A unified theory of variational and quantum Monte Carlo methods and beyond

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We present a unified theory of the variational Monte Carlo (VMC) and determinant quantum Monte Carlo (DQMC) methods using a novel density matrix formulation of VMC. We introduce an efficient algorithm for VMC to compute correlation functions and expectation values based on the auxiliary field Hirsch-Hubbard-Strattonovik transformation. We show that this new approach to VMC converges significantly faster than its traditional implementations. Furthermore, we generalize the Trotter-Suzuki decomposition to finite imaginary time steps \(\tau \sim O(1)\) and develop a variational quantum Monte Carlo (VQMC) method accordingly, which is more accurate than VMC and can incorporate quantum fluctuations more efficiently. The two extreme limits of the VQMC method, namely infinitesimal and infinite imaginary time steps, correspond to the DQMC and VMC techniques, respectively. We demonstrate that our VQMC allows us to access lower temperatures in comparison with the conventional DQMC before the sign problem comes into play. We finally show that our VQMC can also enhance the accuracy of the projector Monte Carlo methods by providing better and less biased candidates for the trial wave functions, requiring shorter projection times for a given accuracy and alleviating the sign problem further.

I. INTRODUCTION

The exact solution of quantum mechanical problems is in general highly nontrivial and in most cases intractable, mainly due to the exponential growth of the Hilbert space dimension with the system size. This obvious fact entails for reliable though approximate solutions of quantum problems. In the past, several reliable approaches capable of solving non-integrable models with arbitrary accuracy have been developed. For example, it has been shown that the ground-state of local (quasi-)one-dimensional gapped Hamiltonians can be obtained through the density-matrix-renormalization group and related quantum entanglement based methods with a finite computational effort independent of the system size [1–4]. Furthermore, quantum Monte Carlo (QMC) methods can solve several non-integrable models in higher dimensions, e.g., the Hubbard model on bipartite lattices at half-filling [5–13]. Nevertheless, these popular methods are inapplicable in most cases. For example, DMRG fails to solve higher-dimensional problems [2–4], or QMC away from half-filling or on frustrated lattices is plagued by the notorious fermionic sign problem [14–19]. The average sign of fermion determinants in these situations vanishes as \(\exp(-V f/T)\), where \(V\) denotes the size of system, \(T\) temperature, and \(f\) is a constant dependent on the interaction strength. Since the number of required Monte Carlo Samplings for a given accuracy scales as \(1/\langle \text{sign} \rangle^2\), the QMC approach becomes infeasible at low temperatures or for large systems for generic models [20–23]. In this paper, we try to ameliorate the sign problem by first reformulating the variational Monte Carlo (VMC) method [24–27] (which does not capture quantum fluctuations efficiently) using a density matrix approach. We then generalize our VMC formulation to incorporate quantum fluctuations as well. The resulting variational quantum Monte Carlo (VQMC) unifies the determinant QMC (DQMC), and VMC methods as the two extreme limits of a single computational approach. Finally, we demonstrate that our VQMC can yield highly accurate results when combined with the projector QMC (PQMC) method [7, 15] through providing better approximate trial ground states.

In this paper, we first show that our density matrix formulation of VMC allows an auxiliary field implementation. Based on this observation we introduce a more efficient algorithm for VMC. The resulting implementation converges faster than its conventional counterparts in coordinate space. Furthermore, we show that measuring correlation functions and expectation values of various operators is more convenient within this new framework. We then discuss our VQMC approach, in which we introduce a generalized Trotter-Suzuki decomposition associated with finite imaginary time steps. The resulting decomposition can be interpreted as a renormalization group transformation along the imaginary time direction. We demonstrate that such coarse graining operations will renormalize various coupling constants of the model Hamiltonian. For example, using the Hubbard model to benchmark our VQMC approach, we show that the onsite Hubbard coupling \(U\) flows to weaker values upon considering larger imaginary time steps. We show that our VQMC yields ground-state properties with a higher accuracy compared to VMC. Furthermore, we argue that VQMC captures low energy quantum fluctuations and despite suffering from the fermionic sign problem (similar to DQMC), the onset of the sign problem emerges at lower temperatures. Having achieved a better ansatz for the ground-state density matrix through applying VQMC, we can feed it into the PQMC machinery as its trial/guiding state and achieve ground-state properties with high confidence using considerably shorter projection times. The latter observation can potentially circumvent the fermionic sign problem.

In this paper, we study the Hubbard model [28] on the square lattice defined as \(H = H_K + H_U\), where its kinetic
part: $H_k = -t_1 \sum_{\langle ij \rangle} c_{i,\sigma}^\dagger c_{j,\sigma}^\dagger$ and the interaction part: $H_U = U \sum_{i,\sigma} n_{i,\uparrow} n_{i,\downarrow}$. In these expressions, $\langle ij \rangle$ denotes nearest neighbors, $c_{i,\sigma}$ electron annihilation operator on site \(i\) with spin $\sigma$, and $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$ the corresponding electron number.

II. A UNIFIED THEORY OF VARIATIONAL, PROJECTOR AND QUANTUM MONTE CARLO METHODS

In this section, we present a unified formulation of the variational and (determinant) quantum Monte Carlo methods. Based on the acquired knowledge we establish a novel technique dubbed as variational quantum Monte Carlo that paves the way between VMC and DQMC. We finally demonstrate that our VQMC-PQMC hybrid approach can outperform all existing QMC methods through providing more accurate initial density matrix (trial state) in the PQMC method.

A. Density matrix formulation of the VMC method

In the conventional VMC approach, we try to come up with a guess for the ground-state wave function. Let us denote the true ground-state by $|\Psi_G\rangle$, and the trial one by $|\Phi_T\rangle$. The guessed/trial wave function $|\Phi_T\rangle$ contains a number of variational parameters, which are tuned to minimize the expectation value of the model Hamiltonian with respect to $|\Phi_T\rangle$. The variational wave function is usually defined through a noninteracting fermion wave function projected by a Gutzwiller-Jastrow operator, namely: $|\Phi_T\rangle = Z^{-1/2} P_G |\Phi_0\rangle$, where $Z$ is a normalization factor, and the (partial) Gutzwiller projection operator is defined as

$$P_G = \prod_i (1 - \hat{g} n_{i,\uparrow} n_{i,\downarrow}) = e^{-\frac{g}{2} \sum_i n_{i,\uparrow} n_{i,\downarrow}},$$

in which $g = -2 \log(1 - \hat{g})$ serves as a variational parameter (which controls the onsite double occupancy). The non-interacting fermionic wave function $|\Phi_0\rangle$ is the groundstate of a variational quadratic fermion Hamiltonian $H_M = -\sum_{ij} \psi_i^\dagger M_{ij} \psi_j$, where $\psi_i = \begin{pmatrix} c_{i,\uparrow}, c_{i,\downarrow}^\dagger \end{pmatrix}^T$ denotes the spinor fields (in Nambu space). Therefore, $H_M$ can in general accommodate pairing terms as well. The main task in VMC is to minimize the expectation value of the Hubbard Hamiltonian w.r.t. the variational wave function, i.e., to minimize $E_{g,M} = \langle \Phi_T | H | \Phi_T \rangle$ functional, from which $g$ and elements of the variational hopping matrix $H_M$ can be obtained. In the conventional implementation of VMC, the variational wave function is written in real space using Slater determinants and the expectation values are computed using Monte Carlo algorithm in which electron coordinates are sampled via Metropolis-Hasting importance sampling [29, 30]. In this approach, even for $g = 0$, we need to sample thousands of configurations to achieve a fair estimate of the expectation value of various operators.

In this paper, we take a different route and instead of working with wave function and Slater determinants, we work with density matrix operators. Our main observation is the following identity:

$$\rho_{VMC} = |\Phi_T\rangle \langle \Phi_T| = \frac{1}{Z} P_G |\Phi_0\rangle \langle \Phi_0| P_G,$$

where we have used the fact that the density matrix associated with noninteracting electrons is unique and identical to the Boltzmann operator when $T = 1/\beta \rightarrow 0$. The above seemingly trivial identity has a profound implication. Indeed, it suggests the following approximate generalization of the Trotter-Suzuki decomposition for gigantic time steps:

$$VMC: \ e^{-\beta (H_K + H_U)} \approx \exp (-\beta H_{eff})^2 e^{-\beta H_M} \exp (-\beta H_{eff})^2,$$

where $U_{eff} = g/\beta$ is the renormalized onsite Hubbard coupling. Although the above relation is clearly an approximation and very far from being accurate, it is the basis of the VMC method and all of its successes as well as limitations. We are now prepared to utilize Monte Carlo methods to evaluate the approximate VMC density matrix $\rho_{VMC}$. To this end, similar to DQMC, we first use the discrete Hubbard-Stratonovic transformation introduced by Hirsch [31] using the following identity:

$$e^{-\frac{g}{2} n_{i,\uparrow} n_{i,\downarrow}} = \frac{1}{2} e^{-\frac{g}{4} (n_{i,\uparrow} + n_{i,\downarrow})} \sum_{s_i = \pm 1} e^{\lambda n_{i,\uparrow} n_{i,\downarrow} + \lambda},$$

where $\cosh(\lambda) = \exp (g/4)$. The above Hubbard-Stratonovic transformation can be employed to rewrite the VMC density matrix in terms of an ensemble of noninteracting (i.e., quadratic) density matrices over the right and left Hubbard-Stratonovic auxiliary binary fields as follows:

$$\rho_{VMC}(\beta) \propto \sum_{\{s_i\}} \sum_{\{j,s_j\}} \exp (-\lambda \sum_{i,\sigma} \sigma s_i^{\sigma} n_{i,\sigma}) \times \exp (-\beta \psi_i^\dagger H_M^\dagger \psi) \exp (-\lambda \sum_{j,\sigma} \sigma s_j^{\sigma} n_{j,\sigma}).$$

Now, we can employ the Metropolis-Hasting algorithm to sample important configurations of the Hubbard-Stratonovic fields. In our calculations we consider large values of $\beta$ and extrapolate to $\beta \rightarrow \infty$. Computing expectation values is more convenient using the above algorithm compared to the conventional VMC implementations. For example, in a single step, we can easily obtain any expectation value for $g = 0$ while the conventional implementation of the VMC method requires thousands of sweeps for the same parameters. On the contrary, our density matrix based method converges faster and expectation values can be obtained with high accuracy by sweeping over Hubbard-Stratonovic fields only a few thousand times even at the large $U$ limit. We would like to stress that the above scheme is spin-problem free due to the fact that the renormalized Hubbard coupling, i.e., $U_{eff} = g/\beta$, is negligible (since $g/U \sim O(1)$) and it is known that such weak couplings do not lead to sign problem (see Figs. 3 and 6).
B. Variational Quantum Monte Carlo

As we argued above, the VMC method can be viewed as a generalized Trotter-Suzuki decomposition for very large imaginary time steps (see Eq. 3). In this section, we generalize VMC and find a smooth path connecting VMC to DQMC. Our main tool to achieve this goal is the following generalized Trotter-Suzuki decomposition for finite imaginary time steps \( \tau \equiv \beta / N \):

\[
e^{-\tau(H_K+H_U)} \approx \rho_{\text{eff}} \equiv e^{-\frac{\tau}{2}H_s}e^{-\frac{\tau}{2}H_e}e^{-\tau H_M}e^{-\frac{\tau}{2}H_s}e^{-\frac{\tau}{2}H_e},
\]

(6)

where \( H_M = \psi^\dagger M \psi \) denotes our variational quadratic Hamiltonian, and \( H_e = 1/2 \sum_{i} V_i n_{i,\uparrow} n_{i,\downarrow} \) and \( H_s = \sum_{\alpha \beta} J_{\alpha \beta} s_{\alpha,\uparrow} s_{\beta,\downarrow} \) are two body density-density and spin-spin interactions with variational couplings \( V_i \) and \( J_{\alpha \beta} \). The above transformation must recover the original Trotter-Suzuki decomposition for infinitesimal time steps which requires \( \tau \rightarrow 0 \): \( H_M \rightarrow H_K, \ V_0 \rightarrow U \) and all other components of \( V \) and \( J \) to vanish. Instead, for finite \( \tau \sim O(1) \), we consider longer range two body interactions to improve the accuracy. Indeed, the long range density-density interaction considered above is a second quantized representation of the Jastrow factors known in the studies of the Bose gas. In this work, we truncate such long range terms to keep the system. More specifically, in this scheme we can define Matsubara frequencies as \( \omega_n = \frac{2\pi}{\beta} n, \) where \( n = 1, \ldots, N \), thus we have kept and considered quantum fluctuations up to \( \omega_{\text{max}} = \frac{2\pi}{\beta} \) energy scale. (iv) Similar to DQMC, considering \( N \gg 1 \) time slices leads to fermionic sign problem, even for \( \tau \sim O(1) \). However, the onset of \( \beta \) above which the sign problem becomes significant is substantially larger than that of the conventional DQMC (see Figs. 1 and 6). This allows us to study the ground-state properties before the sign problem comes into play.

We now argue that although VQMC suffers from the fermionic sign problem in general, which is a consequence of taking quantum fluctuations into account, it does not show up down to extremely low temperatures. This is mainly due to the fact that the renormalized onsite Hubbard interaction is notably weaker than its bare value for \( \tau \sim O(1) \) as shown in Figs. 2 and 3. This pivotal observation along with its higher accuracy and potentials, suggests the VQMC method as a competitive tool for studying strongly interacting fermion systems, especially when combined with the projector quantum Monte Carlo as will be explained in detail later in this section.

To demonstrate the absence of the sign problem down to low enough temperatures, we consider the half filled Hubbard model in this paper. Although the Hubbard model at half filling and on the bipartite lattices does not suffer from the notorious fermionic sign problem, the average sign of spin up (or down) determinants is not positive definite and fluctuates strongly at low temperatures and strong interactions. The absence of the overall sign problem just implies that the sign of spin up determinant equals that of the spin down ones for each realization of the Hubbard-Stratonovic field configuration. Indeed, the emergence of the sign problem and it severity can be readily studied and predicted by studying the average sign of spin up/down determinants at half filling. Thus, in the following we consider the average sign of spin up/down determinants as a metric for measuring the severity of the (product) sign problem in the general case and away from half filling.

C. Beyond VQMC: variational projector quantum Monte Carlo

We now demonstrate that our VQMC can yield highly accurate results when combined with the projector quantum Monte Carlo (PQMC) method while mitigating the sign problem as a corollary. The main idea of the PQMC is the observation that we can achieve the ground state(s) via

\[
|\Psi_G\rangle = \lim_{\beta \rightarrow \infty} Z^{-1/2} e^{-\beta H/2} |\Phi_T\rangle
\]

relation for any trial wave function \( |\Phi_T\rangle \) that has nonzero overlap with the true ground state wave function i.e., \( \langle \Psi_G | \Phi_T \rangle \neq 0 \). Practically, this identity still holds for finite but large enough \( \beta \). However, the convergence speed, i.e., the threshold for \( \beta \) beyond which the identity holds up to a given accuracy, depends on \( \langle |\Psi_G| \Phi_T\rangle^2 \) overlap which measures the distance between the trial and exact ground states. The main advantage of the PQMC method is that the sign problem becomes less severe as we discuss below. It is mostly a consequence of starting with a
good trial wave function which can impose certain constraints on the Hubbard-Stratonovic fields (see section IV).

Similar to our derivation of Eq. 2, the density matrix in PQMC can also be represented as:
\[ \rho_{\text{PQMC}} \equiv |\Psi_G\rangle \langle \Psi_G| \propto e^{-\beta_1 H/2} |\Phi_T\rangle \langle \Phi_T| e^{-\beta_1 H/2} \propto e^{-\beta_1 H/2} \rho_T(\beta_2) e^{-\beta_1 H/2}, \]
where ideally \( \beta_{1,2} \rightarrow \infty \) though in practice we consider finite \( \beta_{1,2} \). Furthermore, we can utilize the original Trotter-Suzuki decomposition to write the outer components as: 
\[ e^{-\tau_1 H} \approx e^{-\tau_1 H_{\text{VQMC}}} e^{-\tau_1 H_K} \] 
for \( \tau_1 \ll 1/\sqrt{U_1} \). This decomposition enables us to employ the Hubbard-Stratonovic transformation and borrow other techniques from DQMC to evaluate various correlation functions (see section IV). It is a common practice to first obtain a good trial wave-function \( |\Phi_T\rangle \) using the mean-field or Hartree-Fock approximations and feed it in the above expression. Alternatively, in this paper we suggest using our VMC or VQMC methods to obtain a better trial density matrix \( \rho_T(\beta_2) \) at temperature \( T_2 = 1/\beta_2 \ll 1 \). Using these alternative approaches, and in particular when \( \tau_2 \sim O(1) \), leads to a shorter threshold for the projection time (i.e., \( \beta_2/2 \)) due to the intrinsic higher accuracy of our VMC/VQMC than the mean-filed or Hartree-Fock approximations (see Fig. 4). More importantly, in this framework we have the choice to use the ergodic form of VQMC where we impose all symmetries of the model Hamiltonian on \( H_{\text{VQMC}} \) in Eq. 6. Alternatively, we could allow symmetry breaking terms in \( H_{\text{VQMC}} \) but instead consider an ensemble over all possible degenerate ground-states.

Intuitively, we can estimate the threshold for \( \beta_1 \) such that
\[ 0 \leq E - E_G < \epsilon, \]
where \( E \) and \( E_G \) are the estimated and exact ground-state energies, respectively as follows. Let us assume the average energy of our trial density matrix \( \rho_T(\beta_2) \) is \( E_2 \). Furthermore, let us assume that we could reach \( E_2 \) in the usual finite temperature DQMC by considering an effective inverse temperature \( \beta^* \). This suggests the following approximation:
\[ \rho_T(\beta) \approx e^{-\beta^* H}, \]
which in turn implies:
\[ \rho_{\text{PQMC}}(\beta_1,\beta_2) = e^{-\beta_1 H/2} \rho_T(\beta_2) e^{-\beta_1 H/2} \approx e^{-\beta_1 + \beta^*} H = \rho_{\text{DQMC}}(\beta_1 + \beta^*). \]
Thus, the density matrix of the PQMC method is related to that of the DQMC at a higher effective inverse temperature \( \beta_1 + \beta^* \). Now, suppose that in the usual finite temperature DQMC method we could reach the desired accuracy \( \epsilon \) in ground-state energy estimation by considering \( \beta \geq \beta_{\text{th}}(\epsilon, \text{DQMC}) \). Consequently, the threshold for \( \beta_1 \) in PQMC is \( \beta_{\text{th}}(\epsilon, \text{PQMC}) = \beta_{\text{th}}(\epsilon, \text{DQMC}) - \beta^* \). Thus, \( \beta_{\text{th}}(\epsilon, \text{PQMC}) < \beta_{\text{th}}(\epsilon, \text{DQMC}) \). This observation suggests that the average sign of fermion determinants in PQMC is comparable to that of the DQMC method at a reduced inverse temperature, shifted down by \( \beta^* \), and therefore the sign problem is less significant in PQMC and has an exponentially larger average sign assuming \( \rho_T(\beta_2) \) does not aggravate the sign problem. Indeed, symmetry breaking choices of \( \rho_T(\beta_2) \) can elevate the average sign since they suppress quantum fluctuation/tunneling between degenerate ground-states.

Figure 1. DQMC results for the half-filled Hubbard model. (a) Ground-state energy per site obtained by DQMC at \( \beta = 20 \) for a \( 16 \times 4 \) square lattice as a function of onsite Hubbard interaction \( U \). These values provide the exact energies for the ground-state (up to 0.0005 statistical error bar) due to the absence of (overall) sign problem. (b) The average sign of spin up determinants for the same parameters. Although the overall sign problem is absent at half filling, the average sign of spin up fermion determinants is highly fluctuating especially at strong couplings.

Considering the above argument, our main message in this paper is that using VQMC with \( \tau_2 \sim O(1) \) leads to the highest possible value for \( \beta^* \) without causing sign problem up to large enough values of \( \beta_2 \). As a result, it minimizes \( \beta_{\text{th}}(\epsilon, \text{PQMC}) \) and maximizes the average sign better than all other existing algorithms. Therefore, it allows us to unravel previously unexplored ground-state properties of models that suffer from the sign problem.

III. IMPLEMENTATION OF OUR UNIFIED QMC ALGORITHM

In this section, we comment on the implementation of our single recipe which unifies several Monte Carlo approaches, namely VMC, its generalization VQMC, DQMC, and PQMC methods. Our starting point is the following identity which was derived before: 
\[ |\Psi_G\rangle \langle \Psi_G| = \lim_{\beta_{1,2} \to \infty} \rho, \]
where \( \rho \) is
defined as:
\[ \rho = e^{-\beta_1 \hat{H}} e^{-\beta_2 \hat{H}}. \]

In the following, we consider \( \beta_1 \ll \beta_2 \) limit. We now break \( \beta_1, \beta_2 \) into \( N_1, N_2 \) time steps and arrive at the following trivial expression for \( \rho \):
\[ \rho = \left( e^{-\tau_1 \hat{H}} \right)^{N_1/2} \left( e^{-\tau_2 \hat{H}} \right)^{N_2} \left( e^{-\tau_1 \hat{H}} \right)^{N_1/2}. \]

Now, we consider \( \tau_1, \tau_2 \) imaginary time steps to be infinitesimal (finite). Therefore, we can employ the conventional Trotter-Suzuki decomposition for \( e^{-\tau_i \hat{H}} \) as follows:
\[ e^{-\tau_i \hat{H}} \approx e^{-\tau_i H_{U}/2} e^{-\tau_i H_{K} /2} e^{-\tau_i H_{U}/2} + O(\tau_i^3), \]
while for \( e^{-\tau_2 \hat{H}} \) we have to use the generalized Trotter-Suzuki decompositions introduced in Eq. 6. Again, for simplicity, we assume that \( V_{r>0} = J_{r>0} = 0 \). At the end of this section, we comment on how to include them in our algorithm.

The above expression for \( \rho \) corresponds to different QMC approaches depending on the values of \( (\beta_1, \beta_2), (\tau_1, \tau_2) \). More specifically, (a) DQMC corresponds to \( \beta_1 > 0, \beta_2 = 0 \) (note that \( \tau_1 \to 0 \), (b) VMC corresponds to \( \beta_1 = 0, \beta_2 > 0 \), and \( \tau_2 = \beta_2 \) (i.e., \( N_2 = 1 \)). (c) VQMC corresponds to \( \beta_1 = 0, \beta_2 > 0 \), and \( N_2 > 1 \), and (d) PQMC corresponds to \( \beta_1 > 0, \beta_2 > 0 \).

Having achieved the above (generalized) Trotter-Suzuki decompositions, we can employ the Hubbard-Stratonovic transformation (see Eq. 4) after which the total density matrix \( \rho \) can be written as an ensemble over non-interacting fermion density matrices subject to space-time dependent auxiliary binary fields. Accordingly, we obtain the following expression for \( Z = \text{Tr} \rho \)
\[ Z = \sum_{\{s_1^{1, L}\}} \sum_{\{s_1^{1, R}\}} \sum_{\{s_2^{2, L}\}} \sum_{\{s_2^{2, R}\}} Z_\sigma \left( \{s_1^{1, L}\}, \{s_1^{1, R}\}, \{s_2^{2, L}\}, \{s_2^{2, R}\} \right) \]
\[ \times \left( \{\hat{S}_1^{1, L}\}, \{\hat{S}_1^{1, R}\}, \{\hat{S}_2^{2, L}\}, \{\hat{S}_2^{2, R}\} \right), \]
in which
\[ Z_\sigma \left( \{s_1^{1, L}\}, \{s_1^{1, R}\}, \{s_2^{2, L}\}, \{s_2^{2, R}\} \right) = \text{Tr} \left[ \hat{F} \left( \{s_1^{1, L}\}, \{s_1^{1, R}\}, \{\lambda_1, \sigma\} \right) \cdots \hat{F} \left( \{s_{N_1}^{1, L}\}, \{s_{N_1}^{1, R}\}, \{\lambda_1, \sigma\} \right) \times \hat{G} \left( \{s_{N_2}^{2, L}\}, \{s_{N_2}^{2, R}\}, \{\lambda_2, \sigma\} \right) \cdots \hat{G} \left( \{s_{N_2}^{2, L}\}, \{s_{N_2}^{2, R}\}, \{\lambda_2, \sigma\} \right) \right]. \]

where \( \hat{F} \) and \( \hat{G} \) operators are defined as follows:
\[ \hat{F} \left( \{s_1^{1, L}\}, \{s_1^{1, R}\}, \{\lambda_1, \sigma\} \right) = e^{-\lambda_1 s_1^{1, L} \sigma n_1^1} e^{-\lambda_1 s_1^{1, R} \sigma n_1^2} e^{\beta_1 H_{U}/2} e^{\beta_1 H_{K} /2} e^{-\beta_1 H_{U}/2}, \]
\[ \hat{G} \left( \{s_2^{2, L}\}, \{s_2^{2, R}\}, \{\lambda_2, \sigma\} \right) = e^{-\lambda_2 s_2^{2, L} \sigma n_1^2} e^{-\lambda_2 s_2^{2, R} \sigma n_1^2} e^{\beta_2 H_{U}/2} e^{\beta_2 H_{K} /2} e^{-\beta_2 H_{U}/2}. \]

Using standard relations for the product of fermion Gaussian forms, individual contributions to the partition function can be evaluated as:
\[ Z_\sigma \left( \{s_1^{1, L}\}, \{s_1^{1, R}\}, \{s_2^{2, L}\}, \{s_2^{2, R}\} \right) = \text{det} \left( I + B_\sigma^{N_1} B_\sigma^{N_2} \cdots + A_\sigma^{N_1} B_\sigma^{N_2} B_\sigma^{N_1/2} \cdots B_\sigma^0 \right), \]

where imaginary time dependent \( A_\sigma^n \), and \( B_\sigma^n \) matrices are defined as:
\[ A_\sigma^n = e^{-\sigma_1 \tau_1 \text{diag}(s_1^{1, L})} e^{-\tau_1 K_{1, \sigma} /2} e^{-\sigma_1 \tau_1 \text{diag}(s_1^{1, R})}, \]
\[ B_\sigma^n = e^{-\sigma_2 \tau_2 \text{diag}(s_2^{2, L})} e^{-\tau_2 K_{2, \sigma} /2} e^{-\sigma_2 \tau_2 \text{diag}(s_2^{2, R})}. \]

In the above expression, \( K_{1, \sigma} = K_{2, \sigma} \) denote the hopping matrices associated with the model Hamiltonian (Hubbard model in our example), and \( K_{2, \sigma} \) denotes the variational hopping matrix. Here, for simplicity we have assumed explicit BCS pairing is absent (as well as spin conservation), though it is straightforward to take them into consideration and generalize the above relations. The fermion Green’s function associated with a fixed Hubbard-Stratonovic binary field configuration
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![Graph](image_url)

**Figure 2.** Results of one and two-parameter families of VMC and
VQMC methods. (a) Gourd-state energy estimation of Free fermions
(with square Fermi surface) as well as VMC and VQMC ansatz with
one variational parameter $U_{\text{eff}}$ (relative to the exact ground-state
energy shown in Fig. 1). Here, we considered $\beta_2 = 80$ (40) for VMC
(VQMC). (b) The corresponding optimal values of $U_{\text{eff}}$. (c) and (d)
plot similar quantities but now by optimizing two variational parame-
ters: $U_{\text{eff}}$ and $m$. These figures show that VMC provides an improve-
ment over the noninteracting mean-field approximation, and VQMC
improves VMC results further via taking quantum fluctuations into
account. Also, considering more variational parameters yields more
accurate results.

s) is Gaussian and noninteracting, we can use the above re-
lation for the two-point functions to compute four-point and
higher order correlation functions by applying Wick’s theo-
rem for the corresponding realization of auxiliary fields. By
sampling enough important field configurations and averag-
ing over them we can achieve the correlation functions for the

![Graph](image_url)

**Figure 3.** Renormalized onsite Hubbard interaction as a function of
imaginary time steps (by optimizing one variational parameter only)
for $U = 4$. As this figure shows, $U_{\text{eff}}$ approaches a constant for
$\tau \geq 1/2$.

![Graph](image_url)

**Figure 4.** Ground-state energy estimated by PQMC with several dif-
dent choices for the trial state. These results correspond to $U = 4$
and $16 \times 4$ rectangular system. Note that PQMC converges faster
than DQMC (which can be imagined as a PQMC with identity trial
density matrix i.e. infinite temperature limit) even by starting from
Fermi surface. Using VQMC with two parameters, $\tau = 1/2$, and
$\beta_2 = 20$ as the trial density matrix yields an accurate energy estima-
tion even for a projection time as short as $\beta_1/2 = 1/2$.

**IV. BEHAVIOR OF THE SIGN PROBLEM**

In this section, we briefly discuss the origin of fermionic
sign problem in DQMC and related methods and argue that
our VQMC as well as our modified PQMC combined with
VQMC can alleviate the sign problem. The sign problem sim-
ply means $Z_\sigma$ (s) defined in Eq. 16 can take negative values
as well depending on the s auxiliary field realization. Since, 
\[ Z_\sigma (s) = \text{Tr} \left( e^{-c_{\sigma}^\dagger h_{\sigma}^N c_{\sigma}} \right) \] it might seem 
surprising why the product of individually positive definite 
terms can give rise to negative values. To understand why 
that can happen, we must note that there exists \( h_{\sigma}^{\text{eff}} \) such that 
\[ e^{-c_{\sigma}^\dagger h_{\sigma}^N c_{\sigma}} = e^{-c_{\sigma}^\dagger h_{\sigma}^{\text{eff}} c_{\sigma}} \] 
where \( h_{\sigma}^{\text{eff}} = e^{h_{\sigma}^N} \cdots e^{h_{\sigma}^1} \). However, it is clear that \( h_{\sigma}^{\text{eff}} \) is 
not necessarily self-conjugate unless \( h_{\sigma}^\dagger = (h_{\sigma}^N)^\dagger \) which is 
not true in general as all Hubbard-Stratonovic fields are 
indeed random binary numbers. Therefore, there is no 
guarantee that \( h_{\sigma}^{\text{eff}} \) contains real eigenvalues in its SVD 
decomposition, and thus \( \text{Tr} \left( e^{-c_{\sigma}^\dagger h_{\sigma}^{\text{eff}} c_{\sigma}} \right) = \text{det} \left( 1 + e^{-h_{\sigma}^{\text{eff}}} \right) \) 
can have a complex phase. However, for real Hamiltonians 
the complex phase can be either 1 or -1. Another way to 
understand the sign problem is to consider the following 
imaginary time evolution operator: 
\[ U_{\sigma}^\tau = \prod_{t=1}^{\tau} e^{-c_{\sigma}^\dagger h_{\sigma} c_{\sigma}} \] [21], and its instantaneous 
many-body lowest right eigenstate denoted as \( |\psi (t)\rangle \). 
This many-body eigenstate has \( t \) dependence and when \( t \) varies slowly, we can define the Berry 
phase for two consecutive instantaneous eigenstates, namely 
\[ e^{i\theta_{\sigma}(t)} = \langle \psi (t+1) | \psi (t) \rangle \] Since, \( h_{\sigma}^{\text{eff}} \) depends on the 
Hubbard-Stratonovic fields which take different values from 
one imaginary time slice to another, \( |\psi (t)\rangle \) can have a 
different phase from its ensuing one. The sign problem occurs 
when \( \langle \psi (N) | \psi (1) \rangle \) (which is correlated with the total Berry 
phase \( \theta_B = \sum_t \theta_B(t) \)) may take negative values. When the 
(renormalized) interaction strength \( U_{\text{eff}}(\tau) \) is weak, random 
parts of \( h_{\tau}^{\text{eff}} \) can be neglected, hence the instantaneous 
eigenstates are close and are all negligible and as a result \( \theta_B(t) \) 
are infinitesimal. However, when \( N = \beta/\tau \gg 1 \), the sum 
of individual contributions may add up to \( \pi \) and cause 
negative signs. The chance of such events increase exponentially 
with \( \beta \), and that is another reason why the average sign dies 
off as \( e^{-\beta V_f} \) with \( \beta \). However, there are two other effects 
that can ameliorate the sign problem. For instance, as we 
discussed previously and Figs. 3 and 6 suggest, \( U_{\text{eff}} \ll 1 \) for 
\( \tau \sim O(1) \) and beyond. Additionally, when symmetry breaking 
terms such as staggered magnetization are allowed, the 
random onsite Hubbard-Stratonovic fields are masked by the 
mean-field terms and their chance to negate the partition functions 
is exponentially suppressed. Moreover, as Fig. 2 shows, 
it is energetically favorable to consider such symmetry breaking 
terms for finite imaginary time steps though their strength 
is attenuated upon decreasing \( \tau \).

To summarize, there are two reasons to push down the on-set temperature for the emergence of the sign problem in our 
VQMC and PQMC methods. Firstly, considering imaginary 
time steps larger than that of the DQMC method surpasses the 
renormalized onsite Hubbard coupling \( U_{\text{eff}} \) as \( 1/\tau \). Secondly, 
for finite imaginary time steps, we find a non-vanishing opti-mal value for the staggered magnetization at half filling and 
other symmetry breaking terms in general. These two ob-servations 
hand in hand ameliorate the sign problem and keep 
the average sign high. As a result, in PQMC, the VQMC 
trial density matrix part of the method is nearly sign free 
and the sign problem is entirely due to the projection part namely 
\( e^{-\beta_1 V_f} \) instead of \( e^{-\beta (\beta_2^2 V_f)} \). Finally, since the VQMC ansatz was already close to the 
exact ground-state, the minimum required projection 
time \( \beta_1/2 \) can be surprisingly short (see Fig. 4).

V. RESULTS

In this section we first benchmark our unifying VQMC algorithm, 
which encompasses VMC and DQMC as its two extreme 
limits (upon varying imaginary time steps \( \tau \)), and later 
employ it to feed PQMC and present the corresponding 
results. In this paper, we focus on the half-filled Hubbard model 
on the square lattice with \( (N_x, N_y) = (16, 4) \) linear dimensions. 
We consider \( U \in [1, 6] \) range for the onsite Hubbard interaction. 
For these model Hamiltonians, the finite temperature 
DQMC method is sign-free and can provide exact results 
up to any desired accuracy by considering large \( \beta \) and sampling 
over enough Hubbard-Stratonovic field configurations. In 
our simulations, we have assumed the following imaginary 
time steps: \( \tau = (1/20, 1/2, 1, 2, 4, 8, \beta) \), and considered
variational parameters. More explicitly, we have considered the matrix obtained through the VQMC method. Here, we have plotted our results for VQMC with one tuning parameter. The average sign does not fluctuate at $\beta = 0$, and only $U_{\text{eff}}$ can vary. In Fig. 2(b) we plot the optimal values of $U_{\text{eff}}$ for these models given $m = 0$ constraint. Similarly, Figs. 2(c) and 2(d) present estimations for the ground-state energy (relative to the exact one) and the corresponding renormalized onsite Hubbard interaction by optimizing both variational parameters namely $U_{\text{eff}}$ and $m$. These two figures suggest a considerable improvement to the mean-field approximation by considering VMC. Furthermore, VQMC improves the results obtained from VMC further which was achieved by taking quantum fluctuations into consideration.

In Fig. 3, we plot the renormalized onsite Hubbard interactions as a function of $\tau$ for $U = 4$. As we expect, $U_{\text{eff}} = U$ for $\tau = 1/20$ (i.e., in DQMC), while it decays as $1/\tau$ for $\tau \geq 1/2$.

In Fig. 4, we compare the estimated ground-state energy of the PQMC method through considering various choices for the trial state/density matrix. This result suggests the VQMC as the best choice for the trial density matrix to feed in PQMC, since a projection time ($\beta_1$) as short as 1 can already result in a highly accurate estimation for the ground-state energy. For the mean-field trial state on the other hand, we must consider $\beta_1 = 3$ to reach that accuracy. We would like to stress that all these results are obtained by allowing at most two variational parameters in VQMC. Using more variational parameters can reduce the threshold of $\beta_1$ ($\beta_{\text{th}} (\epsilon, \text{PQMC})$) further.

Figure 6 presents the average sign of spin up determinants within DQMC at $\beta = 20$ in Fig. 1(b). Note that the average sign diminishes as we increase $U$.

In Fig. 2(a) we compare the estimated ground-state energy (extrapolated to $\beta = \infty$) relative to the ground truth for a range of $U$ values obtained through applying various methods. In this figure we have set $m = 0$, and only $U_{\text{eff}}$ can vary. In Fig. 2(b) we plot the optimal values of $U_{\text{eff}}$ for these models given $m = 0$ constraint. Similarly, Figs. 2(c) and 2(d) present estimations for the ground-state energy (relative to the exact one) and the corresponding renormalized onsite Hubbard interaction by optimizing both variational parameters namely $U_{\text{eff}}$ and $m$. These two figures suggest a considerable improvement to the mean-field approximation by considering VMC. Furthermore, VQMC improves the results obtained from VMC further which was achieved by taking quantum fluctuations into consideration.

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Finally, Fig. 6 presents the average sign of spin up fermion determinants for $U = 4$ versus temperature as well as average energy of the system. These plots show how the average sign (for spin up fermions) can increase exponentially using our modified PQMC (fed by VQMC as its trial density matrix) despite its remarkably high accuracy. This result suggests that our modified PQMC can uncover the ground-state properties of the doped Hubbard model by allowing to access and probe lower temperatures.

VI. SYMMETRY BREAKING, COMPETING ORDERS, AND ERGODICITY

The quadratic Hamiltonian considered in Eqs. 3 and 21 can host terms that break various symmetries associated with the Hubbard model. For example, the staggered magnetization term breaks the spin SU(2) symmetry down to its $Z_2$...
subgroup. It also breaks the lattice translation as well as $C_4$ rotational symmetries and enlarges the unit cell accordingly. However, we would like to stress that considering such terms are not necessary in general. For instance, considering a nonzero value for the $J_1$ term in Eq. 6, we can compensate the effects of staggered magnetization considered in Eq. 21. It can also take quantum fluctuations (such as Goldstone modes) around the symmetry breaking terms into consideration for free. This however, depends on how stable that symmetry breaking phase is compared to other potentially competing orders. If the estimated ground-state energies of those competing symmetry breaking phases are well separated, we may simply consider a symmetry breaking quadratic form. Otherwise, it will be more reasonable to keep the quartic Heisenberg terms to allow for more complicated spin phases, e.g., spin liquids.

VII. SUMMARY AND DISCUSSION

In this work we presented a unified framework for several QMC approaches. We demonstrated that they all can be understood using our generalized Trotter-Suzuki decomposition (see Eq. 6). Based on this understanding we developed a novel technique dubbed as VQMC which paves the way between VMC and DQMC and interpolates between them by smoothly varying imaginary time steps from zero to infinity. We showed that this novel method is more accurate than VMC, captures important (low energy) quantum fluctuations, and can give access to low temperature due to its better behavior for the sign problem. We showed that our VQMC can serve as the best available trial state for the PQMC upon which we can achieve ground-state properties even after short projection time. We investigated various aspects of these related techniques.

There are still several important steps to be taken in future. In this paper, we focused on the unfrustrated Hubbard model at half filling to benchmark our algorithm since we can find the exact solutions using the conventional DQMC algorithm. However, such proposals are more needed away from half filling or for frustrated Hamiltonians that suffer from fermionic sign problem. Hence, it is interesting to see what we can learn from this new approach when applied to doped Hubbard model whose reliable solution (even approximate) is still absent.

In this work, we considered two variational parameters at most, and achieved satisfactory results. However, the VQMC itself can be significantly improved by allowing more variational terms in Eq. 6 such as the longer range Jastrow density-density or Heisenberg spin-spin interactions. We have already seen that considering two variational parameters gives rise to much more accurate results than a single variational parameter (see Fig. 2 for example).

It is worth noting that our algorithm can be useful for the finite temperature DQMC as well. It obviates the need to extrapolate to $\tau \to 0$ to kill the Trotter errors. Instead, we need to consider short enough (imaginary) time steps (e.g., $\tau = 1/4$ or $\tau = 1/8$) and optimize $U_{\text{eff}}$ which will turn out to be slightly less than $U$. Fig. 3 shows that even for $\tau = 1/4$, $U_{\text{eff}} \neq U$. For example, we observed that for $U = 4$ and $\tau = 0.25$, considering $U_{\text{eff}} \approx 3.5$ yields results closer to those of $\tau = 0.05$ than $U_{\text{eff}} = 4$.

Finally, we would like to mention that our two-time representation in Eq. 10 can be straightforwardly generalized to more general situations such as $e^{-\beta_1 H/2} e^{-\beta_2 H/2} e^{-\beta_3 H} e^{-\beta_4 H} e^{-\beta_5 H} e^{-\beta_6 H}/2$, where $\beta_1 \ll \beta_2 \ll \beta_3$ and then consider generalized Trotter-Suzuki decomposition for $\tau_1 \ll 1$, $\tau_2 \sim O(1)$, and $\tau_3 \gg 1$ imaginary time steps. Such additional decorations can enhance the computational time, accuracy, and improve the average sign further.

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