Density functional theory and quantum computation

Frank Gaitan[1,2,3] and Franco Nori[1,3,4]
[1]*Advanced Science Institute, The Institute of Physical and Chemical Research (RIKEN), Wako-shi, Saitama 351-0198, Japan*
[2]*Department of Physics, Southern Illinois University, Carbondale, Illinois 62901-4401, USA*
[3]*CREST, Japan Science and Technology Agency (JST), Kawaguchi, Saitama 332-0012, Japan*
[4]*Department of Physics, Center for Theoretical Physics, University of Michigan, Ann Arbor, Michigan 48109, USA*
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This paper establishes the applicability of density functional theory methods to quantum computing systems. We show that ground state and time-dependent density functional theory can be applied to quantum computing systems by proving the Hohenberg-Kohn and Runge-Gross theorems for a fermionic representation of an N qubit system. As a first demonstration of this approach, time-dependent density functional theory is used to determine the minimum energy gap $\Delta(N)$ arising when the quantum adiabatic evolution algorithm is used to solve instances of the nondeterministic-polynomial-complete problem MAXCUT. It is known that the computational efficiency of this algorithm is largely determined by the large-N scaling behavior of $\Delta(N)$, and so determining this behavior is of fundamental significance. As density functional theory has been used to study quantum systems with $N \sim 10^3$ interacting degrees of freedom, the approach introduced in this paper raises the realistic prospect of evaluating the gap $\Delta(N)$ for systems with $N \sim 10^3$ qubits. Although the calculation of $\Delta(N)$ serves to illustrate how density functional theory methods can be applied to problems in quantum computing, the approach has a much broader range and shows promise as a means for determining the properties of very large quantum computing systems.

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I. INTRODUCTION

The inability of a classical computer to efficiently simulate the dynamics of a quantum system is well known. The problem is that the dimension of the Hilbert space grows exponentially with the number of degrees of freedom of the quantum system, and this in turn causes an exponential growth in the amount of memory and CPU time required to carry out the simulation. This inefficiency is a major stumbling block for numerical studies aiming to determine the asymptotic performance of quantum algorithms. For example, numerical simulation of the dynamics of the quantum adiabatic evolution (QAE) algorithm applied to the nondeterministic-polynomial (NP)-complete problem *Exact Cover 3* has been limited to systems containing $N \leq 20$ qubits.[1,2] Because the algorithm dynamics must be adiabatic, its runtime T must satisfy the inequality

$$T \gg \frac{M}{\Delta^2}, \tag{1}$$

where

$$M = \max_{0 \leq s \leq 1} \left| \langle E_1(s) | \frac{dH(s)}{ds} | E_0(s) \rangle \right|,$$

$$\Delta = \min_{0 \leq s \leq 1} [E_1(s) - E_0(s)], \tag{2}$$

and here t is time; $s = t/T$ is dimensionless time; $H(s)$ is the time-dependent Hamiltonian that drives the dynamics of the QAE algorithm; and $\{E_i(s), |E_i(s)\rangle : i = 0, \ldots, 2^N - 1\}$ are the eigenvalues and eigenstates of $H(s)$. In the usual formulation[3–5] of QAE, $dH(s)/ds$ is an s-independent matrix whose largest eigenvalue bounds M. Typically, this eigenvalue scales polynomially with N. Thus, if the minimum gap $\Delta(N)$ separating the ground- and first-excited states scales polynomially (exponentially) with N, so will the algorithm runtime $T(N)$. An efficient (inefficient) algorithm[6] for a computational problem is one that solves all instances of the problem with polynomial (exponential) $T(N)$. We see then that the computational efficiency of the QAE algorithm is largely determined by the scaling behavior of the minimum gap $\Delta(N)$. Attempts to evaluate $\Delta(N)$ using exact diagonalization[7] have been limited to $N \leq 20$ qubits. Recently, however, the minimum gap $\Delta(N)$ for QAE applied to Exact Cover 3 has been determined for $N \leq 128$ qubits using quantum Monte Carlo methods.[8] This represents a substantial technical advance and has stirred great interest in finding other computational approaches that might allow quantum algorithm performance to be determined for still larger qubit systems.

Quantum computation is not the only research area struggling with the difficulties of simulating quantum systems.[9] Condensed-matter physicists and quantum chemists have been working under the shadow of this problem for decades. A number of computational approaches have been developed which, together with increasingly more powerful computers, have allowed much progress to be made, in spite of the ultimately unavoidable difficulties involved. Among these approaches, density functional theory (DFT) has proven to be one of the most successful.[10–12] DFT is a theory of *interacting* fermion systems. It provides an *exact* treatment of all many-body effects through the exchange-correlation energy functional. It can also handle the coupling of such fermion systems to both static and time-varying electric and magnetic fields. Ground-state density functional theory (GS-DFT) has been used to determine a wide range of ground-state properties of atomic, molecular, and solid state systems;[13,14] while time-dependent density functional theory (TD-DFT) has been used to determine excited-state properties, as well as

the linear and nonlinear response of interacting many-electron systems to electromagnetic fields.[15,16] For our purposes, it is especially significant that DFT has been successfully applied to quantum systems containing $N \sim 10^3$ interacting degrees of freedom.[17–19]

In this paper we establish the applicability of DFT methods to quantum computing systems. By establishing this link, we shall see that a powerful tool becomes available for determining the properties of very large quantum computing systems. Although our analysis can be extended to the case of N qudits (d-level systems) residing on a D-dimensional lattice, we restrict the presentation to N qubits residing on a two-dimensional (2D) lattice since this corresponds to the experimentally interesting cases of qubits placed in a 2D ion trap,[20] or restricted to a planar superconducting qubit circuit.[21]

The outline of this paper is as follows. We begin in Sec. II by showing how an N qubit system can be transformed into a system of N lattice fermions and then, in Sec. III, illustrate this transformation by using it to rewrite the dynamics of the QAE algorithm applied to the NP-complete problem *MAXCUT*.[22] For the resulting interacting fermion system, Sec. IV establishes the Hohenberg-Kohn[13] (HK) and Runge-Gross[15] theorems and sets up the auxiliary Kohn-Sham (KS) system of noninteracting fermions.[14] The results of Sec. IV provide the justification for applying GS- and TD-DFT to quantum computing systems. The proofs given in Sec. IV are adaptations of well-established proofs used for interacting electron systems, and so their validity should not be in doubt. Section V works out the linear response of the system of interacting fermionized qubits using TD-DFT and, as an application, shows how this response can be used to determine the minimum energy gap $\Delta(N)$ for the MAXCUT dynamics. Here we begin to see the value of the newly established link between DFT and quantum computing. Calculation of $\Delta(N)$ boils down to a calculation of excitation energies, and the reliable calculation of excitation energies for very large interacting electron systems was one of the first triumphs of TD-DFT. A straightforward adaptation of standard TD-DFT arguments then determines $\Delta(N)$. In light of earlier remarks, the link established in this paper between DFT and quantum computing raises the realistic prospect of evaluating the minimum gap $\Delta(N)$ for $N \sim 10^3$ qubits, and thus of studying the performance of the QAE algorithm for much larger qubit systems than is currently possible using other approaches. Although we focus on the calculation of the minimum gap in this paper, it is clear that the application of DFT to quantum computing systems has a much broader range and shows genuine promise as a means for determining the properties of very large quantum computing systems. Finally, the paper closes in Sec. VI with a discussion of future work.

II. QUBIT-FERMION TRANSFORMATION

Consider N qubits residing on an N-site 2D lattice with basis vectors $\hat{\mathbf{e}}_k$ $(k=1,2)$ and sites specified by the position vector $\mathbf{r}$. Let $\boldsymbol{\sigma}(\mathbf{r})$ denote the Pauli matrices associated with the qubit at $\mathbf{r}$. We now show how the qubits can be converted into lattice fermions via the 2D Jordan-Wigner (JW) transformation.[23] Note that the following analysis can be extended to N qudits (viz., N d-level systems) on a D-dimensional lattice using the generalized JW transformation[24] that fermionizes a spin s system $(d=2s+1)$ in D spatial dimensions.

For a 2D system of qubits, the JW transformation is

$$\sigma^+(\mathbf{r}) = 2a_{\mathbf{r}}^\dagger Q_{\mathbf{r}},$$

$$\sigma^-(\mathbf{r}) = 2Q_{\mathbf{r}}^\dagger a_{\mathbf{r}},$$

$$\sigma_z(\mathbf{r}) = 2\hat{n}_{\mathbf{r}} - 1. \tag{3}$$

Here, $\sigma^\pm(\mathbf{r}) = \sigma_x(\mathbf{r}) \pm i\sigma_y(\mathbf{r})$; $a_{\mathbf{r}}^\dagger$ $(a_{\mathbf{r}})$ creates (annihilates) a lattice fermion at $\mathbf{r}$; $\hat{n}_{\mathbf{r}} = a_{\mathbf{r}}^\dagger a_{\mathbf{r}}$ is the fermion number operator at $\mathbf{r}$; and

$$Q_{\mathbf{r}} = \exp[-i\phi_{\mathbf{r}}], \quad \phi_{\mathbf{r}} = \left(\frac{1}{2\pi\theta}\right)\sum_{\mathbf{r}'} \Phi(\mathbf{r},\mathbf{r}')\hat{n}_{\mathbf{r}'}. \tag{4}$$

In Eq. (4), $\Phi(\mathbf{r},\mathbf{r}')$ is the angle made by $(\mathbf{r}-\mathbf{r}')$ with respect to some reference direction, say, $\hat{\mathbf{e}}_1$. Thus, (i) $\Phi(\mathbf{r},\mathbf{r}')$ changes by 2π when $(\mathbf{r}-\mathbf{r}')$ traces out a closed loop around $\mathbf{r}'$; and (ii) by convention, $\Phi(\mathbf{r},\mathbf{r}) \equiv 0$. The requirement that the Pauli operators $\boldsymbol{\sigma}(\mathbf{r})$ commute at different lattice sites forces θ to satisfy

$$\frac{1}{2\pi\theta} = 2m+1 \quad (m = 0, \pm 1, \pm 2, \ldots)$$

in Eq. (4).

As shown in Ref. 23, the lattice fermions are spinless and minimally coupled to a gauge field $A_k(\mathbf{r}) = \Delta_k \phi_{\mathbf{r}} \equiv \phi_{\mathbf{r}+\hat{\mathbf{e}}_k} - \phi_{\mathbf{r}}$. The action for the gauge field $A_\mu(\mathbf{r})$ is given by the Chern-Simons term[25]

$$\mathcal{A}_{\mathrm{CS}} = -\frac{\theta}{4}\int dt \sum_{\mathbf{r}} \epsilon^{\mu\nu\lambda} A_\mu(\mathbf{r}) F_{\nu\lambda}(\mathbf{r}).$$

Maxwell's equations for this system take the form

$$j_{\mathbf{r}}^\mu = \epsilon^{\mu\nu\lambda} F_{\nu\lambda}(\mathbf{r}), \tag{5}$$

where $j_{\mathbf{r}}^\mu$ is the fermion current, $F_{\nu\lambda}(\mathbf{r})$ is the gauge-field tensor, $\epsilon^{\mu\nu\lambda}$ is the totally antisymmetric Levi-Civita tensor, and $\mu,\nu,\lambda = 0,1,2$. From Eq. (5), the fermion current $j_{\mathbf{r},\mu}$ has components

$$j_{\mathbf{r},0} = n_{\mathbf{r}},$$

$$j_{\mathbf{r},k} = \frac{1}{2\pi}\sum_{\mathbf{y}} \{\Delta_k G_{\mathbf{r},\mathbf{y}}\}\{\partial_t n_{\mathbf{y}}\} \quad (k = 1,2), \tag{6}$$

where $G_{\mathbf{r},\mathbf{y}}$ is the Green's function for the lattice Laplacian

$$\sum_{k=1,2} \Delta_k \Delta_k G_{\mathbf{r},\mathbf{y}} = -2\pi\delta_{\mathbf{r},\mathbf{y}}.$$

Fermion current conservation, $\partial_\mu j^\mu = 0$, follows immediately from Maxwell's equations.

III. APPLICATION: NP-COMPLETE PROBLEM MAXCUT

In the problem MAXCUT, one considers an N-node undirected graph $\mathcal{G}$ with nodes specified by $\mathbf{r}$. The nodes (edges) are assigned weights $w_{\mathbf{r}}$ ($w_{\mathbf{r},\mathbf{r}'}$), and a binary variable $s_{\mathbf{r}}$ is associated with each node $\mathbf{r}$. A cut of the graph $\mathcal{G}$ is a partition of the nodes into two sets $\mathcal{S}_0$ and $\mathcal{S}_1$. For all nodes belonging to $\mathcal{S}_0$ ($\mathcal{S}_1$), $s_{\mathbf{r}}$ is assigned the value of 0 (1). The node variables are used to construct a string variable $s=s_{\mathbf{r}_1}\cdots s_{\mathbf{r}_N}$, and all possible assignments of the N (binary) node variables lead to 2^N possible string assignments for s. It follows that there is a one-to-one correspondence between cuts of $\mathcal{G}$ and string assignments for s. The MAXCUT problem is to find the cut (viz., string assignment) that maximizes the payoff function $P(s)$ given by

$$P(s) = \sum_{\mathbf{r}} s_{\mathbf{r}} w_{\mathbf{r}} + \sum_{\mathbf{r},\mathbf{r}'} s_{\mathbf{r}}(1 - s_{\mathbf{r}'}) w_{\mathbf{r},\mathbf{r}'}.$$

MAXCUT is known[6] to be NP-complete, and so it belongs to the set of "hardest problems" in the complexity class NP.

The QAE algorithm was applied to MAXCUT in Ref. 22, where the dynamics is driven by the Hamiltonian

$$H(t) = \left(1 - \frac{t}{T}\right) H_0 + \left(\frac{t}{T}\right) H_P. \tag{7}$$

Here T is the algorithm runtime,

$$H_0 = \sum_{\mathbf{r}} \sigma_x(\mathbf{r}), \tag{8}$$

and

$$H_P = \sum_{\mathbf{r}} w_{\mathbf{r}}[1 - \sigma_z(\mathbf{r})]/2 + \sum_{\mathbf{r},\mathbf{r}'} w_{\mathbf{r},\mathbf{r}'}[1 - \sigma_z(\mathbf{r})\sigma_z(\mathbf{r}')]/2. \tag{9}$$

The Hamiltonian H_P is known as the problem Hamiltonian. From Eq. (9), its eigenstates are the simultaneous eigenstates of the $\{\sigma_z(\mathbf{r})\}$,

$$\sigma_z(\mathbf{r})|s_{\mathbf{r}_1}\cdots s_{\mathbf{r}_N}\rangle = (-1)^{s_{\mathbf{r}}}|s_{\mathbf{r}_1}\cdots s_{\mathbf{r}_N}\rangle.$$

By construction,[1,22] each bit string $s=s_1\cdots s_N$ that maximizes the MAXCUT payoff function labels a ground state $|s_1\cdots s_N\rangle$ of H_P. The QAE algorithm places the qubit system in the ground state of the initial Hamiltonian H_0, and for runtime T sufficiently large, $H(t)$ evolves the quantum state adiabatically so that at time T, the system is in the ground state of the final Hamiltonian H_P with probability approaching 1. Measurement of the $\{\sigma_z(\mathbf{r})\}$ at time T yields, with probability approaching 1, a string $s_1\ldots s_N$ that solves the MAXCUT instance.

Using Eq. (3) in $H(t)$ gives the fermionized QAE Hamiltonian for MAXCUT as follows:

$$H(t) = \left(1 - \frac{t}{T}\right)\sum_{\mathbf{r}} [a_{\mathbf{r}}^\dagger Q_{\mathbf{r}} + Q_{\mathbf{r}}^\dagger a_{\mathbf{r}}] + \left(\frac{t}{T}\right)\sum_{\mathbf{r}} v_{\mathbf{r}}\hat{n}_{\mathbf{r}} + \left(\frac{t}{T}\right)\sum_{\mathbf{r}}\sum_{\mathbf{r}'\neq\mathbf{r}} w_{\mathbf{r},\mathbf{r}'}\hat{n}_{\mathbf{r}}\hat{n}_{\mathbf{r}'}], \tag{10}$$

where

$$w_{\mathbf{r}} \equiv v_{\mathbf{r}} + W_{\mathbf{r}},$$

$$W_{\mathbf{r}} = \sum_{\mathbf{r}'\neq\mathbf{r}} w_{\mathbf{r},\mathbf{r}'},$$

and a term proportional to the identity has been suppressed.

IV. DENSITY FUNCTIONAL THEORY

In this section we establish the applicability of the Hohenberg-Kohn and Runge-Gross theorems to the QAE/MAXCUT problem. These theorems justify the use of, respectively, ground state and time-dependent density functional theory to the MAXCUT dynamics. Throughout, the ground state is assumed to be nondegenerate, as would be appropriate for a nonvanishing minimum gap Δ. The formalism can be extended, however, to cover degenerate ground states.[26,27]

A. Ground-state density functional theory

We have seen that the QAE algorithm has an adiabatic dynamics that is driven by a slowly varying Hamiltonian $H(t)$. In this subsection we focus on the MAXCUT Hamiltonian $H(t)$ at a *fixed instant of time* $t=t_*$. By fixing the time, we obtain a well-defined *static* Hermitian operator $H_* \equiv H(t=t_*)$. The aim of this subsection is to show that the Hohenberg-Kohn theorem applies to H_*. With this theorem in place, GS-DFT can be used to study the ground-state properties of $H_*=H(t=t_*)$ for any specific intermediate time $0<t_*<T$. We stress that even though the QAE algorithm works with a slowly varying Hamiltonian, the discussion in this subsection is restricted to the *static* Hermitian operator $H_*=H(t_*)$ that is the value of $H(t)$ at the time $t=t_*$.

Our starting point is the energy functional for the instantaneous MAXCUT Hamiltonian $H_* \equiv H(t=t_*)$,

$$E[n] = \min_{|\psi\rangle\to n} \langle\psi|H_*|\psi\rangle. \tag{11}$$

The domain of $E[n]$ is the set of all N-representable site occupation functions (SOFs) $n_{\mathbf{r}}$ that can be obtained from an N-fermion wave function. The minimization in Eq. (11) is over all $|\psi\rangle$ for which

$$n \equiv n_{\mathbf{r}} = \langle\psi|\hat{n}_{\mathbf{r}}|\psi\rangle,$$

and the minimizing state $|\psi_{\min}[n]\rangle$ is thus a functional of $n_{\mathbf{r}}$. Let $|\psi^g\rangle$ denote the ground state of H_*; E^g is the ground-state energy; and $n_{\mathbf{r}}^g$ is the ground-state SOF. Inserting Eq. (10) into Eq. (11) gives

$$E[n] = (t_*/T)\sum_{\mathbf{r}} v_{\mathbf{r}} n_{\mathbf{r}} + Q[n],$$

where

$$Q[n] \equiv \min_{|\psi\rangle \to n} \langle \psi | (T_{t_*} + U_{t_*}) | \psi \rangle,$$

and T_{t_*} and U_{t_*} are the first and third terms, respectively, on the RHS of Eq. (10) at $t=t_*$.

To establish the HK theorem for H_* we must show:[28]: (i) $E[n^g]=E^g$; (ii) for $n_{\mathbf{r}} \neq n^g_{\mathbf{r}}$, $E[n]>E^g$; and (iii) the ground-state expectation value of any observable is a unique functional of the ground-state SOF $n^g_{\mathbf{r}}$. By the variational principle, $\langle \psi | H_* | \psi \rangle \geq E^g$, with equality when $|\psi\rangle = |\psi^g\rangle$. Thus, for $n=n^g$, the search in Eq. (11) returns the ground state $|\psi^g\rangle$ as the state $|\psi_{\min}[n^g]\rangle$ that minimizes $E[n^g]$. It follows that

$$E[n^g] = \langle \psi^g | H_* | \psi^g \rangle = E^g.$$

This establishes condition (i). For $n \neq n^g$, the minimizing state $|\psi_{\min}[n]\rangle \neq |\psi^g[n^g]\rangle$, and so by the variational principle,

$$E[n] = \langle \psi_{\min}[n] | H_* | \psi_{\min}[n] \rangle > E^g.$$

This establishes condition (ii). Finally, since the ground state $|\psi^g\rangle = |\psi_{\min}[n^g]\rangle$, it is a functional of n^g and, consequently, so are all ground-state expectation values,

$$\langle \hat{\mathcal{O}} \rangle_{\mathrm{gs}} = \langle \psi^g | \hat{\mathcal{O}} | \psi^g \rangle = \langle \psi_{\min}[n^g] | \hat{\mathcal{O}} | \psi_{\min}[n^g] \rangle = \mathcal{O}[n^g].$$

Condition (iii) is thus established, completing the proof of the HK theorem for $H_*=H(t_*)$.

To obtain a practical calculational scheme, an auxiliary system of noninteracting KS fermions is introduced,[14] and it is assumed that the ground-state SOF $n^g_{\mathbf{r}}$ can be obtained from the ground-state density of the KS fermions moving in an external potential $v^{\mathrm{KS}}_{\mathbf{r}}$. For $H_*=H(t_*)$, the KS Hamiltonian $H_{\mathrm{KS}}=T'_{t_*}+V^{\mathrm{KS}}$ is defined to be

$$H_{\mathrm{KS}} = \sum_{\mathbf{r}} \left(1 - \frac{t_*}{T}\right) \{ q_{\mathbf{r}} a^\dagger_{\mathbf{r}} + q^*_{\mathbf{r}} a_{\mathbf{r}} \} + \sum_{\mathbf{r}} \left(\frac{t_*}{T}\right) v^{\mathrm{KS}}_{\mathbf{r}} \hat{n}_{\mathbf{r}},$$

where $q_{\mathbf{r}}=\langle Q_{\mathbf{r}} \rangle$ is the ground-state expectation value of $Q_{\mathbf{r}}$. The effects of $Q_{\mathbf{r}}$ are thus incorporated into the KS dynamics through the mean field $q_{\mathbf{r}}$. The KS energy functional $\epsilon_{\mathrm{KS}}[n]$ is

$$\epsilon_{\mathrm{KS}}[n] = \min_{|\psi\rangle \to n} \langle \psi | H_{\mathrm{KS}} | \psi \rangle = T'_{t_*}[n] + \sum_{\mathbf{r}} \left(\frac{t_*}{T}\right) v^{\mathrm{KS}}_{\mathbf{r}} n_{\mathbf{r}}. \quad (12)$$

To determine the KS external potential $v^{\mathrm{KS}}_{\mathbf{r}}$, we rewrite Eq. (11) as

$$E[n] = T'_{t_*}[n] + \sum_{\mathbf{r}} \left(\frac{t_*}{T}\right) v_{\mathbf{r}} n_{\mathbf{r}} + \xi_{xc}[n], \quad (13)$$

where

$$\xi_{xc}[n] \equiv Q[n] - T'_{t_*}[n]$$

is the exchange-correlation energy functional. As noted in Sec. I, it is through the exchange-correlation energy functional $\xi_{xc}[n]$ that DFT accounts for *all many-body effects*. Since $n^g_{\mathbf{r}}$ minimizes both $\epsilon_{\mathrm{KS}}[n]$ and $E[n]$, Eqs. (12) and (13) are stationary about $n=n^g$. Taking their functional derivatives with respect to n, evaluating the result at $n=n^g$, and eliminating $\delta T'_{t_*}/\delta n|_{n=n^g}$ give

$$v^{\mathrm{KS}}_{\mathbf{r}} = v_{\mathbf{r}} + \left(\frac{T}{t_*}\right) v_{xc}[n^g](\mathbf{r}) \quad (14)$$

for $t_* \neq 0$. Here $v_{xc}[n^g](\mathbf{r})$ is the exchange-correlation potential which is the functional derivative of the exchange-correlation energy functional $\xi_{xc}[n^g]$,

$$v_{xc}[n^g](\mathbf{r}) = \frac{\delta \xi_{xc}[n^g]}{\delta n^g_{\mathbf{r}}}.$$

This sets in place the formulas for a self-consistent calculation of the ground-state properties of $H_*=H(t_*)$ using GS-DFT. Entanglement[29] and its links to quantum phase transitions[30] have been studied using GS-DFT.

B. Time-dependent density functional theory

Here we establish the Runge-Gross theorem[15] for the instantaneous MAXCUT dynamics. Thus we focus on the instantaneous Hamiltonian $H_*=H(t_*)$ for a fixed t_* $(0<t_*<T)$. Now, however, we suppose that the external potential $v_{\mathbf{r}}$ in $H(t_*)$ begins to vary at a moment we call $t=0$. For $t \leq 0$, $v_{\mathbf{r}}(t)=v_{\mathbf{r}}$, and the fermions are in the ground state $|\psi_0\rangle$ of $H(t_*)$. The Runge-Gross theorem states that the SOFs $n_{\mathbf{r}}(t)$ and $n'_{\mathbf{r}}(t)$ evolving from a common initial state $|\psi(0)\rangle = |\psi_0\rangle$ under the influence of the respective potentials $V_{\mathbf{r}}(t)$ and $V'_{\mathbf{r}}(t)$ (both Taylor series expandable about $t=0$) will be different provided that $[V_{\mathbf{r}}(t)-V'_{\mathbf{r}}(t)] \neq C(t)$. For us,

$$V_{\mathbf{r}}(t) = \left(\frac{t_*}{T}\right)\left(1 - \frac{t_*}{T}\right) v_{\mathbf{r}}(t),$$

$$V'_{\mathbf{r}}(t) = \left(\frac{t_*}{T}\right)\left(1 - \frac{t_*}{T}\right) v'_{\mathbf{r}}(t),$$

and

$$V_{\mathbf{r}}(t) = \sum_{k=0}^{\infty} a_k(\mathbf{r}) t^k/k!,$$

$$V'_{\mathbf{r}}(t) = \sum_{k=0}^{\infty} a'_k(\mathbf{r}) t^k/k!.$$

Let $C_k(\mathbf{r}) \equiv a_k(\mathbf{r}) - a'_k(\mathbf{r})$. The condition that $[V_{\mathbf{r}}(t)-V'_{\mathbf{r}}(t)] \neq C(t)$ means that a smallest integer K exists such that $C_k(\mathbf{r})$ is a nontrivial function of $\mathbf{r}$ for all $k \geq K$, while for $k<K$, it is a constant C_k which can be set to zero without loss of generality.

Recall [Eq. (6)] that the conserved fermion current has components

$$\hat{j}_{\mathbf{r},0}(t) = n_{\mathbf{r}}(t),$$

$$\hat{j}_{\mathbf{r},k}(t) = \left(\frac{1}{2\pi}\right) \sum_{\mathbf{y}} (\Delta_k G_{\mathbf{r},\mathbf{y}}) \partial_t n_{\mathbf{y}}(t),$$

with $k=1,2$. Defining $j_{\mathbf{r},k}(t) = \langle \psi_0 | \hat{j}_{\mathbf{r},k}(t) | \psi_0 \rangle$, it follows that

$$\partial_t\{j_{\mathbf{r},k}(t) - j'_{\mathbf{r},k}(t)\} = \langle\psi_0|[\hat{j}_{\mathbf{r},k}(t), H(t) - H'(t)]|\psi_0\rangle. \quad (15)$$

Here $j_{\mathbf{r},k}(t)$ $[j'_{\mathbf{r},k}(t)]$ and $H(t)$ $[H'(t)]$ are the expected fermion current and the Hamiltonian, respectively, when the external potential is $v_{\mathbf{r}}(t)$ $[v'_{\mathbf{r}}(t)]$. The Hamiltonians $H(t)$ and $H'(t)$ differ only in the external potential. Defining

$$\delta j_{\mathbf{r},k}(t) = j_{\mathbf{r},k}(t) - j'_{\mathbf{r},k}(t),$$

and

$$\delta V_{\mathbf{y}}(t) = V_{\mathbf{y}}(t) - V'_{\mathbf{y}}(t),$$

evaluation of the commutator in Eq. (15) eventually gives

$$\partial_t\{\delta j_{\mathbf{r},k}(t)\} = -\left(\frac{1}{2\pi}\right)\sum_{\mathbf{y}} (\Delta_k G_{\mathbf{r},\mathbf{y}})\delta V_{\mathbf{y}}(t)\mathcal{M}_{\mathbf{y}}(t), \quad (16)$$

where

$$\mathcal{M}_{\mathbf{y}}(t) = \langle\psi_0|(a^\dagger_{\mathbf{y}}Q_{\mathbf{y}} + Q^\dagger_{\mathbf{y}}a_{\mathbf{y}})|\psi_0\rangle.$$

With K defined as above, taking K time derivatives of Eq. (16) and evaluating the result at $t=0$ gives

$$\frac{\partial^{K+1}}{\partial t^{K+1}}[\delta j_{\mathbf{r},k}(t)]|_0 = -\left(\frac{1}{2\pi}\right)\sum_{\mathbf{y}} (\Delta_k G_{\mathbf{r},\mathbf{y}})\mathcal{M}_{\mathbf{y}}(0)C_K(\mathbf{r}), \quad (17)$$

where we have used that

$$\frac{\partial^k}{\partial t^k}[\delta V_{\mathbf{y}}(t)]|_{t=0} = C_k(\mathbf{y}) = 0$$

for $k<K$. It is important to note that $\mathcal{M}_{\mathbf{y}}(0) \neq 0$. This follows since

$$[H(t_*), n_{\mathbf{r}}(t_*)] \neq 0$$

for $t_* \neq T$, and so the eigenstates of $H(t_*)$ (specifically, its ground state $|\psi_0\rangle$) cannot be fermion number eigenstates. This ensures that the ground-state expectation value

$$\mathcal{M}_{\mathbf{y}}(0) = \langle\psi_0|(a^\dagger_{\mathbf{y}}Q_{\mathbf{y}} + Q^\dagger_{\mathbf{y}}a_{\mathbf{y}})|\psi_0\rangle \neq 0$$

for $t_* \neq T$. It follows from the continuity equation for the fermion current that

$$\frac{\partial}{\partial t}[n_{\mathbf{r}}(t) - n'_{\mathbf{r}}(t)] = -\sum_{k=1,2} \Delta_k\{\delta j_{\mathbf{r},k}(t)\}.$$

Taking K time derivatives of this equation, evaluating the result at $t=0$, and using Eq. (17) give

$$\frac{\partial^{K+2}}{\partial t^{K+2}}[n_{\mathbf{r}}(t) - n'_{\mathbf{r}}(t)]|_{t=0} = -C_K(\mathbf{r})\mathcal{M}_{\mathbf{r}}(0) \neq 0, \quad (18)$$

where we have used the equation of motion for $G_{\mathbf{r},\mathbf{y}}$. Equation (18) indicates that $n_{\mathbf{r}}(t)$ cannot equal $n'_{\mathbf{r}}(t)$ since it ensures that they will be different at $t=0^+$ and so they cannot be the same function. This proves the Runge-Gross theorem for the instantaneous MAXCUT dynamics.

We have just seen that when potentials $V_{\mathbf{r}}(t)$ and $V'_{\mathbf{r}}(t)$ differ by a time-dependent function $C(t)$, they give rise to the same SOF $n_{\mathbf{r}}(t)$. However, the wave functions produced by these potentials from the same initial state will differ by a time-dependent phase factor. For our purposes, it is important to note that this extra phase factor cancels out when calculating the expectation value of an operator. In particular, it will cancel out when calculating the instantaneous energy eigenvalues $E_n(t) = \langle E_n(t)|H(t)|E_n(t)\rangle$. As a result, this phase factor will not affect our calculation of the minimum energy gap in Sec. V. Having said that, it is worth noting that this subtlety is not expected to cause difficulties in practice since the probe potential $V_{\mathbf{r}}(t)$ is assumed to be under the direct control of the experimenter, and so the precise form of $V_{\mathbf{r}}(t)$ is *known*. When an experimentalist says a sinusoidal probe potential has been applied, this means that $V_{\mathbf{r}}(t) = V_{\mathbf{r}} \sin \omega t$; it does *not* mean $V_{\mathbf{r}}(t) = V_{\mathbf{r}} \sin \omega t + C(t)$. Thus in a well-designed experiment $C(t)=0$.

The KS system of noninteracting fermions can also be introduced in TD-DFT.[15] We must still assume that the interacting SOF $n_{\mathbf{r}}(t)$ can be obtained from the SOF of the noninteracting KS fermions moving in the external potential $v^{\mathrm{KS}}_{\mathbf{r}}(t)$. The potentials $v^{\mathrm{KS}}_{\mathbf{r}}(t)$ and $v_{\mathbf{r}}(t)$ are related via $(t_* \neq 0)$,

$$v^{\mathrm{KS}}_{\mathbf{r}}(t) = v_{\mathbf{r}}(t) + \left(\frac{T}{t_*}\right)v_{xc}[n(t)](\mathbf{r}), \quad (19)$$

though Eq. (19) is to be thought of as defining the time-dependent exchange-correlation potential $v_{xc}[n(t)](\mathbf{r})$.

V. MINIMUM GAP

A problem of longstanding treachery in GS-DFT is the calculation of the excitation energies of a fermion system. TD-DFT was able to find these energies by determining the system's frequency-dependent linear response and relating the excitation energies to poles appearing in that response. The arguments used[31] are quite general and can be easily adapted to determine the energy gap for the instantaneous MAXCUT dynamics.

Previously, we considered an external potential that becomes time varying for $t \geq 0$. Our interest is in the *interacting* fermion linear response, and so we assume that the total potential has the form

$$v^{\mathrm{tot}}_{\mathbf{r}}(t) = v_{\mathbf{r}} + v^1_{\mathbf{r}}(t),$$

with $v^1_{\mathbf{r}}(t)$ a suitably small time-varying perturbation. The probe potential $v^1_{\mathbf{r}}(t)$ generates a first-order response $n^1_{\mathbf{r}}(t)$ in the SOF,

$$n^{\mathrm{tot}}_{\mathbf{r}}(t) = n^g_{\mathbf{r}} + n^1_{\mathbf{r}}(t).$$

The susceptibility $\chi_{\mathbf{r},\mathbf{r}'}(t-t')$ connects the first-order probe potential to the SOF response. The total potential $v^{\mathrm{tot}}_{\mathbf{r}}(t)$ is related to the KS potential $v^{\mathrm{KS}}_{\mathbf{r}}(t)$ through Eq. (19), and by assumption, the SOF for both the interacting and KS fermions is the same. This allows the time-Fourier transform of the SOF response $n^1_{\mathbf{r}}(\omega)$ to be determined from the time-Fourier transforms of the KS susceptibility $\chi^{\mathrm{KS}}_{\mathbf{r},\mathbf{r}'}(\omega)$, the exchange-correlation kernel $f_{xc}[n^g](\mathbf{r},\mathbf{r}';\omega)$, and the probe potential $v^1_{\mathbf{r}}(\omega)$,

$$\sum_{\mathbf{y}'} \{\delta_{\mathbf{r},\mathbf{y}'} - \sum_{\mathbf{r}'} \chi^{\mathrm{KS}}_{\mathbf{r},\mathbf{r}'}(\omega) f_{xc}[n^g](\mathbf{r}',\mathbf{y}';\omega)\} n^1_{\mathbf{y}'}(\omega) = \sum_{\mathbf{r}'} \chi^{\mathrm{KS}}_{\mathbf{r},\mathbf{r}'}(\omega) v^1_{\mathbf{r}'}(\omega). \quad (20)$$

The KS susceptibility[16] depends on the KS static unperturbed orbitals $\phi^j_{\mathbf{r}}$ and the corresponding energy eigenvalues ε_j and orbital occupation numbers f_j,

$$\chi^{\mathrm{KS}}_{\mathbf{r},\mathbf{r}'}(\omega) = \sum_{j,k} (f_k - f_j) \frac{\phi_j(\mathbf{r})\bar{\phi}_k(\mathbf{r})\bar{\phi}_j(\mathbf{r}')\phi_k(\mathbf{r}')}{\omega - (\varepsilon_j - \varepsilon_k) + i\eta}. \quad (21)$$

The exchange-correlation kernel $f_{xc}[n^g]$ incorporates all many-body effects into the linear response dynamics and is related to the exchange-correlation potential $v_{xc}[n^g]$ through a functional derivative,

$$f_{xc}[n^g] = \frac{\delta v_{xc}[n^g]}{\delta n^g}.$$

In general, the *interacting* fermion excitation energies,

$$\Omega_{jk} = E_j - E_k,$$

differ from the KS excitation energies

$$\omega_{jk} = \varepsilon_j - \varepsilon_k.$$

The RHS of Eq. (20) remains finite as $\omega \to \Omega_{jk}$, while the first-order SOF response $n^1_{\mathbf{y}'}(\omega)$ has a pole at each Ω_{jk}. Thus the operator on the LHS acting on $n^1_{\mathbf{y}'}(\omega)$ cannot be invertible. Otherwise, its inverse could be applied to both sides of Eq. (20) with the result that the RHS would remain finite as $\omega \to \Omega_{jk}$, while the LHS would diverge. To avoid this inconsistency, the operator must have a zero eigenvalue as $\omega \to \Omega_{jk}$. Following Ref. 31, one is led to the following eigenvalue problem:

$$\sum_{k',j'} \frac{M_{kj;k'j'}(\omega)}{\omega - \omega_{j'k'} + i\eta} \xi_{k'j'}(\omega) = \lambda(\omega)\xi_{kj}(\omega), \quad (22)$$

where, writing

$$\alpha_{k'j'} = f_{k'} - f_{j'},$$

and

$$\Phi^{kj}_{\mathbf{r}} = \bar{\phi}_k(\mathbf{r})\phi_j(\mathbf{r}),$$

we have

$$M_{k'j';kj}(\omega) = \alpha_{k'j'} \sum_{\mathbf{r}',\mathbf{y}'} \bar{\Phi}^{kj}_{\mathbf{r}'} \{f_{xc}[n^g](\mathbf{r}',\mathbf{y}';\omega)\} \Phi^{k'j'}_{\mathbf{y}'}(\omega).$$

It can be shown that $\lambda(\Omega_{jk}) = 1$.

At this point in the argument, it proves necessary to introduce some form of approximation to proceed further. In the single-pole approximation[31] the KS poles are assumed to be well separated so that we can focus on a particular KS excitation energy $\omega_{jk} = \omega_*$. The eigenvectors $\xi_{k'j'}(\omega)$ and the matrix operator $M_{kj;k'j'}(\omega)$ are finite at ω_*, while the eigenvalue $\lambda(\omega)$ must have a pole there to match the pole on the LHS of Eq. (22),

$$\lambda(\omega) = \frac{A(\omega_*)}{(\omega - \omega_*)} + \mathcal{O}(1).$$

Let ω_* be d-fold degenerate: $\omega_{k_1 j_1}, \ldots, \omega_{k_d j_d} = \omega_*$. Matching singularities in Eq. (22) gives

$$\sum_{l=1}^{d} M_{k_i j_i; k'_l j'_l}(\omega_*) \xi^n_{k'_l j'_l} = A^n(\omega_*) \xi^n_{k_i j_i}(\omega_*), \quad (23)$$

where $i,n = 1,\ldots,d$. For our purposes, the eigenvalues $A^n(\omega_*)$ are of primary interest and are found from Eq. (23). From each $A^n(\omega_*)$, we find

$$\lambda^n(\omega) = \frac{A^n(\omega_*)}{(\omega - \omega_*)}.$$

Since $\lambda^n(\Omega_{jk}) = 1$, it follows that the sum of $\lambda^n(\Omega_{jk})$ and its complex conjugate is 2. Plugging into this sum the singular expressions for $\lambda^n(\Omega_{jk})$ and that of its complex conjugate and solving for Ω^n_{jk} give

$$\Omega^n_{jk} = \omega_* + \mathrm{Re}[A^n(\omega_*)].$$

Interactions will thus generally *split* the ω_* degeneracy. Now let

$$\delta E = \min_n \mathrm{Re}[A^n(\omega_*)]$$

and

$$\bar{\Omega}_{jk} = \min_n \Omega^n_{jk}.$$

Our expression for Ω^n_{jk} then gives

$$\bar{\Omega}_{jk} = \omega_* + \delta E.$$

In the context of the QAE algorithm, our interest is the energy gap,

$$\Delta(t_*) = E_1(t_*) - E_0(t_*),$$

separating the instantaneous ground and first-excited states. In this case, our expression for $\bar{\Omega}_{jk}$ gives

$$\Delta(t_*) = [\varepsilon_1(t_*) - \varepsilon_0(t_*)] + \delta E(t_*). \quad (24)$$

To obtain the minimum gap Δ for QAE numerically, one picks a sufficiently large number of $t_* \in (0,T)$, solves for $\Delta(t_*)$ using the KS system associated with $H(t_*)$ to evaluate the RHS of Eq. (24), and then uses the minimum of the resulting set of $\Delta(t_*)$ to upper bound Δ. Because the KS dynamics is noninteracting, it has been possible to treat KS systems with $N \sim 10^3$ KS fermions.[17–19] This would allow the evaluation of the minimum gap $\Delta(N)$ for the QAE algorithm for $N \sim 10^3$.

VI. DISCUSSION

As with all KS calculations, the minimum gap calculation requires an approximation for the exchange-correlation energy functional $\xi_{xc}[n]$. Note that, because the qubits in a quantum register must be located at fixed positions for the

register to function properly, the associated JW fermions are distinguishable since they are each pinned to a specific lattice site. Consequently, antisymmetrization of the fermion wave function is not required, with the result that the *exchange energy vanishes* in the MAXCUT dynamics. The exchange-correlation energy functional $\xi_{xc}[n]$ is then determined solely by the correlation energy which can be calculated using the methods of Ref. 32. Parametrization of these results yields analytical expressions for the correlation energy per particle which, upon differentiation, give $v_{xc}[n]$ and $f_{xc}[n]$. Replacing $n \to n_{\mathbf{r}}$ in $\xi_{xc}[n]$ gives the local density approximation (LDA) for GS-DFT; while $n \to n_{\mathbf{r}}(t)$ gives the adiabatic local density approximation (ALDA) for TD-DFT. These simple approximations have proven to be remarkably successful and provide a good starting point for the minimum gap calculation. Self-interaction corrections to $\xi_{xc}[n]$ are not necessary since the two-fermion interaction [see Eq. (10)] has no self-interaction terms. Finally, because the fermions are pinned, it will be necessary to test the gap for sensitivity to derivative discontinuities[33] in $\xi_c[n]$.

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