Relation between fermionic and qubit mean fields in the electronic structure problem

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For quantum computing applications, the electronic Hamiltonian for the electronic structure problem needs to be unitarily transformed to a qubit form. We found that mean-field procedures on the original electronic Hamiltonian and on its transformed qubit counterpart can give different results. We establish conditions of when fermionic and qubit mean fields provide the same or different energies. In cases when the fermionic mean-field (Hartree–Fock) approach provides an accurate description (electronic correlation effects are small), the choice of molecular orbitals for the electron Hamiltonian representation becomes the determining factor in whether the qubit mean-field energy will be equal to or higher than that of the fermionic counterpart. In strongly correlated cases, the qubit mean-field approach has a higher chance to undergo symmetry breaking and lower its energy below the fermionic counterpart.

I. INTRODUCTION

An interest in solving quantum chemistry problems on a quantum computer has experienced a rapid growth in the last two decades.  

To address some of the technical difficulties (mainly maintaining long coherence times) associated with the initial quantum phase estimation (QPE) approach, the variational quantum eigensolver (VQE) scheme has been suggested recently and already proven to be feasible in calculating potential energy surfaces (PESs) of small molecules (e.g., H₂, LiH, and BeH₂). The VQE approach searches for unitary rotations \( U_{\text{ENT}}(\tau) \) and \( U_{\text{MF}}(\Omega) \) of qubits encoding the electronic wavefunction

\[
|\Psi(\Omega, \tau)\rangle = U_{\text{ENT}}(\tau)U_{\text{MF}}(\Omega) |0_q\rangle,
\]

that minimize the total electronic energy

\[
E_e = \min_{\Omega, \tau} \langle \Psi(\Omega, \tau) | H | \Psi(\Omega, \tau) \rangle,
\]

where \( \{\Omega, \tau\} \) are parameters of the unitary rotations, \( |0_q\rangle \) is the initial state of qubits, and \( H \) is the system electronic Hamiltonian. A typical starting point of this search is to introduce individual qubit rotations based on the results of a mean-field procedure, \( U_{\text{MF}}(\Omega) \). This qubit mean field (QMF) is followed by the qubit entangling step, employing \( U_{\text{ENT}}(\tau) \). Evaluation of the expectation value in Eq. (2) can be exponentially hard on a classical computer due to the entangling transformation \( U_{\text{ENT}} \), whereas it has a polynomial scaling on a universal quantum computer. Therefore, VQE employs a hybrid scheme where a quantum computer evaluates the energy estimate for a particular set of parameters \( \{\Omega, \tau\} \), and then, a classical computer finds the energy minimum. For calculating the energy expectation value, the Hamiltonian needs to be transformed from its original second-quantized fermionic form to a form operating in the qubit space. This fermion-to-qubit transformation is achieved by either the Jordan–Wigner (JW) or the Bravyi–Kitaev (BK) transformation.

Although the entangling transformation can be generated using the Unitary Coupled Clusters (UCC) approach, which provides energies at the level of chemical accuracy, practical truncated UCC procedures do not guarantee solutions equivalent to the exact Full Configuration Interaction (FCI) solution of the problem. In this case, any practical and approximate entangling scheme will depend on the quality of the mean-field result serving as the first step.

This work is focused on differences in QMF outcomes that originate from representations of the initial electronic Hamiltonian that use different one-particle basis functions. Interestingly, results of the QMF approach are not invariant with respect to different choices of one-electron basis functions. Here, we investigate the origins of this dependence and relations between results of fermionic (Hartree–Fock) and QMF mean fields.

The rest of the paper is organized as follows. First, we briefly recapitulate the relevant basics of the Hartree–Fock (HF) method and formally introduce the QMF method. Second, we illustrate the problem by considering different
QMF solutions for the LiH molecule. Third, we discuss a simple one-electron Hamiltonian that can be treated exactly at the HF level and see what solutions QMF can provide. Finally, we consider a strongly correlated case of a stretched H₂ molecule and discuss the symmetry breaking phenomenon. In conclusions, we summarize all the findings and discuss some of the perils of the QMF method.

II. THEORY

A. Fermionic mean field

An \( N_e \)-electron wavefunction in the HF theory is obtained by application of an ordered string of \( N_e \) fermionic creation operators \( a_i^\dagger \) to the mathematical vacuum state, \( |0\rangle \), the state with zero electrons:

\[
|\Phi\rangle = \prod_{i=1}^{N_e} a_i^\dagger |0\rangle.
\]

Each creation operator \( a_i^\dagger \) adds to a system an electron in a state given by a single-particle molecular spin orbital (MSO), \( \psi_i^\sigma(x) \). Here, \( x = (r, \sigma) \), is a joined spatial and spin coordinate of an electron. For simplicity, we will consider only the restricted version of the HF theory, which implies that for every spatial single-particle function there are two MSOs with the opposite spins.

Individual fermionic operators can be rotated using a unitary transformation, which conserves the fermionic anti-commutation relations,

\[
\hat{a}_i^\dagger(\kappa) = \exp(\hat{\kappa}) a_i^\dagger \exp(-\hat{\kappa}),
\]

where

\[
\hat{\kappa} = \sum_{i>j} \kappa_{ij} (a_j^\dagger a_i - a_i^\dagger a_j)
\]

is an anti-hermitian operator with orbital rotation amplitudes \( \kappa = \{ \kappa_{ij} \} \). Variations of \( \kappa_{ij} \) are used to minimize the expectation value of the electronic energy

\[
E_{HF} = \min_{\kappa} \langle \Phi(\kappa) | H_e | \Phi(\kappa) \rangle,
\]

where \( H_e \) is the second-quantized electronic Hamiltonian,

\[
H_e = \sum_{ij} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} g_{ijkl} a_i^\dagger a_k^\dagger a_l a_j.
\]

Here, \( h_{ij} \) and \( g_{ijkl} \) are one- and two-electron integrals, which depend on the nuclear configuration.\(^{17}\)

If a MSO basis \( \{ \psi_i \} \) contains \( N_b \geq N_e \) orbitals, the first \( N_b \) orbitals are termed occupied, while the remaining \( N_b - N_e \) of them are unoccupied or virtual. Only mixing of occupied and virtual orbitals by means of elements of \( \kappa \) changes the expectation value in Eq. (6). Corresponding orbital rotations are termed non-redundant. The HF method has polynomial complexity in the number of parameters that need to be optimized: there are only \( N_e(N_b - N_e) \) non-redundant orbital rotation amplitudes \( \{ \kappa_{ij} \} \) to be determined. In most computer implementations, optimal parameters are found by iterative diagonalization of an \( N_b \times N_b \) Fock matrix with elements

\[
f_{ij} = \langle \Phi(\kappa) | [a_i^\dagger a_j, H_e] | \Phi(\kappa) \rangle,
\]

which produces orbital energies \( \{ \epsilon_i \} \) as eigenvalues and canonical MSOs (CMSOs) as eigenvectors for the \( N_e \) system.\(^{17}\)

The electronic Hamiltonian in Eq. (7) can be also written using the CMSOs of the \( N_e \) system

\[
\tilde{H}_e = \sum_i \epsilon_i a_i^\dagger a_i + \frac{1}{2} \sum_{ijkl} v_{ijkl} a_i^\dagger a_k^\dagger a_l a_j,
\]

where the one-electron part acquires the diagonal form. Although the HF energy is invariant with respect to the substitution of \( H_e \) by \( \tilde{H}_e \) in Eq. (6), \( \tilde{H}_e \) is often used to start hybrid quantum-classical computations because its form is simpler and classical computers can provide the CMSOs relatively easily for a wide range of systems.

B. Qubit mean field

Quantum computers employ two-level systems (“qubits”) as the basis of computations,\(^{8,12}\) therefore, to address the electronic structure problem they require transforming the fermionic Hamiltonian to an equivalent (isospectral) qubit form. Shorter operator expressions are obtained using the BK transformation, and thus, we will employ it for transforming \( H_e \) to

\[
H_{BK} = \sum_I C_I T_I,
\]

where \( C_I \) are numerical coefficients and \( T_I \) are products of several spin operators \( \omega_i^{(T)} \in \{ x_i, y_i, z_i \} \)

\[
T_I = \omega_{k-1}^{(T)} \cdots \omega_0^{(T)}, \quad 1 \leq k \leq N_e.
\]

Here, \( x_i, y_i, z_i \) are the Pauli matrices for the \( i \) th qubit. The maximum length of \( T_I \)’s determines the degree of locality of the qubit Hamiltonian, which is \( \sim \log_2 N_b \) for the BK transformation. Note that a different qubit Hamiltonian is obtained if the electronic Hamiltonian was presented in the CMSO [Eq. (9)] first and then BK transformed. We will denote such a Hamiltonian as \( \tilde{H}_{BK} \). The structure of \( \tilde{H}_{BK} \) is similar to that of \( H_{BK} \), but values of its coefficients \( C_I \) and components of corresponding operators \( T_I \) are different.

To perform a mean-field treatment of the qubit Hamiltonians we employ the parametrization of the spin-1/2 Hilbert space in terms of the so-called spin coherent states.\(^{18–21}\) This representation is convenient because it provides a simple parametrization of the electronic energy functional.
A spin coherent state (also known as a “Bloch state”) for a single particle with spin \( J \) is defined by the action of an appropriately scaled exponent of the lowering operator \( \hat{S}_- \) on the normalized eigenfunction of \( \hat{S}_z \) operator, \( \hat{S}_z |JM\rangle = M |JM\rangle \), with maximal projection \( M = J \):\(^{21}\)

\[
|\Omega\rangle = \cos^J\left(\frac{\theta}{2}\right) \exp \left[ \tan \left(\frac{\theta}{2}\right) e^{i\phi} \hat{S}_- \right] |JJ\rangle = \sum_{M=-J}^{J} \left(\frac{2J}{M+J}\right)^{1/2} \cos^{J+M}\left(\frac{\theta}{2}\right) \sin^{J-M}\left(\frac{\theta}{2}\right) e^{i(J-M)\phi} |JM\rangle , \tag{12}
\]

where \( \Omega = (\phi, \theta) \), \( 0 \leq \phi < 2\pi \), \( 0 \leq \theta \leq \pi \), are the spherical coordinates on a unit sphere (“Block sphere”). States \( |JM\rangle \) are normalized as:

\[
|JM\rangle = \left(\frac{2J}{M+J}\right)^{1/2} [(J-M)!]^{-1} S^{J-M}_{-M} |JJ\rangle . \tag{13}
\]

For the qubits used in quantum computing, \( J = 1/2 \).

A direct product of the spin-coherent states for \( N_e \) qubits, \( \{\Omega_1, \Omega_2, \ldots, \Omega_{N_e}\} \) is used as an analog of the HF wavefunction, Eq. (3). Also, by analogy with the HF energy functional in the right-hand side of Eq. (6), we introduce the QMF energy functional as:

\[
E_{\text{QMF}}(\Omega) = \langle \Omega | H_{\text{BK}} | \Omega \rangle . \tag{14}
\]

The explicit form of this functional can be easily obtained using the substitution suggested by Lieb\(^{21}\) for every \( T_I \) term in \( H_{\text{BK}} \). Minimization of the QMF functional in Eq. (14) with respect to all Bloch angles (\( \phi_1, \theta_1, \phi_2, \theta_2, \ldots \)) gives the QMF energy corresponding to the electronic Hamiltonian \( H_e \)

\[
E_{\text{QMF}} = \min_{\Omega} E_{\text{QMF}}(\Omega) . \tag{15}
\]

If a different initial electronic Hamiltonian is used, for instance \( \hat{H}_e \), the qubit mean-field energy can potentially be different, \( E_{\text{QMF}} = \min_{\Omega} \langle \Omega | \hat{H}_e | \Omega \rangle \neq E_{\text{QMF}} \).

### III. RESULTS AND DISCUSSION

#### A. LiH molecule

A numerical comparison of fermionic and qubit mean fields was conducted by calculating the LiH molecule in the STO-3G basis set at the interatomic distance \( R = 1.45 \) Å (at this distance the HF mean-field description is quite accurate). In this example, the electronic structure problem has \( N_b = 12 \) MSOs. The electronic Hamiltonians were considered in two sets of MSOs: 1) the HF CMSOs of the LiH molecule [Eq. (9)], and 2) MSOs from LiH\(^{2+}\) that keep the electronic Hamiltonian in the form of Table I.

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within the occupied-virtual subspace

\[ b_2 = \cos \tau \tilde{a}_2 + \sin \tau \tilde{a}_3, \]
\[ b_3 = -\sin \tau \tilde{a}_2 + \cos \tau \tilde{a}_3, \] (18)

the creation counterparts (Hermite conjugates) of \( \tilde{a}_2 \) and \( \tilde{a}_3 \) are transformed accordingly, and all the remaining operators are left untouched.\textsuperscript{24} The new fermionic operators \( (\tilde{b}_1^\dagger, \tilde{b}_1) \) satisfy the same commutation relations as the old ones. Of course, this transformation can be easily undone by taking \( \tau' = -\tau \), and hence, the HF method applied to the transformed fermionic Hamiltonian will recover the original value for the minimum. However, the rotated electronic Hamiltonian defines a new BK image, which for the particular choice \( \tau = \pi/6 \) reads

\[
H_{BK}^{(1)} = -2.4009 - 0.08175 z_0 (1 + 2 z_5 z_3) \\
+ 1.1731 z_0 (1 + z_1) + 0.14875 z_2 - 0.03965 z_4 \\
+ 0.10165 z_1 z_2 z_1 + 0.00745 z_5 z_4 \\
- 0.0815796 (2 z_2^2 z_4 + y_5 y_3 z_2 z_1). \] (19)

Here, the pairs of \( x_i \) and \( y_i \) operators introduce entanglement in eigenstates of the rotated Hamiltonian and make the QMF ground state solution higher in energy than the exact one: \( E_{QMF}^{(1)} = -5.2081 \) a.u. > \( E_0 \).

Further testing with random unitary transformations involving more MSOs than in Eq. (18) showed that the QMF minima are always higher than \( E_0 \) as long as the occupied-virtual rotations are included in the unitary transformation. Thus, the source of the QMF problems can be related to its inability to perform rotations equivalent to the unitary one-particle transformations that are easily achieved by the one-electron operators in Eq. (4).

The last example can make an impression that the fermionic mean-field approach is more powerful than its qubit counterpart. The following example shows that it is not the case. A simple qubit Hamiltonian that allows for the exact solution by QMF can be written as

\[
H_q^{(1)} = \alpha z_0 + \beta x_1 + \gamma y_2, \] (20)

it can be converted to a fermionic form using the inverse of the JW transformation (see Ref. 25):

\[
H_c^{(1q)} = \alpha (1 - 2 a_1^\dagger a_1) + \beta (1 - 2 a_2^\dagger a_2) \\
+ \gamma (1 - 2 a_1^\dagger a_1)(1 - 2 a_2^\dagger a_2)(a_3^\dagger - a_3). \] (21)

It is easy to see that the \( H_c^{(1q)} \) Hamiltonian is quintic in terms of powers of elementary fermionic operators, and it does not conserve the number of electrons. Thus, any HF procedure that uses Slater determinants with a fixed number of electrons will give the minimum energy that is higher than the exact one.

### C. Symmetry breaking

If electron correlation is large, which is usually the case when the system ground state becomes quasi-degenerate, it is possible to have \( E_{QMF} \) ≤ \( E_{HF} \). A specific example is a stretched \( H_2 \) molecule in the STO-3G basis (Fig. 1). For \( R(H-H) \) ≥ 1.5 Å the QMF energy plunges below the restricted (singlet) HF energy and the potential energy curve in this region displays a “kink”. This takes place because the energy of a triplet state becomes lower than the HF singlet and QMF readily switches to the triplet solution. This phenomenon is known as the symmetry breaking, and QMF is prone to it: QMF solutions may easily violate such physical constraints as the number of electrons in the system or the state multiplicity as in the given example.\textsuperscript{26} On the other hand, the fermionic mean-field approach is organized so that the unitary rotations [Eq. (4)] commute with the operators of the number of electrons, the total electron spin \( z \)-projection, and even with the square of the total spin \( S^2 \) in some cases. Therefore, the fermionic mean-field approach conserves many symmetries by construction.\textsuperscript{27}

### IV. CONCLUSIONS

We introduced and studied properties of the QMF approach, which is the simplest parametrized molecular wavefunction ansatz possible on a quantum computer. We considered the representation of quantum states of individual qubits in terms of the spin coherent states that depend on a set of Bloch angles. This representation leads to extremely simple form of the energy functional and allows us to draw parallels between the fermionic mean-field approach (the restricted HF method) and QMF. We compared the results of HF energy minimization with those given by QMF and found that generally, the QMF method provides energies that are higher than their restricted HF counterparts. This result emphasizes the importance of specifying the electronic Hamiltonian representation (the MSO set) used for any VQE simulations. Also, our observations suggest that prior HF calculations on a classical computer may be beneficial to decrease
computational burden placed on a quantum computer. However, this supremacy of fermionic mean-field stems from a somewhat biased starting point of the electronic Hamiltonian, which is formulated using the fermionic operators. It is easy to find an oppositely biased starting point of a spin Hamiltonian that can be treated exactly by QMF but whose treatment with the HF method will be only approximate.

Another significant aspect of the relation between qubit and fermionic mean-fields is their behavior in strongly correlated cases where mean-field solutions become inaccurate. The fermionic mean-field approach usually conserves many symmetries by construction, and the symmetry breaking requires relaxing some constraints built in its variational ansatz. QMF is prone to breaking physical symmetries because arbitrary qubit rotations are generally incompatible with symmetries of the electronic Hamiltonian. In the symmetry breaking case, PESs exhibit characteristic “kinks” due to drastic change of the physical nature of the wavefunction. Although in such cases $E_{\text{QMF}} \leq E_{\text{HF}}$, one should prefer to stay on the same physical branch of a solution. A treatment producing continuous PESs in symmetry breaking situations is proposed in Ref. 26, and the current work emphasizes additionally the importance of physical constraints for variational methods working with qubits.

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22. These MSOs were obtained as the HF CMSOs for the singlet LiH\(^1\)\(^+\) cation.
23. The BK Hamiltonians are generated using the OpenFermion software.
24. The list of the MSOs is enumerated so that all spin $z$-projection $+1/2$ orbits in the ascending order of the orbital energies are followed by the corresponding spin $z$-projection $-1/2$ subset.
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