \hat{\rho}]. \tag{5}$$

To simulate these equations, we therefore need identities that describe the action of the Hamiltonian on the density operator as derivatives on elements of the Gaussian basis. With our ordering notation given above, the necessary operator identities can be written:

$$\begin{aligned} \hat{\Lambda} &= \Omega\frac{\partial}{\partial\Omega}\hat{\Lambda}, \qquad :\underline{\hat{a}}\hat{a}^\dagger\hat{\Lambda}: = \underline{\underline{\sigma}}\,\hat{\Lambda} - \underline{\underline{\sigma}}\frac{\partial\hat{\Lambda}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\sigma}}, \\ \{\underline{\hat{a}}:\underline{\hat{a}}^\dagger\hat{\Lambda}:\} &= -\underline{\underline{\sigma}}\hat{\Lambda} + (\underline{\underline{\sigma}} - \underline{\underline{I}})\frac{\partial\hat{\Lambda}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\sigma}}, \\ \{\underline{\hat{a}}\hat{a}^\dagger\hat{\Lambda}\} &= (\underline{\underline{\sigma}} - \underline{\underline{I}})\hat{\Lambda} - (\underline{\underline{\sigma}} - \underline{\underline{I}})\frac{\partial\hat{\Lambda}}{\partial\underline{\underline{\sigma}}}(\underline{\underline{\sigma}} - \underline{\underline{I}}). \end{aligned} \tag{6}$$

The matrix derivative is here defined as $(\partial/\partial\underline{\underline{\sigma}})_{\mu,\nu} = \partial/\partial\sigma_{\nu\mu}$. There are no Pfaffians or determinants to be calculated in these identities.

We make use of the representation by expanding the density operator in Eq. (5) in terms of Gaussian operators and by applying the identities in Eq. (6). After integrating by parts, we arrive at an equation for the distribution function, which we can sample numerically, by solving stochastic phase-space equations. Although there is never any need to calculate determinants with these methods, the sampling error typically grows in (imaginary) time unless a suitable choice of "stochastic gauge" is made [12], in which one exploits the overcomplete nature of the basis to keep the distribution compact. Stochastic gauges can also be used to eliminate boundary terms that may arise in the partial integration step.

As an application of the fermionic representation, consider the well-known Hubbard model:

$$H(\hat{\mathbf{n}}_\uparrow, \hat{\mathbf{n}}_\downarrow) = -\sum_{ij\sigma} t_{ij}\hat{n}_{ij,\sigma} + U\sum_j \hat{n}_{jj\uparrow}\hat{n}_{jj\downarrow} - \mu\sum_{j\sigma}\hat{n}_{jj\sigma}, \tag{7}$$

where $\hat{n}_{ij\sigma} = \hat{a}_{i\sigma}^\dagger\hat{a}_{j\sigma} = (\hat{\mathbf{n}}_\sigma)_{ij}$, t_{ij} gives the strength of hopping, or tunneling, between sites, U is strength of on-site interactions, and μ is the chemical potential, included to control the total particle number. The index σ denotes spin $(\uparrow, \downarrow)$, and the indices i, j label lattice location. The Hubbard model is the simplest nontrivial model for strongly interacting electrons and is thus an important system in condensed matter physics, with relevance to the theory of high-temperature superconductors [2]. It also describes an ultracold Fermi gas in a optical lattice potential. The physics of the model is not yet fully understood, and although there are known solutions in the 1D case [13], this is not so for higher dimensions.

The 2D problem, in particular, is an important testing ground for QMC methods. Traditional methods are prone to sign problems in the repulsive case ($U > 0$) away from half filling. These are particularly severe for large systems, higher dimensions, stronger interaction, and open-shell configurations [3,7].

Before applying the Gaussian method to the Hubbard model, we first rewrite the interaction terms as

$$U\hat{n}_{jj\uparrow}\hat{n}_{jj\downarrow} = -|U|/2:(\hat{n}_{jj\uparrow} - s\hat{n}_{jj\downarrow})^2:, \quad (8)$$

where $s = U/|U|$. The extra terms here vanish because of the anticommuting property of fermion operators, but they do lead to additional stochastic terms. Such terms are examples of a new type of stochastic gauge, and one that is unique to fermions: vanishing operator products can be used to modify the stochastic behavior of the phase-space equations without affecting the averaged results. With this choice of terms, we map the imaginary-time calculation onto a set of *real* Stratonovich stochastic equations:

$$\frac{d\mathbf{n}_\sigma}{d\tau} = \frac{1}{2}\{(\mathbf{I} - \mathbf{n}_\sigma)\mathbf{\Delta}_\sigma^{(1)}\mathbf{n}_\sigma + \mathbf{n}_\sigma\mathbf{\Delta}_\sigma^{(2)}(\mathbf{I} - \mathbf{n}_\sigma)\}. \quad (9)$$

Here we have introduced the matrix:

$$\Delta_{ij\sigma}^{(r)} = t_{ij} - \delta_{ij}\left\{|U|\left(sn_{jj-\sigma} - n_{jj\sigma} + \frac{1}{2}\right) - \mu + f\xi_j^{(r)}\right\},$$

where $f = -s$ for $\sigma = \downarrow$ and one otherwise. The real Gaussian noise $\xi_j^{(r)}(\tau)$ is defined by the correlations $\langle \xi_j^{(r)}(\tau)\xi_{j'}^{(r')}(\tau')\rangle = 2|U|\delta(\tau - \tau')\delta_{jj'}\delta_{rr'}$. The weights for each trajectory evolve as physically expected for energy-weighted averages, with $d\Omega/d\tau = -\Omega H(\mathbf{n}_\uparrow, \mathbf{n}_\downarrow)$. Because the equations for the variables $n_{ij\sigma}$ are all real, the weights remain positive, thereby avoiding the traditional manifestation of the sign problem.

Consider first the case without tunnel coupling ($t_{ij} = 0$), which describes an ultracold Fermi gas in a deep optical lattice potential. In Fig. 1, we plot the correlation function $g^{(2)} \equiv \langle \hat{n}_\uparrow \hat{n}_\downarrow \rangle / \langle \hat{n}_\uparrow \rangle \langle \hat{n}_\downarrow \rangle$ for $U > 0$, revealing a strong antibunching effect at low temperatures, as expected from the fermion-fermion repulsion.

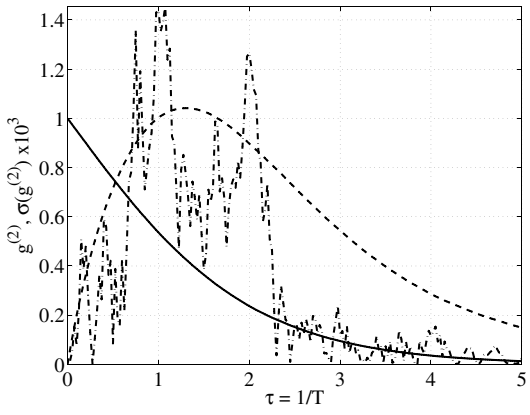

FIG. 1. Second-order correlation function $g^{(2)}$ versus inverse temperature τ for $t_{ij} = 0$, $U = 2$, and $\mu = 1$, for which $\langle n_\sigma \rangle = 0.5$. The solid curve gives the simulation result, and the dashed and dot-dashed lines show the estimated sampling error and deviation from the analytic result, respectively (on a $\times 1000$ scale). Calculated from 100 000 trajectories.

Whether the method can overcome the fundamental cause of the sign problem, which is the complexity of fermionic states, must be demonstrated by calculating physical quantities in cases where the sign problem is known to occur in other methods. Thus we calculate the total energy for $U = 4$ in two dimensions with the nearest-neighbor coupling of strength one as a function of temperature, for different fillings. The results for a 16×16 lattice are shown in Fig. 2, in which to obtain good sampling with the spreading weights we use a branching technique [14].

For a 4×4 lattice at an inverse temperature of $\tau = 20$, we calculate, from 5000 paths, $E = -13.40 \pm 0.80(-13.62)$ at $n = 0.5$ and $E = -19.56 \pm 0.70(-19.57)$ at $n = 0.3125 \pm 0.0028$. These results agree very well with the zero-temperature, exact-diagonalization results given in brackets [15]. Improving the sampling error is simply a matter of including more trajectories. At a filling of $n = 0.3998 \pm 0.0082$, for which the sign deteriorates for a projector QMC calculation [7], we calculate $E = -16.9 \pm 1.1$. Unlike projector QMC techniques, the Gaussian method can calculate any correlation function, at any temperature.

As an application of the method to a dynamical calculation, we consider the process of the dissociation of a molecular Bose condensate into its constituent atoms, which may be fermions or bosons. For simplicity, we consider two atomic modes, representing, for example, states of different spin or momenta, coupled to a single molecular mode via the effective interaction $\hat{H} = \hat{a}^\dagger \hat{b}_1 \hat{b}_2 + \text{H.c.}$, where $\hat{b}_j^\dagger$ and $\hat{b}_j$ are the atomic creation and annihilation operators and $\hat{a}^\dagger$ and $\hat{a}$ are the bosonic molecular operators. Realistic models of the atomic-

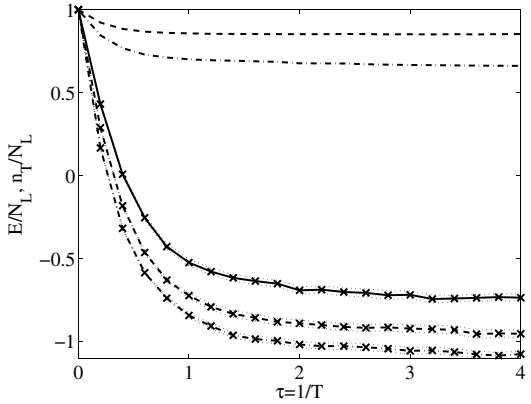

FIG. 2. Energy E per site versus inverse temperature τ for a 16×16 2D lattice for chemical potentials $\mu = 2$ (solid line), $\mu = 1$ (dashed line), and $\mu = 0$ (dot-dashed line). Curves without crosses give the number of particles per site for $\mu = 1$ (dashed line) and $\mu = 0$ (dot-dashed line). $t_{ij} = 1$ for nearest neighbors, $U = 4$, and 50 paths initially. Dotted curves give sampling error estimate.

molecular Feshbach resonances contain such terms to describe the coupling, and it is important to illustrate how this method can represent them. Because the normal spin-spin correlations $\langle \hat{b}_1^\dagger \hat{b}_2 \rangle$ will remain zero in this system (if initially zero), the phase space of the system reduces to $\vec{\lambda} = (\alpha, \alpha^+, n_1, n_2, m, m^+)$, i.e., four complex atomic variables and two complex molecular amplitudes. Applying the identities in Eq. (6) and in [9], we derive the following phase-space equations for the time evolution (where $+ \longrightarrow$ bosonic and $- \longrightarrow$ fermionic):

$$\begin{aligned} \dot{n}_j &= i(\alpha^+ m - \alpha m^+) \pm \sqrt{i} n_j (m\zeta_1^* + m^+ \zeta_2^*), \\ \dot{m} &= -i\alpha(1 \pm n_1 \pm n_2) + \sqrt{i}(\pm m^2 \zeta_1^* + n_1 n_2 \zeta_2^*), \\ \dot{m}^+ &= i\alpha^+(1 \pm n_1 \pm n_2) + \sqrt{i}(n_1 n_2 \zeta_1^* \pm m^{+2} \zeta_2^*), \\ \dot{\alpha} &= -im - \sqrt{i}\zeta_1, \dot{\alpha}^+ = im^+ + \sqrt{i}\zeta_2, \end{aligned} \tag{10}$$

where $j = 1, 2$ and where the $\zeta_k(t)$ are two complex Gaussian noises, defined by the correlations $\langle \zeta_k(t)\zeta_{k'}(t') \rangle = 0, \langle \zeta_k(t)\zeta_{k'}^*(t') \rangle = \delta_{kk'}\delta(t - t')$. The simulations of Eq. (10) are compared with the truncated number-state-based calculations in Fig. 3. Although the initial rates of conversion are the same in each case, a Pauli blocking effect soon slows the fermionic conversion, in contrast to an enhanced bosonic conversion. In these real-time calculations, a growing sampling error appears to be a generic property, although a prudent gauge choice may control the growth rate for a certain time.

In summary, we have introduced here an operator representation that is able to represent arbitrary physical states of fermions. Together with the corresponding bosonic representation, it is the largest class of representations that can be constructed using an operator basis that is Gaussian in the ladder operators. We have presented identities for first-principles calculations of the time evolution of quantum systems, both dynamical (real time) and canonical (imaginary time). Many-body quantum systems map exactly to stochastic equations, provided a suitable stochastic gauge is chosen that eliminates all boundary terms. No computationally intensive determinant calculations are involved.

The simple examples given here show how one, unified method can solve both fermionic and bosonic problems, making it well suited for simulating Bose-Fermi mixtures (e.g., the Bose-Einstein condensate-BCS crossover). Importantly, a new type of Fermi stochastic freedom can be used to map canonical calculations of the Hubbard type onto a real subspace. We have thereby been able to numerically simulate the Hubbard model without sign error, even without employing any of the sophisticated sampling techniques that have been developed over time to optimize more conventional QMC methods. The application of such techniques to the Gaussian approach is yet to be explored.

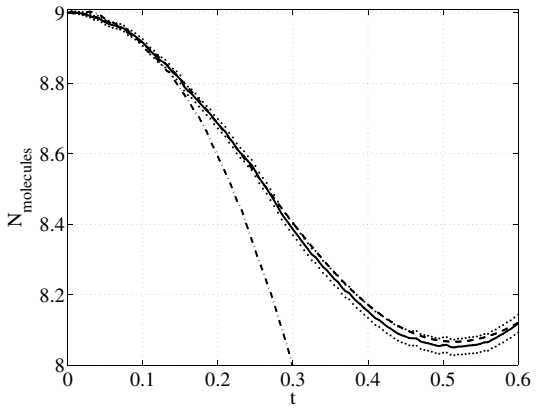

FIG. 3. Molecular dissociation into pairs of fermionic (solid line) or bosonic (dot-dashed line) atoms. For the fermionic case, the dashed curve gives the truncated number-state calculation, and the dotted lines the estimated sampling error. In the bosonic case, the estimated sampling error is too small to be distinctly plotted on this graph. The initial state is a molecular coherent state [$N_{\text{molecules}}(0) = 9$]. Calculated from 10 000 trajectories.

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