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Gaussian phase-space representations for fermions

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We introduce a positive phase-space representation for fermions, using the most general possible multimode Gaussian operator basis. The representation generalizes previous bosonic quantum phase-space methods to Fermi systems. We derive equivalences between quantum and stochastic moments, as well as operator correspondences that map quantum operator evolution onto stochastic processes in phase space. The representation thus enables first-principles quantum dynamical or equilibrium calculations in many-body Fermi systems. Potential applications are to strongly interacting and correlated Fermi gases, including coherent behavior in open systems and nanostructures described by master equations. Examples of an ideal gas and the Hubbard model are given, as well as a generic open system, in order to illustrate these ideas.

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I. INTRODUCTION

The study of strongly correlated Fermi gases is one of the most active areas in modern condensed matter and atomic, molecular, and optical (AMO) physics. In quantum degenerate electron gases, improvements in condensed matter materials have led to sophisticated experiments, typically in reduced dimensional environments. Many interesting quantum phenomena are observed in these systems, including such features as the quantum Hall effect,[1] metal-insulator phase-transitions,[2] high *T*-*c* superconductors,[3] and single electron gates in nanostructures.[4]

Recently, pioneering experiments in strongly interacting ultracold Fermi gases have opened up novel experiments of unprecedented simplicity and precision, both in the crossover between Bose-Einstein condensate (BEC) and BCS regimes[5] and in lattices.[6] The underlying atomic interactions are extremely well-understood, and the dynamics, interactions, and geometry are all highly adaptable. Measurement techniques are also rapidly improving, with direct measurements of collective modes,[7] thermodynamic properties,[8] vortices,[9] and even momentum correlations being recently reported.[10]

This situation provides a substantial opportunity to develop and test first-principles theoretical methods for the investigation of correlations and dynamical effects in quantum degenerate Fermi gases. To this end, we introduce a generalized phase-space representation for correlated fermionic systems. The representation is based on a Gaussian operator basis for fermionic density operators. Like the analogous basis for bosons,[11] the fermionic operator basis enables the representation of arbitrary physical density operators as a positive distribution over a phase space. This representation allows quantum evolution, either in real time or in inverse temperature, to be viewed as a stochastic evolution of covariances or Green's functions.

Phase-space methods based on coherent states[12] have long been used for bosonic systems, with great success. These approaches include the Wigner function,[13] the *Q* function,[14] as well as the well-known Glauber-Sudarshan *P* function,[15] and its generalizations.[16,17] The early methods based on classical phase spaces were later generalized to give the positive-*P* distribution,[18] which has proved a successful way to simulate quantum many-body systems from first principles.[19] This method reduces quantum dynamics to the time evolution of a positive distribution on an overcomplete basis set of coherent-state projection operators, which are special cases of the bosonic Gaussian operators. Applications have been to quantum statistics of lasers,[20] superfluorescence,[21] parametric amplifiers,[18,22] and quantum solitons,[23] as well as quantum dynamics[24] and thermal correlations[25] in Bose-Einstein condensates.

Fermionic phase-space representations are relevant to a long-standing problem in theoretical physics, which is the sign problem that occurs in quantum Monte-Carlo (QMC) calculations of many-body fermionic physics.[26–28] There are many different approximate techniques that can be used, but the intention of this paper is to establish fundamentally exact procedures that avoid the Fermi sign problem. As reported earlier,[29–31] the Gaussian method has been successfully applied to the difficult case of the repulsive Hubbard model.[32] Here, we concentrate on the foundational issues of the Gaussian representation method, presenting the general identities required to apply the method to a wide range of problems in fermionic many-body physics, including both ultracold atomic and condensed matter systems.

To proceed, we make use of three important results, proved elsewhere,[33] (i) the Gaussian fermion operators form a complete basis for any physical density operator, (ii) the distribution can always be chosen positive, and (iii) there are mappings to a second-order differential form for all two-body operators. From these properties, we show that positive-definite Fokker-Planck equations exist for many-body fermionic systems, provided that the distribution tails remain sufficiently bounded. Such Fokker-Planck equations enable first-principles stochastic simulation methods, either in real time or at finite temperature. As is usual in such methods, care must be taken with sampling errors and boundary terms due to the distribution tails. Due to the nonuniqueness of the representation, there is a type of gauge freedom in the choice of stochastic equation. We show how this stochastic gauge freedom, which has been successfully used to remove boundary terms in bosonic representations,[34] can in principle also be used here.

Representations for fermionic density operators were introduced by Cahill and Glauber[35] using fermionic coherent states.[36] These provide a means of defining quasiprobabilities for fermionic states analogous to the well-known bosonic distributions.[35,37] However, the resulting quasiprobabilities are functions of noncommuting Grassmann variables and are thus not directly computationally accessible. Nevertheless, fermion coherent states and Grassmann algebra are useful for deriving analytical results in Fermi systems.

The Gaussian method introduced here overcomes the problems inherent in using Grassmann algebra variables. The Gaussian expansion utilizes an operator basis constructed from pairs of operators, instead of a state-vector basis. Because pairs of fermion operators obey commutation relations rather than anticommutation relations, a natural solution of the anticommutation problem is achieved. The resulting phase space thus exists on a domain of commuting c numbers, rather than anticommuting Grassmann variables. Furthermore, the phase-space equations obviate the need to evaluate large determinants in simulations. This method substantially generalizes and extends earlier phase-space techniques used in quantum optics to treat electronic transitions in atoms.[20,38] It is different than auxiliary field quantum Monte Carlo (AFQMC) methods[39] in condensed matter theory, which use Gaussian operators, but involve path integrals rather than positive expansions of the density matrix.

We begin in Sec. II by defining the Gaussian operator basis on which the representation is based and introducing some convenient notations. In Sec. III, we define the Gaussian representation as an expansion in Gaussian operators, and then show how the representation establishes a novel class of exact Monte Carlo type methods for simulating the real-time dynamics or finite-temperature equilibrium of a quantum system. We show how to map quantum operator evolution onto a set of stochastic (real or complex) differential equations and give the correspondences necessary to calculate physical moments.

Finally, in Sec. V, we give examples of the application of the method. These are intended to be illustrative rather than exhaustive, and further examples and applications in greater detail will be given elsewhere. In particular, we note that any nonlinear application requires a careful analysis of the issues of sampling error and boundary term behavior. For simplicity, we focus on the ideal Fermi gas, a generic open system master equation and the finite-temperature Hubbard model, as well as showing how to apply gauges to modify the drift evolution.

Appendix A summarizes the mathematical properties of the Gaussian operators proved in Ref. 33 that are essential to making use of the phase-space representation, and Appendix B gives an alternative form of the operator mappings.

II. GAUSSIAN OPERATORS

Before discussing the Gaussian representation, we first introduce the fermion operators on which it is based. Fermionic Gaussian operators are defined as exponentials of quadratic forms in the Fermi annihilation or creation operators. This simple definition encompasses a wide range of physical applicability. Obviously, it includes the well-known thermal density matrices of the free field. Since the definition includes quadratic forms involving pairs of annihilation or creation operators, it also encompasses the pure-state density matrices that correspond to the BCS states used in superconductivity.

A more subtle issue is that the definition is not restricted to Hermitian operators. This has the advantage of leading to completeness properties that are much stronger than if the definition were restricted to only Hermitian operators. Some of these issues are discussed elsewhere, in a more formal derivation of the mathematical properties of the Gaussian operators.[33]

A. Notation

Before giving mathematical results, we summarize the notation that will be used. We can decompose a given fermionic system into a set of M orthogonal single-particle modes or orbitals. With each of these modes, we associate creation and annihilation operators $\hat{b}_j^\dagger$ and $\hat{b}_j$, with anticommutation relations

$$[\hat{b}_k,\hat{b}_j^\dagger]_+ = \delta_{kj}$$

$$[\hat{b}_k,\hat{b}_j]_+ = 0, \tag{2.1}$$

where $j,k=1,\ldots,M$. Thus, $\hat{\boldsymbol{b}}$ is a column vector of the M annihilation operators, and $\hat{\boldsymbol{b}}^\dagger$ is a row vector of the corresponding creation operators.

For products of operators, we make use of normal and antinormal ordering concepts. 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., $:\hat{b}_i\hat{b}_j^\dagger: = -\hat{b}_j^\dagger\hat{b}_i$. The sign changes are necessary so that the anticommuting natures of the Fermi operators can be accommodated without ambiguity.

To enable the general Gaussian operator to be written in a compact form, we use an extended-vector notation

$$\underline{\hat{b}} = \begin{pmatrix} \hat{\boldsymbol{b}} \\ \hat{\boldsymbol{b}}^{\dagger T} \end{pmatrix} \tag{2.2}$$

is defined as an extended column vector of all $2M$ operators, with an adjoint row vector defined as

$$\underline{\hat{b}}^\dagger = (\hat{\boldsymbol{b}}^\dagger,\hat{\boldsymbol{b}}^T). \tag{2.3}$$

Throughout the paper, we print vectors of length M and $M\times M$ matrices in bold type, and index them where necessary with Latin indices: $j=1,\ldots,M$. Vectors of length $2M$ we denote with an underline, while $2M\times 2M$ matrices are indicated by a double underline. These extended vectors and matrices are indexed where necessary with Greek indices: $\mu=1,\ldots,2M$. For further examples of this notation, see Refs. 11 and 33. More general kinds of vectors are denoted with an arrow notation: $\vec{\lambda}$.

B. Definition of the Gaussian operator

We define a Gaussian operator to be any normally ordered, Gaussian form of annihilation and creation operators. Like a complex number Gaussian, the operator Gaussian is an exponential of a quadratic form, with the exponential defined by its series representation. The most general Gaussian form is a cumbersome object to manipulate, unless products of odd numbers of operators are excluded. Fortunately, restricting the set of Gaussians to those containing only even products can be physically justified on the basis of superselection rules for fermions. Because it is constructed from pairs of operators, this type of Gaussian operator contains no Grassmann variables.

With the extended-vector notation, we can write any general Gaussian operator $\hat{\Lambda}$ as

$$\hat{\Lambda}(\vec{\lambda}) = \Omega \frac{1}{\mathcal{N}} :\exp[-\underline{\hat{b}}^{\dagger} \underline{\underline{\Sigma}} \underline{\hat{b}}/2]:, \tag{2.4}$$

where Ω is an amplitude, $\mathcal{N}$ is a normalizing factor defined so that $\mathrm{Tr}[\hat{\Lambda}(\vec{\lambda})]=\Omega$, and $\underline{\underline{\Sigma}}$ is a $2M \times 2M$ complex matrix. For later identification with physical observables, it proves useful to write $\underline{\underline{\Sigma}}$ in the form

$$\underline{\underline{\Sigma}} = (\underline{\underline{\sigma}}^{-1} - 2\underline{\underline{I}}), \tag{2.5}$$

where $\underline{\underline{\sigma}}$ is a generalized covariance matrix and $\underline{\underline{I}}$ is the constant matrix is defined as

$$\underline{\underline{I}} = \begin{bmatrix} -\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}. \tag{2.6}$$

It is convenient to introduce complex $M \times M$ matrices $\mathbf{n}$ and $\tilde{\mathbf{n}}=\mathbf{I}-\mathbf{n}$ which, as we show later, correspond to normal Green's functions for particles and holes, respectively. We also introduce two independent antisymmetric complex $M \times M$ matrices $\mathbf{m}$ and $\mathbf{m}^{+}$ that correspond to anomalous Green's functions. These are related to the covariance matrix $\underline{\underline{\sigma}}$ by

$$\underline{\underline{\sigma}} = \begin{bmatrix} -\tilde{\mathbf{n}}^{T} & \mathbf{m} \\ \mathbf{m}^{+} & \tilde{\mathbf{n}} \end{bmatrix} = \begin{bmatrix} \mathbf{n}^{\mathbf{T}} - \mathbf{I} & \mathbf{m} \\ \mathbf{m}^{+} & \mathbf{I} - \mathbf{n} \end{bmatrix}. \tag{2.7}$$

Thus the covariance matrix has a type of antisymmetry, which can be written as $\underline{\underline{\sigma}}=-\underline{\underline{\sigma}}^{+}$, where "+" denotes a generalized transpose operation defined by

$$\begin{bmatrix} \mathbf{a} & \mathbf{b} \\ \mathbf{c} & \mathbf{d} \end{bmatrix}^{+} \equiv \begin{bmatrix} \mathbf{d} & \mathbf{c} \\ \mathbf{b} & \mathbf{a} \end{bmatrix}^{T}. \tag{2.8}$$

In summary, the Gaussian operators are parametrized by

$$\vec{\lambda} = (\Omega, \mathbf{n}, \mathbf{m}, \mathbf{m}^{+}), \tag{2.9}$$

corresponding to $1+p=1+M(2M-1)$ complex parameters. Where necessary, we will index over all the independent phase-space variables with the notation λ_a, $a=0,\ldots p$.

The normalization $\mathcal{N}$ contains a Pfaffian, whose square is equal to a matrix determinant. We will show that $\mathcal{N}$ does not appear explicitly in later results. The additional variable Ω plays the role of a weighting factor in the expansion. This allows us to represent unnormalized density operators like $\exp(-\beta\hat{H})$ and to introduce stochastic gauges that change these relative weighting factors in order to stabilize trajectories.

C. Moments

Just as with classical Gaussian forms, these generalized fermionic Gaussians are completely characterized by their first-order moments (to within a weight factor). From Eq. (A3) of Appendix A, we have

$$\mathrm{Tr}[\hat{b}_i \hat{b}_j \hat{\Lambda}] = \Omega m_{ij},$$

$$\mathrm{Tr}[\hat{b}_i^{\dagger} \hat{b}_j \hat{\Lambda}] = \Omega n_{ij},$$

$$\mathrm{Tr}[\hat{b}_j \hat{b}_i^{\dagger} \hat{\Lambda}] = \Omega \tilde{n}_{ij},$$

$$\mathrm{Tr}[\hat{b}_i^{\dagger} \hat{b}_j^{\dagger} \hat{\Lambda}] = \Omega m_{ij}^{+}. \tag{2.10}$$

If the Gaussian operator happens to be a physical density matrix, these quantities correspond to the first-order correlations or Green's functions. Thus, in many-body terminology, $\mathbf{n}$ and $\tilde{\mathbf{n}}$ are the normal Green's functions of particles and holes, respectively, and $\mathbf{m}$ and $\mathbf{m}^{+}$ are anomalous Green's functions. From this, we see that, for the subset of Gaussians that are physical density matrices, we must have that $\mathbf{m}^{\dagger}=\mathbf{m}^{+}$ and $\mathbf{n}^{\dagger}=\mathbf{n}$. Furthermore, $\mathbf{n}$ and $\tilde{\mathbf{n}}$ must be positive semidefinite (because $0 \leqslant \langle \hat{b}_j^{\dagger} \hat{b}_j \rangle \leqslant 1$).

More generally, the phase-space function $O(\vec{\lambda})$ corresponding to the normally ordered operator $\hat{O}$ is defined as a phase-space correspondence, according to

$$O(\vec{\lambda}) \equiv \langle \hat{O} \rangle_{\vec{\lambda}} \equiv \mathrm{Tr}(\hat{O}\hat{\Lambda}(\vec{\lambda}))/\Omega. \tag{2.11}$$

For higher-order moments, a form of Wick's theorem applies to any normally ordered product. One simply writes down the sum of all distinct factorizations into pairs, with a minus sign in front of any product that is an odd permutation of the original form. The term distinct factorization means that neither permutation of pair ordering nor reordering inside a pair is regarded as significant, since these do not change the result. Thus, an Nth order correlation (expectation value of a product of $2N$ operators), is the sum of $(2N)!/(2^N N!)$ distinct terms, as follows:

$$\langle :\hat{b}_{\mu_1} \cdots \hat{b}_{\mu_{2N}}: \rangle_{\vec{\lambda}} = \sum_{P} (-1)^P \langle :\hat{b}_{\mu_{P(1)}} \hat{b}_{\mu_{P(2)}}: \rangle_{\vec{\lambda}} \times \cdots \times \langle :\hat{b}_{\mu_{P(2N-1)}} \hat{b}_{\mu_{P(2N)}}: \rangle_{\vec{\lambda}}. \tag{2.12}$$

Here the sum is over all $(2N)!/(2^N N!)$ distinct pair permutations $P(1),\ldots,P(2N)$ of $1,\ldots,2N$, and where $(-1)^P$ is the parity of the permutation (i.e., the number of pairwise transpositions required to perform the permutation).

Thus, for example, the second-order number correlation moment is

$$\langle \hat{b}_i^{\dagger} \hat{b}_j^{\dagger} \hat{b}_j \hat{b}_i \rangle_{\vec{\lambda}} = n_{ii} n_{jj} - n_{ij} n_{ji} + m_{ij}^{+} m_{ji}. \tag{2.13}$$

D. Generalized thermal states

An important subset of the Gaussian operators is the set of generalized thermal operators, for which $\mathbf{m}=\mathbf{m}^{+}=\mathbf{0}$. These include the canonical density matrices for free Fermi gases in the case that $\mathbf{n}$ and $\tilde{\mathbf{n}}$ are each Hermitian and positive-definite. More generally, however, we do not require $\mathbf{n}$ to be Hermitian. In all cases, the generalized thermal operators in normally ordered Gaussian form can be written most directly in terms of the hole population, $\tilde{\mathbf{n}}=\mathbf{I}-\mathbf{n}$

$$\hat{\Lambda}(\vec{\lambda})=\Omega\,\det[\tilde{\mathbf{n}}]:\exp[\hat{\mathbf{b}}^{\dagger}(\tilde{\mathbf{n}}^{-1}-2\mathbf{I})^{T}\hat{\mathbf{b}}]:. \tag{2.14}$$

Of course, there is a symmetry here: in an antinormally ordered Gaussian, the role of $\hat{\mathbf{b}}^{\dagger}$ and $\hat{\mathbf{b}}$ is reversed and, consequently, so is the role of $\mathbf{n}$ and $\tilde{\mathbf{n}}$. Our choice of normal ordering is in fact arbitrary from a physical point of view, and antinormal ordering would also serve our purpose equally well, provided all the identities were redefined.

By comparison, the usual canonical form of the fermionic thermal state with a diagonal Hamiltonian $H=\hat{\mathbf{b}}^{\dagger}\boldsymbol{\omega}\hat{\mathbf{b}}$ and a chemical potential μ, is an unordered form, namely

$$\hat{\rho}(\beta)=\exp[\beta\hat{\mathbf{b}}^{\dagger}(\mu\mathbf{I}-\boldsymbol{\omega})\hat{\mathbf{b}}]/Z. \tag{2.15}$$

Here, Z is the partition function and $\beta=1/k_{B}T$ is the inverse temperature. In this case, the mean occupation numbers are diagonal and well-known. They are given by the Fermi-Dirac distribution,

$$\langle\hat{b}_{i}^{\dagger}\hat{b}_{j}\rangle=\bar{n}_{ij}=\frac{\delta_{ij}}{1+e^{\beta(\omega_{i}-\mu)}}. \tag{2.16}$$

However, both Gaussian forms are equivalent. A normally ordered thermal Gaussian can always be chosen so that $\mathbf{n}$ is Hermitian, and hence $\hat{\rho}(\beta)=\hat{\Lambda}(\vec{\lambda})$, if and only if $\Omega=1$ and $n_{ij}=\bar{n}_{ij}$.

A rather trivial example is the vacuum state, in which $\mathbf{n}=\mathbf{0}$, so that

$$\hat{\Lambda}(1,\mathbf{0},\mathbf{0},\mathbf{0})=|\mathbf{0}\rangle\langle\mathbf{0}|=:\exp[-\hat{\mathbf{b}}^{\dagger}\hat{\mathbf{b}}]:. \tag{2.17}$$

We emphasize that since the Gaussian forms used here are not necessarily Hermitian, the generalized thermal operators are a much larger set of operators than the usual canonical thermal density matrices.

E. Generalized BCS states

A second important subset of the Gaussian operators is the generalization of the Bardeen-Cooper-Schreiffer (BCS) states, which are an excellent approximation to the ground state of a weakly interacting (BCS) superconductor. The BCS states are the fermionic equivalent of the squeezed states found in quantum optics and are composed only of correlated fermion pairs. In the case of fermions, these are the fundamental pure states that carry phase information. In Bose gases, coherent states can also carry phase information (as in a laser or Bose-Einstein condensate), but the fermionic equivalent of these is an unphysical Grassmann coherent state.

An unnormalized pure BCS state is defined as[40]

$$|\Psi_{\mathrm{BCS}}\rangle=\exp[\hat{\mathbf{b}}^{\dagger}\mathbf{g}\hat{\mathbf{b}}^{\dagger}/2]|\mathbf{0}\rangle, \tag{2.18}$$

so that the corresponding density matrix is

$$\begin{aligned}\hat{\rho}_{\mathrm{BCS}}&=|\Psi_{\mathrm{BCS}}\rangle\langle\Psi_{\mathrm{BCS}}|=\exp[\hat{\mathbf{b}}^{\dagger}\mathbf{g}\hat{\mathbf{b}}^{\dagger}/2]|\mathbf{0}\rangle\langle\mathbf{0}|\exp[\hat{\mathbf{b}}\mathbf{g}^{\dagger}\hat{\mathbf{b}}/2]\\&=:\exp[\hat{\mathbf{b}}^{\dagger}\mathbf{g}\hat{\mathbf{b}}^{\dagger}/2-\hat{\mathbf{b}}^{\dagger}\hat{\mathbf{b}}+\hat{\mathbf{b}}\mathbf{g}^{\dagger}\hat{\mathbf{b}}/2]:.\end{aligned} \tag{2.19}$$

Apart from being unnormalized, this corresponds directly to a Gaussian in our normal form.

More general non-Hermitian BCS type states are obtained by replacing $\mathbf{g}^{\dagger}$ by an independent matrix $\mathbf{g}^{+}$. This generalized BCS Gaussian has an extended covariance matrix of

$$\underline{\underline{\sigma}}=\begin{bmatrix}(\mathbf{I}+\mathbf{g}\mathbf{g}^{+})^{-1} & 0\\ 0 & (\mathbf{I}+\mathbf{g}^{+}\mathbf{g})^{-1}\end{bmatrix}\begin{bmatrix}-\mathbf{I} & \mathbf{g}\\ \mathbf{g}^{+} & \mathbf{I}\end{bmatrix}. \tag{2.20}$$

Clearly, from this we can see that the occupation numbers and correlations for a generalized BCS state are given by

$$\begin{aligned}\mathbf{n}&=\mathbf{g}^{+}(\mathbf{I}+\mathbf{g}\mathbf{g}^{+})^{-1}\mathbf{g},\\ \tilde{\mathbf{n}}&=(\mathbf{I}+\mathbf{g}^{+}\mathbf{g})^{-1}\\ \mathbf{m}&=(\mathbf{I}+\mathbf{g}\mathbf{g}^{+})^{-1}\mathbf{g}\\ \mathbf{m}^{+}&=\mathbf{g}^{+}(\mathbf{I}+\mathbf{g}\mathbf{g}^{+})^{-1},\end{aligned} \tag{2.21}$$

which gives the expected result that $\mathbf{m}^{+}\mathbf{m}=\tilde{\mathbf{n}}\mathbf{n}$.

In summary, the usual BCS states have a density matrix which is Gaussian and has $\mathbf{g}^{+}=\mathbf{g}^{\dagger}$. These pure states exist as a subset of a more general class of BCS-like Gaussian operators. This class also includes operators which have $\mathbf{g}^{+}\neq\mathbf{g}^{\dagger}$ and are, therefore, not Hermitian. While these operators do not correspond to any physical state, a linear combination of them can still correspond to a possible physical fermionic many-body state, provided the result is Hermitian and positive-definite.

III. GAUSSIAN REPRESENTATION

While the Gaussian operators include a large and interesting set of physical density operators, there are many cases where the existence of interparticle interactions leads to more general fermionic states whose correlations are of more complex, non-Gaussian forms. In all such cases, the overall physical density operator can still be expressed as a positive distribution over the Gaussian operators. Furthermore, any two-body operator acting on a generalized Gaussian can be written as a second-order derivative. These important results, proved in Ref. 33, mean that probabilistic, random sampling methods may be used to calculate physical observables, as we show below.

A. Definition

The Gaussian representation is defined as an expansion of the density matrix for any physical state $\hat{\rho}(\tau)$ as a positive distribution over the Gaussian basis. That is

$$\hat{\rho}(\tau) = \int P(\vec{\lambda}, \tau)\hat{\Lambda}(\vec{\lambda})d\vec{\lambda}, \tag{3.1}$$

where the expansion coefficients are normalized to one

$$\int P(\vec{\lambda}, \tau)d\vec{\lambda} = 1. \tag{3.2}$$

Here, the variable τ can either be real time t or imaginary time (inverse temperature) β.

This expansion defines a type of phase-space representation of the state: the vector $\vec{\lambda}$ of Gaussian parameters becomes a generalized phase-space coordinate, the function $P(\vec{\lambda}, \tau)$ is then a probability distribution function over the generalized phase space, and $d\vec{\lambda} = d^{2(p+1)}\vec{\lambda}$ is the phase-space integration measure.

B. Completeness and positivity

The Gaussian representation as we have defined it here always exists for any physical state. In other words, a distribution always exists and can always be chosen to be positive. This property follows from the overcompleteness of the Gaussian basis, which can be stated as follows:

For any physical density matrix $\hat{\rho}$, a positive set of coefficients P_j exists such that

$$\hat{\rho} = \sum_j P_j \hat{\Lambda}(\vec{\lambda}^{(j)}), \tag{3.3}$$

or, in a continuous formulation, a positive semidefinite function $P(\vec{\lambda})$ exists such that

$$\hat{\rho} = \int P(\vec{\lambda})\hat{\Lambda}(\vec{\lambda})d\vec{\lambda}, \tag{3.4}$$

where the Gaussian operators $\hat{\Lambda}(\vec{\lambda})$ are as defined in Eq. (2.4).

By "physical density matrix," we mean one in which there are no coherences between states that differ by an odd number of fermions. The proof of this result, given in Ref. 33, does not rely on the complex amplitudes Ω that are part of the most general Gaussian operator (i.e., we set $\Omega = 1$), since using these with complex values is equivalent to having a complex distribution, although this may be useful when constructing particular exact solutions, depending on the problem. The property is analogous to a similar result known for the positive-P bosonic representation.[18]

Note that the expansion P_j or $P(\vec{\lambda})$ is not guaranteed to be unique. In fact, there may be many possible positive expansions that correspond to the same physical state. This nonuniqueness is a further aspect of the overcompleteness of the Gaussian operators. It allows the resulting phase-space representation to be used for calculating time evolution and is the basis of stochastic gauges, which we discuss further in Sec. IV D.

As a simple example, consider the single-mode density operator. In this case, a complete operator basis for fermions would be the number state projection operators, both of which are in fact Gaussian operators $\hat{\Lambda}(\Omega, n)$

$$|0\rangle\langle 0| = \hat{\Lambda}(1,0),$$

$$|1\rangle\langle 1| = \hat{\Lambda}(1,1). \tag{3.5}$$

Because superselection rules prohibit superpositions of states differing by odd numbers of fermions, this is the most general case possible, and clearly the Pauli exclusion principle means that there can be no anomalous moments m or m^+ in a single-mode Gaussian.

Equation (3.5) implies that just two single-mode Gaussians are sufficient to form a complete basis set for all possible single-mode density matrices, and of course, these must have a positive expansion coefficient to ensure overall positivity of $\hat{\rho}$. Thus, a single-mode density matrix can always be expanded as a discrete sum of Gaussians with *positive* coefficients, as in Eq. (3.3), since for $0 \leqslant \bar{n} \leqslant 1$

$$\hat{\rho}(\bar{n}) = (1 - \bar{n})\hat{\Lambda}(1,0) + \bar{n}\hat{\Lambda}(1,1). \tag{3.6}$$

However, there are other possible expansions as well. In the single-mode case, all physical density operators are also Gaussian operators: $\hat{\rho} = \hat{\Lambda}_1(1, \bar{n})$. This means that a continuous expansion of form given in Eq. (3.4) is also possible, with

$$P(\vec{\lambda}) = \delta^2(\Omega - 1)\,\delta^2(\bar{n} - n). \tag{3.7}$$

It is clear from these examples that the Gaussian operators are *overcomplete*: a physical density matrix may be represented by more than one positive distribution over the Gaussians. So far, we have only considered examples in which the Gaussians are themselves physical density operators. However, single-mode Gaussian operators as defined here can have n complex. Including such operators, which do not correspond directly to any physical density operators, provides even more freedom of choice in constructing expansions.

C. Moments

Some basic properties of $P(\vec{\lambda}, \tau)$ follow from those of the Gaussian operators. For example, using the normalization of the Gaussian operators, we find that

$$\mathrm{Tr}[\hat{\rho}] = \int P(\vec{\lambda}, \tau)\Omega d\vec{\lambda} \equiv \overline{\Omega}. \tag{3.8}$$

Thus, the normalized distribution P can represent unnormalized density operators by incorporating the normalization into the mean weight $\overline{\Omega}$.

More generally, the expectation value of an operator $\hat{O}$ evaluates to

$$\langle \hat{O} \rangle \equiv \mathrm{Tr}[\hat{O}\hat{\rho}]/\mathrm{Tr}[\hat{\rho}] = \int P(\vec{\lambda}, \tau)\mathrm{Tr}[\hat{O}\hat{\Lambda}]d\vec{\lambda}/\overline{\Omega} \equiv \langle O(\vec{\lambda}) \rangle_P, \tag{3.9}$$

where the weighted average $\langle \ldots \rangle_P$ is defined as[41]

$$\langle O(\vec{\lambda})\rangle_P = \int P(\vec{\lambda},\tau)\Omega O(\vec{\lambda})d\vec{\lambda}/\overline{\Omega}. \tag{3.10}$$

The phase-space function $O(\vec{\lambda})$ corresponding to the operator $\hat{O}$ is defined as previously in Eq. (2.11) and can be evaluated using the generalized Wick result of Eq. (2.12).

Physical quantities thus correspond to (weighted) moments of P. For example, from traces evaluated in Sec. II C, we find that the normal and anomalous Green's functions correspond to first-order moments

$$\langle \hat{b}_i \hat{b}_j\rangle = \langle m_{ij}\rangle_P,$$

$$\langle \hat{b}_i^\dagger \hat{b}_j\rangle = \langle n_{ij}\rangle_P,$$

$$\langle \hat{b}_i^\dagger \hat{b}_j^\dagger\rangle = \langle m_{ij}^+\rangle_P. \tag{3.11}$$

Number-number correlations correspond to averages of products of these moments

$$\langle :\hat{n}_i\hat{n}_j:\rangle = \langle n_{ii}n_{jj} - n_{ij}n_{ji} + m_{ij}^+ m_{ji}\rangle_P, \tag{3.12}$$

where $\hat{n}_i \equiv \hat{b}_i^\dagger \hat{b}_i$.

Similarly, higher-order correlations correspond to higher-order moments, the form of which are also determined by the generalized Wick result of Eq. (2.12).

We note that the expectation value of any odd product of operators must vanish, e.g., $\langle \hat{b}_i\rangle = 0$. Thus the distribution cannot represent a superposition of states whose total number differ by an odd number. Such superposition states we exclude from our definition of the physical state, as they are not generated by evolution under any known physical Hamiltonian. The Gaussian distribution can, however, represent systems in which particles are coherently added or removed in pairs, leading to nonzero anomalous correlations $\langle m_{ij}\rangle_P$. On the other hand, if the total number of particles is conserved or changed only via contact with a thermal reservoir, then the anomalous correlations will be identically zero, and we can represent the system via an expansion in only the thermal subset of Gaussian operators.

IV. TIME EVOLUTION

Here we show how these positive representations of density matrices can be put to use. By use of these representations, any quantum evolution arising from one-body and two-body interactions can be sampled by classical stochastic processes. To see this, note that the evolution of a density operator is determined by a master equation, of the general form

$$\frac{d}{d\tau}\hat{\rho}(\tau) = \hat{L}[\hat{\rho}(\tau)], \tag{4.1}$$

where the $\hat{L}$ is a superoperator that premultiplies and postmultiplies the density operator by combinations of annihilation and creation operators and where τ can represent either real or imaginary time.

A. Types of evolution

We consider three general time-evolution categories.

1. Hamiltonian quantum dynamics

For unitary evolution in real time t, the superoperator is a commutator with the Hamiltonian

$$\hat{L}[\hat{\rho}] = -\frac{i}{\hbar}[\hat{H},\hat{\rho}]. \tag{4.2}$$

2. Irreversible quantum dynamics

More generally, for an open quantum system, there will be additional terms of Lindblad form[42,43] to describe the coupling to the environment

$$\hat{L}[\hat{\rho}] = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] + \sum_K (2\hat{O}_K\hat{\rho}\hat{O}_K^\dagger - [\hat{O}_K^\dagger\hat{O}_K,\hat{\rho}]_+), \tag{4.3}$$

where the operators $\hat{O}_K$ depend on the correlations of the environment or reservoir, within the Markov approximation.

3. Thermal equilibrium ensemble

To calculate the canonical thermal equilibrium state at temperature $T = 1/k_B\beta$, one can solve an inverse temperature equation for the unnormalized density operator

$$\frac{d}{d\beta}\hat{\rho} = -\frac{1}{2}[\hat{H} - \mu\hat{N},\hat{\rho}]_+, \tag{4.4}$$

the solution of which will generate the unnormalized density operator for a grand canonical distribution: $\hat{\rho}(\beta) = \exp[-\beta(\hat{H} - \mu\hat{N})]$.

B. Operator mappings

We wish to show how to transform a general operator time-evolution equation [Eq. (4.1)] into a Fokker-Planck equation for the distribution and, hence, into a stochastic equation. A crucial part of this procedure is to be able to transform the operator equations into a differential form.

The first step is to substitute for $\hat{\rho}$ the expansion in Eq. (3.1)

$$\int \frac{dP(\vec{\lambda},\tau)}{d\tau}\hat{\Lambda}(\vec{\lambda})d\vec{\lambda} = \int P(\vec{\lambda},\tau)\hat{L}[\hat{\Lambda}(\vec{\lambda})]d\vec{\lambda}. \tag{4.5}$$

Second, we use the differential identities summarized in Eq. (A5) of Appendix A to convert the superoperator $\hat{L}[\hat{\Lambda}]$ into an operator $\mathcal{L}[\hat{\Lambda}]$ that contains only derivatives of $\hat{\Lambda}$. Next, we integrate by parts to obtain, provided that no boundary terms arise,

$$\int \frac{dP(\vec{\lambda},\tau)}{d\tau}\hat{\Lambda}(\vec{\lambda})d\vec{\lambda} = \int \mathcal{L}'[P(\vec{\lambda},\tau)]\hat{\Lambda}(\vec{\lambda})d\vec{\lambda}, \tag{4.6}$$

where $\mathcal{L}'$ is a reordered form of $\mathcal{L}$, with a sign change to derivatives of odd order. Finally, we see that this equation

holds if the distribution function satisfies the evolution equation

$$\frac{d}{d\tau}P(\vec{\lambda},\tau)=\mathcal{L}'[P(\vec{\lambda},\tau)]. \tag{4.7}$$

This procedure for going from the master equation for $\hat{\rho}$ to the evolution equation for P can be implemented using a set of operator mappings. To write these mappings in a compact form, we introduce *anti*normal ordering as the opposite of normal ordering and denote it via curly braces: $\{\hat{b}_j^\dagger\hat{b}_i\}=-\hat{b}_i\hat{b}_j^\dagger$. We also use nested orderings, in which the outer ordering does not reorder the inner one. For example, $\{:\hat{\rho}\hat{b}_j^\dagger:\hat{b}_i\}=-\hat{b}_i\hat{b}_j^\dagger:\hat{\rho}:$, where $\hat{\rho}$ is some density operator. When ordering products that contain the density operator $\hat{\rho}$, we do not change the ordering of $\hat{\rho}$ itself; the other operators are merely reordered around it.

Including all possible orderings, we obtain the following mappings:

$$\hat{\rho}\to-\frac{\partial}{\partial\Omega}\Omega P,$$

$$:\hat{\rho}\underline{\hat{b}}\underline{\hat{b}}^\dagger:\to\left[\underline{\underline{\sigma}}+\underline{\underline{\sigma}}\frac{\overleftrightarrow{\partial}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\sigma}}\right]P,$$

$$:\{\hat{\rho}\underline{\hat{b}}\}\underline{\hat{b}}^\dagger:\to\left[\underline{\underline{\tilde{\sigma}}}+\underline{\underline{\tilde{\sigma}}}\frac{\overleftrightarrow{\partial}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\sigma}}\right]P,$$

$$:\underline{\hat{b}}\{\underline{\hat{b}}^\dagger\hat{\rho}\}:\to\left[\underline{\underline{\tilde{\sigma}}}+\underline{\underline{\sigma}}\frac{\overleftrightarrow{\partial}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\tilde{\sigma}}}\right]P,$$

$$\{\hat{\rho}\underline{\hat{b}}\underline{\hat{b}}^\dagger\}\to\left[-\underline{\underline{\tilde{\sigma}}}+\underline{\underline{\tilde{\sigma}}}\frac{\overleftrightarrow{\partial}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\tilde{\sigma}}}\right]P, \tag{4.8}$$

where $\underline{\underline{\tilde{\sigma}}}=\underline{\underline{I}}-\underline{\underline{\sigma}}$. The notation $\frac{\overleftrightarrow{\partial}}{\partial x}$ indicates a differentiation on both left and right sides with the ordering of matrix multiplication preserved, so that

$$\left[\underline{\underline{\sigma}}\frac{\overleftrightarrow{\partial}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\sigma}}\right]_{\mu\nu}\equiv\frac{\partial}{\partial\sigma_{\mu'\nu'}}\sigma_{\mu\nu'}\sigma_{\mu'\nu}. \tag{4.9}$$

For convenience of the reader, these identities are summarized in a more explicit form using the $M\times M$ submatrices, in Appendix B. We note here that the mixed identities involving nested orderings are not independent—one can always be obtained from the other. Also, since the kernel is analytic, the distinct analytic derivatives of the kernel are all interchangeable and lead to equivalent identities, so that generically if $\lambda_a=\lambda_a^x+i\lambda_a^y$, then $\partial/\partial\lambda_a=\partial/\partial\lambda_a^x=-i\,\partial/\partial\lambda_a^y$.

If there are higher than quadratic terms present, the differential mappings are applied in sequence. The operator set closest to the operator $\hat{\rho}$ leads to the innermost differential operator acting on P. Thus, for example,

$$:\hat{\rho}\hat{b}_\mu\hat{b}_\nu^\dagger\hat{b}_{\mu'}\hat{b}_{\nu'}^\dagger:\to\left[\sigma_{\mu'\nu'}+\frac{\partial}{\partial\sigma_{\alpha\beta}}\sigma_{\mu'\beta}\sigma_{\alpha\nu'}\right]\times\left[\sigma_{\mu\nu}+\frac{\partial}{\partial\sigma_{\gamma\delta}}\sigma_{\mu\delta}\sigma_{\gamma\nu}\right]P. \tag{4.10}$$

For a system in which the total number is conserved, one can use the simpler thermal subset of these correspondences, i.e., including only those that contain terms that remain when all anomalous correlations vanish

$$\hat{b}_i^\dagger\hat{\rho}\hat{b}_j\to\left[\tilde{n}_{ij}-\frac{\partial}{\partial n_{lk}}\tilde{n}_{ik}\tilde{n}_{lj}\right]P,$$

$$\hat{b}_i^\dagger\hat{b}_j\hat{\rho}\to\left[n_{ij}-\frac{\partial}{\partial n_{lk}}\tilde{n}_{ik}n_{lj}\right]P,$$

$$\hat{\rho}\hat{b}_i^\dagger\hat{b}_j\to\left[n_{ij}-\frac{\partial}{\partial n_{lk}}n_{ik}\tilde{n}_{lj}\right]P,$$

$$\hat{b}_j\hat{\rho}\hat{b}_i^\dagger\to\left[n_{ij}+\frac{\partial}{\partial n_{lk}}n_{ik}n_{lj}\right]P. \tag{4.11}$$

C. Fokker-Planck equation

To be able to sample the time evolution of P with stochastic phase-space equations, which is the final goal, we must have an evolution equation that is in the form of a Fokker-Planck equation, containing first-order and second-order derivatives

$$\frac{d}{d\tau}P(\vec{\lambda},\tau)=\left[-\sum_{a=0}^{p}\frac{\partial}{\partial\lambda_a}A_a(\vec{\lambda})+\frac{1}{2}\sum_{a,b=0}^{p}\frac{\partial}{\partial\lambda_a}\frac{\partial}{\partial\lambda_b}D_{ab}(\vec{\lambda})\right]P(\vec{\lambda},\tau), \tag{4.12}$$

where $a=0,\ldots,p$ is an index that ranges over all the variables in the phase space. The matrix D_{ab} must be positive-definite when the Fokker-Planck equation is written in terms of real variables. Fortunately, the fact that the representation kernel $\hat{\Lambda}(\vec{\lambda})$ is analytic in the phase-space variables $\vec{\lambda}$ means that the matrix D_{ab} can *always* be chosen positive-definite after it is divided into real and imaginary parts,[18] through appropriate choices of the equivalent analytic forms $\partial/\partial\lambda_a=\partial/\partial\lambda_a^x=-i\,\partial/\partial\lambda_a^y$.

A Monte Carlo type sampling of Eq. (4.12) can be realized by integrating the Ito stochastic equations

$$d\lambda_a(\tau)=A_a(\vec{\lambda})d\tau+\sum_b B_{ab}(\vec{\lambda})dW_b(\tau), \tag{4.13}$$

where $dW_b(\tau)$ are Weiner increments, obeying $\langle dW_b(\tau)dW_{b'}(\tau')\rangle=\delta_{b,b'}\delta(\tau-\tau')d\tau$, i.e., Gaussian white noise. The noise matrix B_{ab} is related to the diffusion matrix by $D_{ab}=\Sigma_c B_{ac}B_{bc}$. This equation is directly equivalent to a path integral in phase space, so that the procedures outlined here can be regarded as a route to obtaining a path integral without Grassmann variables.

Auxiliary field methods[39] can also be used to obtain a non-Grassmann path integral, but these are generally more restrictive.

D. Stochastic gauges

The final phase-space equations are far from being unique. This freedom in the final form arises from different choices that are made at different points in the procedure. The choices at some points are constrained by the need to generate a genuine Fokker-Planck equation with a positive-definite diffusion matrix and vanishing boundary terms. Other than this, the choices are in principle free; they affect the final stochastic behavior without changing observable moments. They are thus a stochastic analogue of a gauge choice in field theories, and a good choice of stochastic gauge can dramatically improve the performance of the simulations.[34]

Because the Gaussian basis is analytic, methods previously used for the (bosonic) stochastic gauge positive-P representation are, therefore, applicable.[34,44,45] In the fermionic case, there are three sources of gauge freedom.

1. Fermi gauges

For fermionic systems, there is a freedom in the choice of operator correspondences, arising from vanishing operator products; any term involving a square of a fermion operator, like $\hat{a}_i^2\hat{O}$, is zero. Terms like this (and products of such terms) can be added to the Hamiltonian or Liouville equation without modifying the density matrix. The corresponding additional differential terms may not vanish, hence generating a different but equivalent stochastic equation. Such a fermionic stochastic gauge is necessary to avoid complex weights in imaginary-time simulations of interacting systems, such as the Hubbard model.[29]

2. Diffusion gauges

Diffusion gauges arise from the fact that the matrix square root $D_{ab}=\Sigma_c B_{ac}B_{bc}$, has multiple solutions, especially if one notes that there is no restriction on the second dimension of B_{ab}. This changes the stochastic noise term and can lead to a reduction in sampling error.[45]

3. Drift gauge

As well as the Fermi-gauge and diffusion-gauge freedoms, it is also possible to introduce a gauge freedom in the choice of drift terms. Drift gauges are obtained by trading off trajectory weight against trajectory direction. The possibility for drift gauges arises from the weight Ω in the density-operator expansion. The first of the correspondences in Eq. (4.8) can be used to convert drift terms for the phase-space variables into diffusion terms for the weight.[19] As a result, one can add an arbitrary gauge $g_a(\vec{\lambda})$ of the same dimension as the noise vector. Assuming $B_{0b}=0$, and using Einstein summation conventions, one obtains

$$d\Omega(\tau) = A_0 d\tau + \Omega g_b dW_b(\tau),$$

$$d\lambda_a(\tau) = A_a d\tau + B_{ab}[dW_b(\tau) - g_b d\tau]. \tag{4.14}$$

Previous work[34,44] has shown that drift gauges can remove boundary terms in bosonic positive-P representation by stabilizing deterministic trajectories.

V. EXAMPLES

The virtue of phase-space representation is that, whereas, the Hilbert space dimension grows exponentially with the number of modes M, the phase-space dimension only grows quadratically. Thus, for example, a problem involving $M=1000$ fermion modes has a Hilbert space dimension of $D=2^{1000}=10^{301}$ dimensions. This is larger than the number of particles in the observable universe (which is perhaps 10^{85} by current astrophysical reckoning). By contrast, the fermion phase-space dimension is 4×10^6. While large, this is not astronomical.

Hamiltonians and general time-evolution equations that are only quadratic in the Fermi ladder operators, i.e., constructed from one-body operators, will map to a Fokker-Planck equation that contains only first-order derivatives. The evolving quantum state can thus be sampled by a single, deterministic trajectory. More generally, quartic terms and cubic terms (if bosonic operators are included) can also be handled, and these result in stochastic equations or their equivalent path integrals.

Examples of how some typical Fermi problems are mapped into phase-space equations are given as follows.

A. Free gas

As an example of quadratic evolution, consider the thermal equilibrium calculation for a gas of noninteracting particles. The governing Hamiltonian (including the chemical potential) is always diagonalizable and can be written as

$$\hat{H} = \hat{\mathbf{b}}^\dagger \boldsymbol{\omega} \hat{\mathbf{b}}, \tag{5.1}$$

where $\omega_{ij}=\delta_{ij}\omega_j$ are the single-particle energies. The grand canonical distribution at temperature $T=1/k_B\beta$ is found from the equation

$$\frac{\partial}{\partial\beta}\hat{\rho} = -\frac{1}{2}(\hat{\mathbf{b}}^\dagger\boldsymbol{\omega}\hat{\mathbf{b}}\hat{\rho} + \hat{\rho}\hat{\mathbf{b}}^\dagger\boldsymbol{\omega}\hat{\mathbf{b}}). \tag{5.2}$$

Now this master equation can be mapped to an equivalent equation for the distribution P by use of the thermal correspondences in Eq. (4.11). However, because the solution is an unnormalized density operator, there will be zeroth-order terms in the equation. We can convert such terms to first order by applying the weight (Ω) identity in Eq. (4.8), thus obtaining the Fokker-Planck equation

$$\frac{\partial P}{\partial\beta} = \sum_k \omega_k \left[\frac{\partial}{\partial n_k}(1-n_k) + \frac{\partial}{\partial\Omega}\Omega\right] n_k P. \tag{5.3}$$

This Fokker-Planck equation with first-order derivatives corresponds to deterministic characteristic equations

$$\dot{\Omega} = -\sum_k \omega_k \Omega n_k, \tag{5.4}$$

$$\dot{n}_k = -\omega_k n_k (1 - n_k). \tag{5.5}$$

Integrating the deterministic equation for the mode occupation n_k leads to the usual Fermi-Dirac distribution

$$n_k = \frac{1}{e^{\omega_k \beta} + 1}. \tag{5.6}$$

From integration of the weight equation, one finds that normalization of the density operator is

$$\mathrm{Tr}[\hat{\rho}_u] = \Omega(\beta) = \Omega_0 \Pi_k e^{-\omega_k n_k \beta}, \tag{5.7}$$

i.e., the weight decays exponentially, at a rate given by the total energy.

B. General quadratic evolution

More generally, one can have a quadratic Liouville operator in situations involving nonthermal terms like $\hat{b}_i \hat{b}_j$. This can occur for, example, when fermion pairs are generated from molecule or exciton dissociation. These are even associated with certain spin-chain problems,[46] where the Jordan-Wigner theorem is used to transform spins to fermion operators. Other quadratic Liouville operators are commonly found in cases involving coupling to reservoirs.[43]

The generic phase-space equations for a general Fermi system with a quadratic Liouville operator can be easily obtained, for evolution both through time t and through inverse temperature β. The most general master equation that covers both kinds of evolution can be written

$$\frac{d}{d\tau}\hat{\rho} = K\hat{\rho} - \frac{1}{2}\sum_{\mu\nu} (\mathcal{A}_{\nu\mu} :\hat{b}_\mu \hat{b}^\dagger_\nu \hat{\rho}: + \mathcal{B}_{\nu\mu}\{\hat{b}_\mu \hat{b}^\dagger_\nu \hat{\rho}\} + \mathcal{C}_{\nu\mu} :\{\hat{\rho}\hat{b}_\mu\}\hat{b}^\dagger_\nu : + \mathcal{C}^*_{\mu\nu}\{:\hat{\rho}\hat{b}_\mu : \hat{b}^\dagger_\nu\}), \tag{5.8}$$

where the elements of $2M \times 2M$ matrices $\underline{\underline{\mathcal{A}}}$, $\underline{\underline{\mathcal{B}}}$, and $\underline{\underline{\mathcal{C}}}$ are determined by the coefficients of the Hamiltonian or master equation. By applying the mappings of Eq. (4.8)), we find the evolution of the covariance matrix to be

$$\frac{d}{d\tau}\underline{\underline{\sigma}} = \underline{\underline{\sigma}}(\underline{\underline{\mathcal{A}}} - \underline{\underline{\mathcal{A}}}^+)\underline{\underline{\sigma}} + \underline{\underline{\tilde{\sigma}}}(\underline{\underline{\mathcal{B}}} - \underline{\underline{\mathcal{B}}}^+)\underline{\underline{\tilde{\sigma}}} + \underline{\underline{\sigma}}(\underline{\underline{\mathcal{C}}} - \underline{\underline{\mathcal{C}}}^+)\underline{\underline{\tilde{\sigma}}} + \underline{\underline{\tilde{\sigma}}}(\underline{\underline{\mathcal{C}}}^\dagger - \underline{\underline{\mathcal{C}}}^{\dagger+})\underline{\underline{\sigma}}. \tag{5.9}$$

This equation simply corresponds to the characteristic or drift equations given by the vector $\vec{A}$ in the Ito stochastic equation (4.13), and in these cases, there is no diffusion or stochastic term. Unlike a conventional path integral, we see that a quadratic Hamiltonian or Liouville equation simply results in a noise-free, deterministic trajectory on phase space. For deterministic evolution such as this, the weight Ω does not affect physical observables, so we do not consider it here.

In the examples that follow, we assume for simplicity (but without loss of generality) that the constant matrices have been chosen with an antisymmetry such that

$$\underline{\underline{A}} = -\underline{\underline{A}}^+,$$

$$\underline{\underline{B}} = -\underline{\underline{B}}^+,$$

$$\underline{\underline{C}}^\dagger = -\underline{\underline{C}}^+. \tag{5.10}$$

1. Temperature evolution

For temperature evolution, the structure of the master equation [Eq. (4.4)] is such that $\underline{\underline{A}} = \underline{\underline{B}}$ and $\underline{\underline{C}} = \underline{\underline{C}}^\dagger$, giving the simpler result

$$\frac{d}{d\beta}\underline{\underline{\sigma}} = \frac{1}{2}(\underline{\underline{I}} - 2\underline{\underline{\sigma}})\underline{\underline{T}}(\underline{\underline{I}} - 2\underline{\underline{\sigma}}) + \underline{\underline{\sigma}}^0, \tag{5.11}$$

where we have introduced

$$\underline{\underline{T}} = \underline{\underline{\mathcal{B}}} - \underline{\underline{\mathcal{C}}},$$

$$\underline{\underline{\sigma}}^0 = \frac{1}{2}\underline{\underline{I}}(\underline{\underline{\mathcal{B}}} + \underline{\underline{\mathcal{C}}})\underline{\underline{I}}. \tag{5.12}$$

For the case of a number conserving Hamiltonian $H = \mathbf{b}^\dagger \boldsymbol{\omega} \mathbf{b}$, we find that $\underline{\underline{B}} = 0$ and

$$\underline{\underline{\mathcal{C}}} = \frac{1}{2}\begin{bmatrix} -\boldsymbol{\omega}^T & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\omega} \end{bmatrix}. \tag{5.13}$$

The phase-space equations then reduce to

$$\frac{d}{d\beta}\mathbf{n} = -\frac{1}{2}(\mathbf{n}\boldsymbol{\omega}\tilde{\mathbf{n}} + \tilde{\mathbf{n}}\boldsymbol{\omega}\mathbf{n}), \tag{5.14}$$

which reproduces the free gas example above.

2. Dynamical evolution

For real-time evolution, with possible coupling to the environment, there is a different symmetry to the master equation [Eq. (4.3)] that means that $\underline{\underline{\mathcal{A}}} + \underline{\underline{\mathcal{B}}} - \underline{\underline{\mathcal{C}}} - \underline{\underline{\mathcal{C}}}^\dagger = \underline{\underline{0}}$. A formal solution to the phase-space equations can now be explicitly written down

$$\underline{\underline{\sigma}}(t) = \exp(-\underline{\underline{U}}^\dagger t)(\underline{\underline{\sigma}}(0) - \underline{\underline{\sigma}}^\infty)\exp(-\underline{\underline{U}} t) + \underline{\underline{\sigma}}^\infty, \tag{5.15}$$

where $\underline{\underline{U}} = (\underline{\underline{\mathcal{B}}} - \underline{\underline{\mathcal{C}}})\underline{\underline{I}}$ and where $\underline{\underline{\sigma}}^\infty$ satisfies

$$\underline{\underline{I}}\underline{\underline{\mathcal{B}}}\underline{\underline{I}} = \underline{\underline{U}}^\dagger \underline{\underline{\sigma}}^\infty + \underline{\underline{\sigma}}^\infty \underline{\underline{U}}. \tag{5.16}$$

To illustrate the physical meaning of these matrices, we consider the simplest model of a small quantum dot coupled to a zero-temperature reservoir

$$\dot{\hat{\rho}} = -i\omega \hat{b}^\dagger \hat{b}\hat{\rho} + i\omega\hat{\rho}\hat{b}^\dagger \hat{b} + \gamma\left(\hat{b}\hat{\rho}\hat{b}^\dagger - \frac{1}{2}\hat{b}^\dagger \hat{b}\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{b}^\dagger \hat{b}\right). \tag{5.17}$$

In terms of the general form, this corresponds to $\underline{\underline{\mathcal{A}}} = \underline{\underline{0}}$, $\underline{\underline{\mathcal{B}}} = \gamma \underline{\underline{I}}$, and

$$\underline{\underline{C}} = \begin{bmatrix} -i\omega - \frac{1}{2}\gamma & 0 \\ 0 & -i\omega + \frac{1}{2}\gamma \end{bmatrix}. \tag{5.18}$$

The general solution then reduces to

$$\underline{\underline{\sigma}}(t) = \begin{bmatrix} e^{(-i\omega-\gamma/2)t} & 0 \\ 0 & e^{(i\omega-\gamma/2)t} \end{bmatrix} (\underline{\underline{\sigma}}(0) - \underline{\underline{I}}) \times \begin{bmatrix} e^{(i\omega-\gamma/2)t} & 0 \\ 0 & e^{(-i\omega-\gamma/2)t} \end{bmatrix} + \underline{\underline{I}}, \tag{5.19}$$

which implies that the density decays as $n(t)=e^{-\gamma t}n(0)$, as expected.

The solution to a multimode quantum dot model also follows from Eq. (5.15). The relevant master equation is

$$\dot{\hat{\rho}} = -i\omega_{ji}\hat{b}_i^\dagger \hat{b}_j \hat{\rho} + i\omega_{ji}\hat{\rho}\hat{b}_i^\dagger \hat{b}_j + \gamma_{ij}\left(\hat{b}_i \hat{\rho}\hat{b}_j^\dagger - \frac{1}{2}\hat{b}_j^\dagger \hat{b}_i \hat{\rho} - \frac{1}{2}\hat{\rho}\hat{b}_j^\dagger \hat{b}_i\right), \tag{5.20}$$

for which the evolution matrix is

$$\underline{\underline{U}} = \begin{bmatrix} e^{-i\boldsymbol{\omega}+\boldsymbol{\gamma}/2} & \mathbf{0} \\ \mathbf{0} & e^{i\boldsymbol{\omega}+\boldsymbol{\gamma}/2} \end{bmatrix}, \tag{5.21}$$

where we have assumed that $\boldsymbol{\omega}^T=\boldsymbol{\omega}$ and $\boldsymbol{\gamma}^T=\boldsymbol{\gamma}$. Physically, this corresponds, as expected, to damped oscillatory behavior (taking $\boldsymbol{\gamma}$ to be positive definite) in the moments

$$\mathbf{n} = e^{(i\boldsymbol{\omega}-\boldsymbol{\gamma}/2)t}\mathbf{n}(0)e^{(-i\boldsymbol{\omega}-\boldsymbol{\gamma}/2)t},$$

$$\mathbf{m} = e^{(-i\boldsymbol{\omega}-\boldsymbol{\gamma}/2)t}\mathbf{m}(0)e^{(-i\boldsymbol{\omega}-\boldsymbol{\gamma}/2)t}. \tag{5.22}$$

Here, of course, there are no electron-electron interactions included. However, such interactions can be dealt with via a stochastic sampling methods, as we show in Sec. V C.

C. Interacting gas

1. Two-body interactions

For systems of particles with two-body interactions, the Gaussian representation gives nonlinear, stochastic phase-space equations, which must be solved numerically. Consider a two-body interaction of the form

$$\hat{H}_2 = \sum_{ij} U_{ij}\hat{n}_{ii}\hat{n}_{jj}, \tag{5.23}$$

where $\hat{n}_{ij}=\hat{b}_i^\dagger \hat{b}_j$. For a number-conserving system, we can use correspondences of Eq. (4.11) to generate a Fokker-Planck equation for the grand-canonical evolution. The diffusion matrix $D_{u,v}$ in this equation is

$$D_{ij,kl} = -\sum_{pq} U_{pq}\{n_{ip}\tilde{n}_{pj}n_{kq}\tilde{n}_{ql} + \tilde{n}_{ip}n_{pj}\tilde{n}_{kq}n_{ql}\}. \tag{5.24}$$

Suppose that the interaction matrix U_{pq} is negative-definite, such that we can write it as a sum of negative squares: $U_{pq}=-\Sigma_\alpha b_{p,\alpha}b_{q,\alpha}$. Then the diffusion matrix is positive definite, as it can be written in the form

$$D_{ij,kl} = \sum_\alpha \{B^{(1)}_{ij,\alpha}B^{(1)}_{kl,\alpha} + B^{(2)}_{ij,\alpha}B^{(2)}_{kl,\alpha}\}, \tag{5.25}$$

where the noise matrices are

$$B^{(1)}_{ij,\alpha} = \sum_p b_{p,\alpha}n_{ip}\tilde{n}_{pj},$$

$$B^{(2)}_{ij,\alpha} = \sum_p b_{p,\alpha}\tilde{n}_{ip}n_{pj}. \tag{5.26}$$

Thus for an interaction of this type, the noise terms in the final stochastic equations will be real. The form of noise terms for a more general interaction is considered in Ref. 31.

2. Hubbard model

As an example, we show how to apply the representation to the Hubbard model. Some simulations of the resulting equations were reported in Refs. 29–31, along with details of the numerical implementations and comparisons with other methods. Here we focus on how these equations are derived and on the possible gauge choices available.

The Hubbard model is the simplest nontrivial model for strongly interacting fermions on a lattice. It is an important system in condensed matter physics, with relevance to the theory of high-temperature superconductors,[26] and in ultracold atomic physics. The full phase diagram in two dimensions is not fully understood as yet. Due to developments in atomic lattices, this model is directly experimentally accessible.[6,47]

The Hamiltonian for the model is[32]

$$H(\hat{\mathbf{n}}_1,\hat{\mathbf{n}}_{-1}) = -\sum_{ij,\sigma} t_{ij}\hat{n}_{ij,\sigma} + U\sum_j \hat{n}_{jj,1}\hat{n}_{jj,-1}, \tag{5.27}$$

where $\hat{n}_{ij,\sigma}=\hat{a}^\dagger_{i,\sigma}\hat{a}_{j,\sigma}=\{\hat{\mathbf{n}}_\sigma\}_{ij}$. The index σ denotes spin (±1), the indices i,j label lattice location. Here, $t_{ij}=t$ if the i,j correspond to nearest neighbor sites, $t_{ij}=\mu$ if $i=j$ and is otherwise 0. The chemical potential μ is included to control the total particle number.

Because the Hubbard model conserves total number and spin, one can map this problem to a reduced phase space of $\lambda=(\Omega, n_{ij,1}, n_{ij,-1})$. Thus the simpler mappings of Eq. (4.11) can be used for each spin component. The one-body terms generate drift terms only and can be dealt with as above. The two-body terms generate both drift and diffusion terms. Applying the mappings directly to the Hubbard model as written above, we obtain the diffusion matrix

$$D_{ij\sigma,kl\sigma'} = -U\delta_{\sigma,-\sigma'}\sum_p \{n_{ip\sigma}\tilde{n}_{pj\sigma}n_{kp\sigma'}\tilde{n}_{pl\sigma'} + \tilde{n}_{ip\sigma}n_{pj\sigma}\tilde{n}_{kp\sigma'}n_{pl\sigma'}\}, \tag{5.28}$$

which, because it has zeros on the diagonal, cannot be put into a positive-definite form with real variables.

However, using the anticommuting properties of the Fermi operators, we can rewrite the interaction term in the Hubbard Hamiltonian as

$$H_I = -\frac{|U|}{2}\sum_j :(\hat{n}_{jj,1} - S\hat{n}_{jj,-1})^2: = \sum_j U_{i\sigma,j\sigma'} :\hat{n}_{ii,\sigma}\hat{n}_{jj,\sigma'}:, \tag{5.29}$$

where $S = U/|U| = \pm 1$. Now in this form, the interaction matrix is negative-definite

$$U_{i\sigma,j\sigma'} = -\frac{|U|}{2}\delta_{ij}(\delta_{\sigma,\sigma'} - S\delta_{\sigma,-\sigma'}) = -\frac{|U|}{2}\sum_k \delta_{i,k}\sigma^s\delta_{j,k}\sigma'^s, \tag{5.30}$$

where $s = (S+1)/2$, so that $s=0$ for the attractive case and $s=1$ for the repulsive case.

From Eq. (5.25), the diffusion matrix is positive-definite, with corresponding noise matrices

$$B^{(1)}_{ij\sigma,\alpha} = \sqrt{|U|/2}\sigma^s n_{i\alpha,\sigma}\tilde{n}_{\alpha j,\sigma},$$

$$B^{(2)}_{ij\sigma,\alpha} = \sqrt{|U|/2}\sigma^s \tilde{n}_{i\alpha,\sigma} n_{\alpha j,\sigma}. \tag{5.31}$$

With this choice of noise terms, the final phase-space equations are, in Itô form,

$$\frac{d\mathbf{n}_\sigma}{d\beta} = \frac{1}{2}\{\tilde{\mathbf{n}}_\sigma \boldsymbol{T}^{(1)}_\sigma \mathbf{n}_\sigma + \mathbf{n}_\sigma \boldsymbol{T}^{(2)}_\sigma \tilde{\mathbf{n}}_\sigma\}, \tag{5.32}$$

where we have introduced the stochastic propagation matrix

$$T^{(r)}_{ij,\sigma} = t_{ij} - \delta_{ij}\{Un_{jj,-\sigma} + \sigma^s \xi^{(r)}_j\}. \tag{5.33}$$

The real Gaussian noise $\xi^{(r)}_j(\beta)$ is defined by the correlations

$$\langle \xi^{(r)}_j(\beta)\xi^{(r')}_{j'}(\beta')\rangle = 2|U|\delta(\beta-\beta')\delta_{jj'}\delta_{rr'}. \tag{5.34}$$

Because the diffusion can be realized in terms of real noise, the phase-space equations will not be driven off the real manifold. This has an important implication for the weight Ω, which enters the problem because the solution will be an unnormalized density operator. The weights for each trajectory evolve as physically expected for energy-weighted averages, with weights depending exponentially on the inverse temperature β and the effective trajectory Hamiltonian H:

$$\frac{d\Omega}{d\beta} = -\Omega H(\mathbf{n}_1, \mathbf{n}_{-1}). \tag{5.35}$$

Because the equations for the phase-space variables $n_{ij,\sigma}$ are all real, the weights will all remain positive, thereby eliminating the traditional manifestation of the sign problem. In contrast, the analogous equation in AFQMC does not guarantee the weights to be positive, and this is where the sign problem enters in such calculations.

This method can calculate any correlation function, at any temperature, to the precision allowed by the sampling error and subject to there being no boundary terms in Eq. (4.6). Simulations in one,[48] two,[29,30] and three dimensions are shown in Figs. 1–4. They demonstrate that sampling error is well-controlled, even for very low temperatures and for cases in which the sign deteriorates for projector QMC.

However, more extensive simulations of the two-dimensional (2D) Hubbard model have shown that, at half filling, certain correlation functions do not appear to converge to the correct zero-temperature results at these very low temperatures.[31] Because the Gaussian basis does not possess many of the symmetries of the Hubbard model, they must be restored in the distribution over Gaussian basis elements. For finite sampling, this restoration may be incomplete, giving the departure from exact results at low temperatures. There may also be systematic errors if boundary terms are present. Both of these possibilities imply that further optimization via stochastic gauge choices may be required to keep the low-temperature distributions compact and free from tails and features that would lead to biasing.

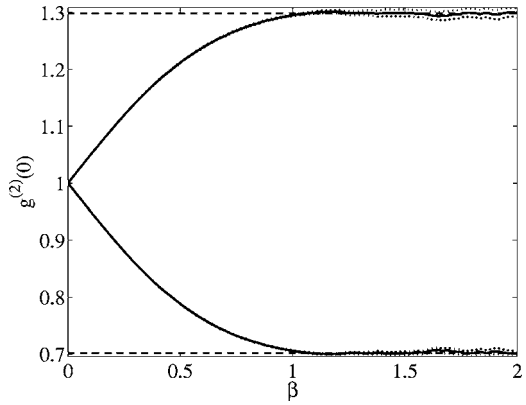

FIG. 1. Second-order correlation function $g^{(2)} = (1/N_L)\Sigma_j \langle \hat{n}_{jj,1}\hat{n}_{jj,-1}\rangle / \langle \hat{n}_{jj,1}\rangle\langle \hat{n}_{jj,-1}\rangle$ for a $N_L = 100$ site one-dimensional lattice at half filling. Lower curves are for $U=2$ (repulsive) and upper curves are for $U=-2$ (attractive). Solid lines give the numerical results, dashed lines give the zero-temperature analytic result[49] for an infinite system, and dotted lines indicate sampling error. $t=1$ and 1000 paths.

Nevertheless, it has already been shown that the correct results can be obtained by applying a projection onto a symmetric subspace.[31] Importantly, accurate results were then obtained even in cases that are beyond the reach of AFQMC.

3. Drift gauges

Here, we outline how the performance of the Hubbard simulations may be improved by means of drift gauges. We

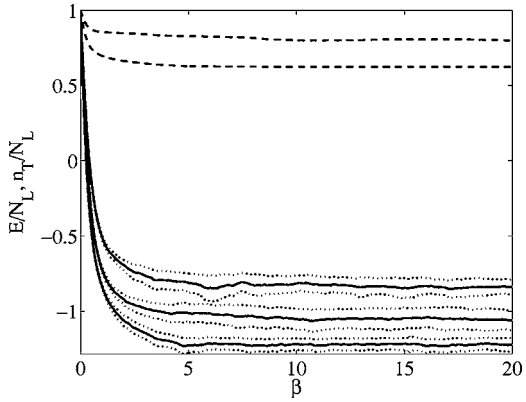

FIG. 2. Two-dimensional Hubbard model with $N_L = 16$ sites. Solid lines give energy E per lattice site for chemical potentials (in order of decreasing energy) $\mu=2$, $\mu=1$, and $\mu=0$. Dashed lines give number of particles per site for $\mu=1$ (upper) and $\mu=0$ (lower). Dotted lines indicate sampling error. $U=4$, $t=1$ and 5000 paths.

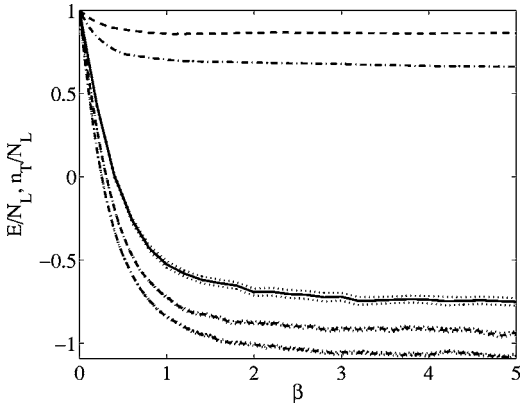

FIG. 3. Two-dimensional Hubbard model with $N_L=256$ sites. Solid lines give energy E per lattice site for chemical potentials (in order of decreasing energy) $\mu=2$, $\mu=1$, and $\mu=0$. Dashed lines give number of particles per site for $\mu=1$ (upper) and $\mu=0$ (lower). Dotted lines indicate sampling error. $U=4$, $t=1$. Breeding algorithm used with approximately 100 paths.

can modify the Hubbard drift according to Eq. (4.14) by adding a term $\mathbf{G}_\sigma$ to the stochastic propagation matrices $\mathbf{T}_\sigma^{(r)}$. Because of the diagonal nature of the noise terms, the added term will also be diagonal: $G_{ij\sigma}=\delta_{ij}\sigma^s G_j$. The additional diffusion term in the weight equation is then

$$\left(\frac{d\Omega}{d\beta}\right)_g = \frac{\Omega}{2|U|}\sum_{jr} G_j \xi_j^{(r)}. \tag{5.36}$$

The choice of gauge term $\mathbf{G}_\sigma$ is guided, on the one hand, by the need to ensure the phase-space distribution remains bounded and, on the other, by the requirement of introducing only the minimum amount of diffusion into the weight. The function should thus act only when necessary to control large trajectories and should be zero otherwise.

However, because of the coupling terms t_{ij}, a diagonal drift gauge is insufficient to remove all instabilities, making it necessary to introduce off-diagonal gauge terms. This in turn requires additional, off-diagonal noise terms in the propagation matrix. Such noises can be introduced by use of additional Fermi gauges. For example, the vanishing term[50]

$$0 = \sum_{ij\sigma} \frac{1}{2} V_{ji,\sigma}\{(\delta_{ij}-\hat{n}_{ij,\sigma})\hat{n}_{ij,\sigma}\hat{\rho} + \hat{\rho}\hat{n}_{ij,\sigma}(\delta_{ij}-\hat{n}_{ij,\sigma})\}, \tag{5.37}$$

where $V_{ij,\sigma}$ are positive numbers, gives the additional stochastic contribution to the propagation matrix

$$T_{ij,\sigma}^{(r)} \to T_{ij,\sigma}^{(r)} + \zeta_{ij,\sigma}^{(r)}(\beta), \tag{5.38}$$

where the new noises $\zeta_{ij,\sigma}^{(r)}(\beta)$ have the correlations

$$\langle \zeta_{ij,\sigma}^{(r)}(\beta)\zeta_{i'j',\sigma'}^{(r')}(\beta')\rangle = 4V_{ij,\sigma}\delta(\beta-\beta')\delta_{ii'}\delta_{jj'}\delta_{rr'}\delta_{\sigma\sigma'}. \tag{5.39}$$

We can now introduce arbitrary off-diagonal gauge terms $G_{ij,\sigma}^{(r)}$ into the propagation matrix, with the corresponding diffusion term in the weight equation

$$\left(\frac{d\Omega}{d\beta}\right)_g = -\Omega\sum_{ijr\sigma} G_{ij,\sigma}^{(r)}\zeta_{ij,\sigma}^{(r)}/4V_{ij,\sigma}. \tag{5.40}$$

Again there is a tradeoff between gauge strength and additional diffusion. But there is also a freedom (in the choice of $V_{ij,\sigma}$) as to whether the noise appears in the weight equation or in the propagation matrix.

With such a combination of Fermi and drift gauges, it is possible to introduce terms to stabilize the drift evolution of any of the phase-space variables $n_{ij,\sigma}$, and so maintain a bounded phase-space distribution.

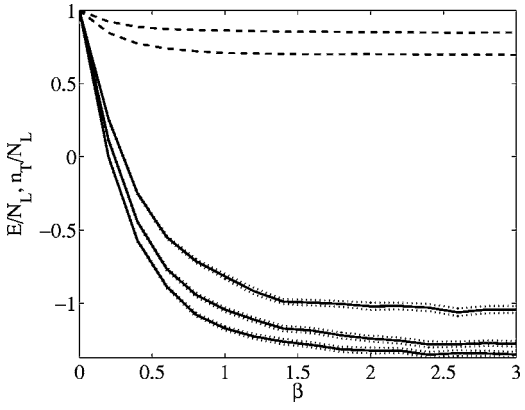

FIG. 4. Three-dimensional Hubbard model with $N_L=216$ sites. Solid lines give energy E per lattice site for chemical potentials (in order of decreasing energy) $\mu=2$, $\mu=1$, and $\mu=0$. Dashed lines give number of particles per site for $\mu=1$ (upper) and $\mu=0$ (lower). Dotted lines indicate sampling error. $U=4$, $t=1$ and 50 paths.

VI. CONCLUSION

In summary, we have introduced a phase-space representation for many-body fermionic states, enabling new types of first-principles calculations and simulations of highly correlated systems. Systems with one-body and two-body interactions can be solved by the use of stochastic sampling methods, since they can be transformed into a second-order Fokker-Planck equation, provided a suitable stochastic gauge is chosen to ensure that the distribution remains sufficiently bounded.

These techniques are potentially applicable to a wide range of fermionic problems, including both real-time and finite-temperature calculations. Generalized master equations for nonequilibrium fermionic open systems coupled to reservoirs are a particularly suitable type of application. We have given examples of the use of fermionic differential identities to transform multimode master equations into deterministic phase-space equations, although more general interactions typically lead to stochastic equations. These equations have exponentially less complexity than the full Hilbert space equations.

In contrast to Grassmann-based approaches, the Gaussian representation does not involve anticommuting variables and thus avoids the associated complexity issues. In contrast to standard QMC methods, the phase-space approach is based

on a positive expansion of the density matrix, rather than a path integral. This approach makes the method very flexible and general in its application. It is also what allows problems of the Hubbard type to be simulated with positive weights, thereby avoiding the traditional manifestation of the sign problem. The current limiting factor to the Gaussian method is the need to develop appropriate gauges, but as we have indicated here, there are many avenues to consider.

The application to the Hubbard model demonstrates the immediate utility of the Gaussian method to solving long-standing problems in many-body quantum physics, provided suitable gauges can be found to ensure that boundary terms to not arise. Rapid experimental advances in the area of ultracold fermionic atoms[5] mean that direct and quantitative tests of precise theoretical predictions should be feasible in the near future. Demonstration of a quantum degenerate Fermi gas in a lattice has already taken place.[6]

The general technique established here potentially also has broad applicability in many other areas of quantum many-body theory and quantum field theory.

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APPENDIX A: ESSENTIAL GAUSSIAN OPERATOR RESULTS

We here summarize the algebraic properties of Gaussian operators Eq. (2.4) that are essential to making use of the Gaussian phase-space representation. These results are proved and extensively discussed in Ref. 33.

1. Definition and trace properties

The Gaussian operator $\hat{\Lambda}$ is defined as the most general Gaussian form of fermionic annihilation and creation operators, with zero displacement. Using the extended-vector notation introduced in Sec. II A, we can write the general Gaussian operator as

$$\hat{\Lambda} = \Omega \frac{1}{\mathcal{N}} :\exp[-\underline{\hat{b}}^{\dagger}(\underline{\underline{\sigma}}^{-1} - 2\underline{\underline{I}})\underline{\hat{b}}/2]:, \tag{A1}$$

where Ω is a complex amplitude, $\underline{\underline{\sigma}}$ is a $2M \times 2M$ complex matrix, and $\underline{\underline{I}}$ is the constant matrix is defined as

$$\underline{\underline{I}} = \begin{bmatrix} -\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix}. \tag{A2}$$

The normalization factor N contains the Pfaffian of an antisymmetric form of the generalized covariance matrix

$$\mathcal{N} = \mathrm{Pf}[\underline{\underline{\sigma}}_A^{-1}].$$

Some elementary traces are

$$\mathrm{Tr}[\hat{\Lambda}] = \Omega,$$

$$\mathrm{Tr}[\underline{b}\hat{\Lambda}] = 0,$$

$$\mathrm{Tr}[:\underline{\hat{b}}\underline{\hat{b}}^{\dagger}\hat{\Lambda}:] = \Omega\underline{\underline{\sigma}}. \tag{A3}$$

The first of these is the normalization, proved in Sec. B.2 of Ref. 33. That the second is zero follows from the fact that the Gaussians are constructed from pairs of ladder operators and thus cannot correspond to a superposition of states whose total fermion numbers differ by an odd number. The third trace, proved in Sec. B.3 of Ref. 33, allows us to calculate first-order correlations.

As proved in Sec. B.4 of Ref. 33, traces involving higher-order products reduce to these elementary traces

$$\mathrm{Tr}[:\hat{b}_{\mu_1}\cdots\hat{b}_{\mu_{2r}}\hat{\Lambda}:] = \sum_P (-1)^P \mathrm{Tr}[:\hat{b}_{\nu_1}\hat{b}_{\nu_2}\hat{\Lambda}:]\times\cdots \times \mathrm{Tr}[:\hat{b}_{\nu_{2r-1}}\hat{b}_{\nu_{2r}}\hat{\Lambda}:], \tag{A4}$$

where $\nu_j = \mu_{P(j)}$. The sum is over all $(2r)!/(2^r r!)$ distinct pair permutations $P(1),\ldots,P(2r)$, and the sign $(-1)^P$ is the parity of the permutation.

2. Differential properties

The action of any pair of ladder operators on a Gaussian operator can be written as a first-order derivative, as follows:

$$\hat{\Lambda} = \Omega\frac{\partial}{\partial\Omega}\hat{\Lambda},$$

$$:\underline{\hat{b}}\underline{\hat{b}}^{\dagger}\hat{\Lambda}: = \underline{\underline{\sigma}}\hat{\Lambda} - \underline{\underline{\sigma}}\frac{\partial\hat{\Lambda}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\sigma}},$$

$$\{\underline{\hat{b}}:\underline{\hat{b}}^{\dagger}\hat{\Lambda}:\} = -\underline{\underline{\sigma}}\hat{\Lambda} - \underline{\underline{\tilde{\sigma}}}\frac{\partial\hat{\Lambda}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\sigma}},$$

$$\{:\hat{\Lambda}\underline{\hat{b}}:\underline{\hat{b}}^{\dagger}\} = -\underline{\underline{\sigma}}\hat{\Lambda} - \underline{\underline{\sigma}}\frac{\partial\hat{\Lambda}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\tilde{\sigma}}},$$

$$\{\underline{\hat{b}}\underline{\hat{b}}^{\dagger}\hat{\Lambda}\} = -\underline{\underline{\tilde{\sigma}}}\hat{\Lambda} - \underline{\underline{\tilde{\sigma}}}\frac{\partial\hat{\Lambda}}{\partial\underline{\underline{\sigma}}}\underline{\underline{\tilde{\sigma}}}, \tag{A5}$$

where $\underline{\underline{\tilde{\sigma}}} \equiv \underline{\underline{I}} - \underline{\underline{\sigma}}$. Here normal ordering is denoted with $:\cdots:$ and antinormal ordering with $\{\cdots\}$, as discussed in Sec. IV B. The proof of these identities is given in Secs. 5.4 and B.5–B.7 of Ref. 33.

For the subset of Gaussian operators that correspond to (generalized) thermal states, i.e., $\mathbf{m}^{+} = \mathbf{m} = \mathbf{0}$, the differential identities reduce to a simpler form

$$\hat{\boldsymbol{b}}^{\dagger T}\hat{\boldsymbol{b}}^{T}\hat{\Lambda} = \boldsymbol{n}\hat{\Lambda} + \tilde{\boldsymbol{n}}\frac{\partial\hat{\Lambda}}{\partial\boldsymbol{n}}\boldsymbol{n},$$

$$\hat{\Lambda}\hat{\boldsymbol{b}}^{\dagger T}\hat{\boldsymbol{b}}^{T} = \boldsymbol{n}\hat{\Lambda} + \boldsymbol{n}\frac{\partial\hat{\Lambda}}{\partial\boldsymbol{n}}\tilde{\boldsymbol{n}},$$

$$\hat{\boldsymbol{b}}^{\dagger T}\hat{\Lambda}\hat{\boldsymbol{b}}^{T} = \tilde{\boldsymbol{n}}\hat{\Lambda} + \tilde{\boldsymbol{n}}\frac{\partial\hat{\Lambda}}{\partial\boldsymbol{n}}\tilde{\boldsymbol{n}},$$

$$(\hat{\boldsymbol{b}}\hat{\Lambda}\hat{\boldsymbol{b}}^{\dagger})^{T} = \boldsymbol{n}\hat{\Lambda} - \boldsymbol{n}\frac{\partial\hat{\Lambda}}{\partial\boldsymbol{n}}\boldsymbol{n}. \tag{A6}$$

These identities mean that there are mappings to a second-order differential form for all two-body operators and allow us to map the evolution of the density operator onto an evolution of the expansion coefficients P_j.

APPENDIX B: MAPPINGS IN GREEN'S FUNCTION FORM

It is sometimes more convenient to work explicitly with $\mathbf{n}$, $\mathbf{m}$, and $\mathbf{m}^{+}$ submatrices rather than the total covariance. In fully indexed notation, using the $M\times M$ submatrices, the Fermi operator correspondences [Eq. (4.8)] become

$$\hat{b}_i^{\dagger}\hat{b}_j\hat{\rho} \to \left[n_{ij} - \frac{\partial}{\partial n_{lk}}\{n_{lj}\tilde{n}_{ik} + m_{li}^{+}m_{jk}\} - \frac{\partial}{\partial m_{lk}}\{m_{lj}\tilde{n}_{ik} + \tilde{n}_{il}m_{jk}\} + \frac{\partial}{\partial m_{lk}^{+}}\{n_{lj}m_{ik}^{+} + m_{li}^{+}n_{kj}\}\right]P,$$

$$\hat{\rho}\hat{b}_i^{\dagger}\hat{b}_j \to \left[n_{ij} - \frac{\partial}{\partial n_{lk}}\{\tilde{n}_{lj}n_{ik} + m_{li}^{+}m_{jk}\} + \frac{\partial}{\partial m_{lk}}\{m_{lj}n_{ik} + n_{il}m_{jk}\} - \frac{\partial}{\partial m_{lk}^{+}}\{\tilde{n}_{lj}m_{ik}^{+} + m_{li}^{+}\tilde{n}_{kj}\}\right]P,$$

$$\hat{b}_i^{\dagger}\hat{\rho}\hat{b}_j \to \left[\tilde{n}_{ij} - \frac{\partial}{\partial n_{lk}}\{\tilde{n}_{lj}\tilde{n}_{ik} - m_{li}^{+}m_{jk}\} + \frac{\partial}{\partial m_{lk}}\{m_{lj}\tilde{n}_{ik} + \tilde{n}_{il}m_{jk}\} + \frac{\partial}{\partial m_{lk}^{+}}\{\tilde{n}_{lj}m_{ik}^{+} + m_{li}^{+}\tilde{n}_{kj}\}\right]P,$$

$$\hat{b}_j\hat{\rho}\hat{b}_i^{\dagger} \to \left[n_{ij} - \frac{\partial}{\partial n_{lk}}\{m_{li}^{+}m_{jk} - n_{lj}n_{ik}\} + \frac{\partial}{\partial m_{lk}}\{m_{lj}n_{ik} + n_{il}m_{jk}\} + \frac{\partial}{\partial m_{lk}^{+}}\{n_{lj}m_{ik}^{+} + m_{li}^{+}n_{kj}\}\right]P,$$

$$\hat{b}_i\hat{b}_j\hat{\rho} \to \left[m_{ij} - \frac{\partial}{\partial n_{lk}}\{n_{li}m_{jk} - n_{lj}m_{ik}\} - \frac{\partial}{\partial m_{lk}}\{m_{li}m_{jk} - m_{lj}m_{ik}\} - \frac{\partial}{\partial m_{lk}^{+}}\{n_{lj}n_{ki} - n_{li}n_{kj}\}\right]P,$$

$$\hat{\rho}\hat{b}_i\hat{b}_j \to \left[m_{ij} - \frac{\partial}{\partial n_{lk}}\{\tilde{n}_{lj}m_{ik} - \tilde{n}_{li}m_{jk}\} - \frac{\partial}{\partial m_{lk}}\{m_{li}m_{jk} - m_{lj}m_{ik}\} - \frac{\partial}{\partial m_{lk}^{+}}\{\tilde{n}_{lj}\tilde{n}_{ki} - \tilde{n}_{li}\tilde{n}_{kj}\}\right]P,$$

$$\hat{b}_j\hat{\rho}\hat{b}_i \to \left[m_{ij} + \frac{\partial}{\partial n_{lk}}\{\tilde{n}_{li}m_{jk} + n_{lj}m_{ik}\} - \frac{\partial}{\partial m_{lk}}\{m_{li}m_{jk} - m_{lj}m_{ik}\} - \frac{\partial}{\partial m_{lk}^{+}}\{\tilde{n}_{li}n_{kj} - \tilde{n}_{lj}n_{ki}\}\right]P,$$

$$\hat{b}_i^{\dagger}\hat{b}_j^{\dagger}\hat{\rho} \to \left[m_{ij}^{+} - \frac{\partial}{\partial n_{lk}}\{m_{lj}^{+}\tilde{n}_{ik} - m_{li}^{+}\tilde{n}_{jk}\} - \frac{\partial}{\partial m_{lk}}\{\tilde{n}_{jl}\tilde{n}_{ik} - \tilde{n}_{il}\tilde{n}_{jk}\} - \frac{\partial}{\partial m_{lk}^{+}}\{m_{li}^{+}m_{jk}^{+} - m_{lj}^{+}m_{ik}^{+}\}\right]P,$$

$$\hat{\rho}\hat{b}_i^{\dagger}\hat{b}_j^{\dagger} \to \left[m_{ij}^{+} - \frac{\partial}{\partial n_{lk}}\{m_{li}^{+}n_{jk} - m_{lj}^{+}n_{ik}\} - \frac{\partial}{\partial m_{lk}}\{n_{jl}n_{ik} - n_{il}n_{jk}\} - \frac{\partial}{\partial m_{lk}^{+}}\{m_{li}^{+}m_{jk}^{+} - m_{lj}^{+}m_{ik}^{+}\}\right]P,$$

$$\hat{b}_j^{\dagger}\hat{\rho}\hat{b}_i^{\dagger} \to \left[m_{ij}^{+} + \frac{\partial}{\partial n_{lk}}\{m_{lj}^{+}n_{ik} + m_{li}^{+}\tilde{n}_{jk}\} - \frac{\partial}{\partial m_{lk}}\{n_{il}\tilde{n}_{jk} - \tilde{n}_{jl}n_{ik}\} - \frac{\partial}{\partial m_{lk}^{+}}\{m_{li}^{+}m_{jk}^{+} - m_{lj}^{+}m_{ik}^{+}\}\right]P, \tag{B1}$$

where we have used the Einstein summation convention for repeated indices. Furthermore, we have explicitly written out the extra terms involving anomalous $(\mathbf{m},\mathbf{m}^{+})$ derivatives that arise from their antisymmetry, such that the summation of these terms is only for $k>l$.

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[50] This form of Fermi gauge is also used in Ref. 31 to generate phase-space equations for the general electronic structure problem.