Density functional theory and quantum computation

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Abstract

We establish 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 NP-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 treat quantum systems with $N \sim 10^3$ interacting degrees of freedom, the approach presented here 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 broader range and shows promise as a means for determining the properties of very large quantum computing systems.

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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 NP-Complete problem Exact Cover 3 has been limited to systems containing $N \leq 20$ qubits [1]. Because the algorithm requires adiabatic dynamics, its performance is highly sensitive to the minimum energy gap $\Delta(N)$ separating the instantaneous ground- and first-excited states, with the gap's asymptotic limit, $(N \gg 1)$, largely determining the algorithm's computational efficiency. Attempts to evaluate $\Delta(N)$ using exact diagonalization have been limited to $N \leq 20$ qubits [2]. 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 [3]. 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. 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, has 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 [4]. DFT applies to *interacting* fermion systems. It captures all many-body effects through the exchange-correlation energy functional. 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 [5, 6]; while time-dependent density functional theory (TD-DFT) has been used to determine excited-state properties, as well as the linear and non-linear response of interacting many-electron systems to electromagnetic fields [7, 8]. 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 [9–11].

Here we show how DFT can be applied to quantum computing systems [12]. 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 2D lattice since this corresponds to the experimentally interesting cases of qubits placed in a 2D ion trap, or restricted to a planar superconducting qubit circuit. We begin by showing how the N qubit system can be transformed into a system of N lattice fermions. We illustrate this transformation by using it to re-write the dynamics of the QAE algorithm applied to the NP-Complete problem MAXCUT [13]. For the resulting interacting fermion system, we establish the Hohenberg-Kohn [5] and Runge-Gross [7] theorems, and set-up the auxiliary Kohn-Sham system of non-interacting fermions [6]. This justifies the application of GS- and TD-DFT to the dynamics of the interacting fermion system. The linear response of the interacting fermions is determined using TD-DFT, which is then used to obtain the energy gap $\Delta(N)$ for the MAXCUT dynamics. In light of earlier remarks, this approach would allow evaluation of the minimum gap $\Delta(N)$ for $N \sim 10^3$ qubits.

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 [14]. Note that the following analysis can be extended to N qudits on a D-dimensional lattice using the generalized JW transformation [15] that fermionizes a spin s system in D spatial dimensions ($d = 2s + 1$).

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

$$
\begin{aligned}
\sigma^+(\mathbf{r}) &= 2a_{\mathbf{r}}^\dagger Q_{\mathbf{r}}; \\
\sigma^-(\mathbf{r}) &= 2Q_{\mathbf{r}}^\dagger a_{\mathbf{r}}; \\
\sigma_z(\mathbf{r}) &= 2\hat{n}_{\mathbf{r}} - 1.
\end{aligned}
\tag{1}
$$

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 $\mathbf{r}$; $\hat{n}_{\mathbf{r}} = a_{\mathbf{r}}^\dagger a_{\mathbf{r}}$; and

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

In Eq. (2), $\Phi(\mathbf{r}, \mathbf{r}')$ 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) $\Phi(\mathbf{r}, \mathbf{r}) \equiv 0$. The requirement that the Pauli operators $\boldsymbol{\sigma}(\mathbf{r})$ commute at different

lattice sites forces θ to satisfy

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

in Eq. (2).

As shown in Ref. [14], 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[16]

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

Maxwell's equations for this system take the form

$$j^\mu = \epsilon^{\mu\nu\lambda} F_{\nu\lambda}, \tag{3}$$

where j^μ is the fermion current, $F_{\nu\lambda}$ is the gauge field tensor, $\epsilon^{\mu\nu\lambda}$ is the totally anti-symmetric Levi-Civita tensor, and $\mu, \nu, \lambda = 0, 1, 2$. Fermion current conservation, $\partial_\mu j^\mu = 0$, follows immediately from Maxwell's equations.

NP-Complete Problem MAXCUT: In this problem, one considers an N-node undirected graph 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 is a partition of the nodes into two sets $\mathcal{S}_0$ and $\mathcal{S}_1$. For the nodes belonging to $\mathcal{S}_0$ ($\mathcal{S}_1$), $s_\mathbf{r}$ is assigned the value 0 (1). The problem is to find the cut that maximizes the payoff function

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

The QAE algorithm was applied to MAXCUT in Ref. [13], where the dynamics is driven by the time-dependent Hamiltonian

$$H(t) = (1 - t/T)H_0 + (t/T)H_P. \tag{4}$$

Here T is the algorithm runtime; the initial Hamiltonian H_0 is

$$H_0 = \sum_\mathbf{r} \frac{1}{2}\left[1 - \sigma_x(\mathbf{r})\right]; \tag{5}$$

and the final/problem Hamiltonian H_P is

$$H_P = \sum_\mathbf{r} w_\mathbf{r}(1 - \sigma_z(\mathbf{r}))/2 + \sum_{\mathbf{r},\mathbf{r}'} w_{\mathbf{r},\mathbf{r}'}(1 - \sigma_z(\mathbf{r})\sigma_z(\mathbf{r}'))/2. \tag{6}$$

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Using Eqs. (1) in $H(t)$ gives the fermionized QAE Hamiltonian for MAXCUT:

$$
\begin{aligned}
H(t) = {} & (1 - t/T) \sum_{\mathbf{r}} [a_{\mathbf{r}}^{\dagger} Q_{\mathbf{r}} + Q_{\mathbf{r}}^{\dagger} a_{\mathbf{r}}] \\
& + (t/T) \sum_{\mathbf{r}} v_{\mathbf{r}} \hat{n}_{\mathbf{r}} + (t/T) \sum_{\mathbf{r}} \sum_{\mathbf{r}' \neq \mathbf{r}} w_{\mathbf{r},\mathbf{r}'} \hat{n}_{\mathbf{r}} \hat{n}_{\mathbf{r}'}],
\end{aligned}
\tag{7}
$$

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. We now show that GS-DFT can be applied to the dynamics of the instantaneous MAXCUT Hamiltonian $H(t)$ for each $t \in (0, T)$.

Note: Throughout the remainder of this paper, the instantaneous groundstate is assumed to be non-degenerate as would be appropriate for the case of a non-vanishing gap Δ.

GS-DFT: The QAE algorithm has an adiabatic dynamics that is driven by a slowly varying Hamiltonian $H(t)$. In our discussion of GS-DFT 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 $H_* \equiv H(t = t_*)$. We aim 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 following GS-DFT discussion is restricted to the _static_ Hermitian operator H_* that is the value of $H(t)$ at $t = t_*$.

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

$$
E[n] = \min_{|\psi\rangle \to n} \langle \psi | H_* | \psi \rangle.
\tag{8}
$$

The domain of $E[n]$ is the set of all N-representable site occupation functions (SOF) $n_{\mathbf{r}}$ that can be obtained from an N-fermion wavefunction. The minimization in Eq. (8) 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 the ground-state energy; and $n_{\mathbf{r}}^g$ the ground-state SOF. Inserting Eq. (7) into (8) 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. (7) at $t = t_*$.

To establish the Hohenberg-Kohn (HK) theorem for H_* we must show [17]: (i) $E[n^g] = E^g$; (ii) for $n_{\mathbf{r}} \neq n_{\mathbf{r}}^g$, $E[n] > E^g$; and (iii) the ground-state expectation value of any observable is a unique functional of the ground-state SOF $n_{\mathbf{r}}^g$. 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. (8) returns the ground-state $|\psi^g\rangle$ as the state $|\psi_{\min}[n^g]\rangle$ that minimizes $E[n^g]$. It follows that

$$E[n^g] = \langle\psi^g|H(t)|\psi^g\rangle = E^g.$$

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,

$$E[n] = \langle\psi_{\min}[n]|H(t)|\psi_{\min}[n]\rangle > E^g.$$

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

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

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 non-interacting Kohn-Sham (KS) fermions is introduced [6], and it is assumed that the ground-state SOF $n_{\mathbf{r}}^g$ can be obtained from the ground-state density of the KS fermions moving in an external potential $v_{\mathbf{r}}^{ks}$. For $H_* = H(t_*)$, the KS Hamiltonian $H_{ks} = T_t' + V^{ks}$ is defined to be

$$H_{ks} = \sum_{\mathbf{r}}(1 - t_*/T)\{q_{\mathbf{r}}a_{\mathbf{r}}^\dagger + q_{\mathbf{r}}^*a_{\mathbf{r}}\} + \sum_{\mathbf{r}}(t_*/T)v_{\mathbf{r}}^{ks}\hat{n}_{\mathbf{r}},$$

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 $\epsilon_{ks}[n]$ is:

$$\epsilon_{ks}[n] = \min_{|\psi\rangle \to n} \langle\psi|H_{ks}|\psi\rangle = T_{t_*}'[n] + \sum_{\mathbf{r}}(t_*/T)v_{\mathbf{r}}^{ks}n_{\mathbf{r}}. \tag{9}$$

To determine the KS external potential $v_{\mathbf{r}}^{ks}$, we re-write Eq. (8) as

$$E[n] = T_{t_*}'[n] + \sum_{\mathbf{r}}(t_*/T)v_{\mathbf{r}}n_{\mathbf{r}} + \xi_{xc}[n], \tag{10}$$

where

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

is the exchange-correlation energy functional. Recall that it is through the exchange-correlation energy functional $\xi_{xc}[n]$ that DFT accounts for *all many-body effects*. Since $n_{\mathbf{r}}^g$ minimizes $\epsilon_{ks}[n]$ and $E[n]$, Eqs. (9) and (10) are stationary about $n = n^g$. Taking their functional derivatives with respect to n, evaluating the result at $n = n^g$, and eliminating $\delta T'/\delta n|_{n=n^g}$ gives

$$v_{\mathbf{r}}^{ks} = v_{\mathbf{r}} + (T/t_*)v_{xc}[n^g], \tag{11}$$

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 $\xi_{xc}[n^g]$,

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

This sets in place the formulas for a self-consistent calculation of the ground-state properties of $H_* = H(t_*)$ using GS-DFT. Entanglement [18] and its links to quantum phase transitions [19] have been studied using GS-DFT.

TD-DFT: Here we establish the Runge-Gross theorem [7] for the instantaneous MAX-CUT 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,

$$V_{\mathbf{r}}(t) = (t_*/T)(1 - t_*/T)v_{\mathbf{r}}(t),$$
$$V'_{\mathbf{r}}(t) = (t_*/T)(1 - t_*/T)v'_{\mathbf{r}}(t),$$

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 a smallest integer K exists such that $C_k(\mathbf{r})$ is a non-trivial 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.

It follows from Eq. (3) that the conserved fermion current $j_{\mathbf{r},\mu}$ has components

$$\hat{j}_{\mathbf{r},0}(t) = n_\mathbf{r}(t);$$
$$\hat{j}_{\mathbf{r},k}(t) = (1/2\pi) \sum_\mathbf{y} (\Delta_k G_{\mathbf{r},\mathbf{y}}) \partial_t n_\mathbf{y}(t),$$

with $k = 1, 2$ [14]. Here $G_{\mathbf{r},\mathbf{y}}$ is the Green's function for the lattice Laplacian,

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

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

$$\partial_t \{ j_{\mathbf{r},k}(t) - j'_{\mathbf{r},k}(t) \} = \langle \psi_0 | [\hat{j}_{\mathbf{r},k}(t), H(t) - H'(t)] | \psi_0 \rangle. \tag{12}$$

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. (12) eventually gives

$$\partial_t \{ \delta j_{\mathbf{r},k}(t) \} = -(1/2\pi) \sum_\mathbf{y} (\Delta_k G_{\mathbf{r},\mathbf{y}}) \, \delta V_\mathbf{y}(t) \, \mathcal{M}_\mathbf{y}(t), \tag{13}$$

where

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

With K defined as above, taking K time-derivatives of Eq. (13) and evaluating the result at $t = 0$ gives

$$\left. \frac{\partial^{K+1}}{\partial t^{K+1}} (\delta j_{\mathbf{r},k}(t)) \right|_0 = \frac{-1}{2\pi} \sum_\mathbf{y} (\Delta_k G_{\mathbf{r},\mathbf{y}}) \mathcal{M}_\mathbf{y}(0) C_K(\mathbf{r}), \tag{14}$$

where we have used that

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

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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

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

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

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

Taking K time-derivatives of this equation, evaluating the result at $t = 0$, and using Eq. (14) gives

$$\frac{\partial^{K+2}}{\partial t^{K+2}} (n_{\mathbf{r}}(t) - n'_{\mathbf{r}}(t))|_{t=0} = -C_K(\mathbf{r}) \mathcal{M}_{\mathbf{r}}(0) \neq 0, \tag{15}$$

where we have used the equation of motion for $G_{\mathbf{r},\mathbf{y}}$. Eq. (15) indicates that $n_{\mathbf{r}}(t)$ cannot equal $n'_{\mathbf{r}}(t)$ since it insures that they will be different at $t = 0^+$, and so 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 to be described below. Having said this, 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 $V_{\mathbf{r}}(t) = V_{\mathbf{r}} \sin \omega t$; it does *not* mean $V_{\mathbf{r}}(t) = V_{\mathbf{r}} \sin \omega t + C(t)$. Thus in a well-defined experiment $C(t) = 0$.

The KS system of non-interacting fermions can also be introduced in TD-DFT [7]. We must still assume that the interacting SOF $n_{\mathbf{r}}(t)$ can be obtained from the SOF of the non-interacting KS fermions moving in the external potential $v_{\mathbf{r}}^{ks}(t)$. The potentials $v_{\mathbf{r}}^{ks}(t)$ and $v_{\mathbf{r}}(t)$ are related via ($t_* \neq 0$)

$$v^{ks}_{\mathbf{r}}(t) = v_{\mathbf{r}}(t) + (T/t_*)\, v_{xc}[n_{\mathbf{r}}(t)], \tag{16}$$

though Eq. (16) is to be thought of as defining the exchange-correlation potential $v_{xc}[n_{\mathbf{r}}(t)]$.

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 [20]. The arguments used 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 the *interacting* fermion linear response, and so we assume that the total potential has the form

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

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:

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

The susceptibility $\chi_{\mathbf{r},\mathbf{r}'}(t - t')$ connects the first-order probe potential to the SOF response. The total potential $v^{\text{tot}}_{\mathbf{r}}(t)$ is related to the KS potential $v^{ks}_{\mathbf{r}}(t)$ through Eq. (16), 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 $\chi^{ks}_{\mathbf{r},\mathbf{r}'}(\omega)$, the exchange-correlation kernel $f_{xc}[n^g](\mathbf{r}, \mathbf{r}'; \omega)$, and the probe potential $v^1_{\mathbf{r}}(\omega)$:

$$\sum_{\mathbf{y}'} \{\delta_{\mathbf{r},\mathbf{y}'} - \sum_{\mathbf{r}'} \chi^{ks}_{\mathbf{r},\mathbf{r}'}(\omega) f_{xc}[n^g](\mathbf{r}', \mathbf{y}'; \omega)\} n^1_{\mathbf{y}'}(\omega) = \sum_{\mathbf{r}'} \chi^{ks}_{\mathbf{r},\mathbf{r}'}(\omega) v^1_{\mathbf{r}'}(\omega). \tag{17}$$

The KS susceptibility [8] depends on the KS static unperturbed orbitals $\phi_j(\mathbf{r})$; and the corresponding energy eigenvalues ε_j and orbital occupation numbers f_j,

$$\chi^{ks}_{\mathbf{r},\mathbf{r}'}(\omega) = \sum_{j,k} (f_k - f_j) \frac{\phi_j(\mathbf{r})\overline{\phi}_k(\mathbf{r})\overline{\phi}_j(\mathbf{r}')\phi_k(\mathbf{r}')}{\omega - (\varepsilon_j - \varepsilon_k) + i\eta}. \tag{18}$$

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. (17) 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. (17) 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. [20], one is led to the following eigenvalue problem:

$$\sum_{k',j'} \frac{M_{kj;k'j'}(\omega)}{\omega - \omega_{j'k'} + i\eta} \xi_{k'j'}(\omega) = \lambda(\omega) \xi_{kj}(\omega), \tag{19}$$

where, writing

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

and

$$\Phi^{kj}_{\mathbf{r}} = \overline{\phi}^k_{\mathbf{r}} \phi^j_{\mathbf{r}},$$

we have

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

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

So far, the argument is exact. To proceed further some form of approximation must be introduced. In the single-pole approximation [20] 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. (19):

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

Let ω_* be d-fold degenerate: $\omega_{k_1j_1}, \cdots, \omega_{k_dj_d} = \omega_*$. Matching singularities in Eq. (19) gives

$$\sum_{l=1}^{d} M_{k_ij_i;k'_lj'_l}(\omega_*) \xi^n_{k'_lj'_l} = A^n(\omega_*) \xi^n_{k_ij_i}(\omega_*), \tag{20}$$

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where $i, n = 1, \ldots, d$. For our purposes, the eigenvalues $A^n(\omega_*)$ are of primary interest and are found from Eq. (20). 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_{jk}^n gives

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

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

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

and

$$\overline{\Omega}_{jk} = \min_n \Omega_{jk}^n.$$

Our expression for Ω_{jk}^n then gives

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

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 $\overline{\Omega}_{jk}$ gives

$$\Delta(t_*) = [\varepsilon_1(t_*) - \varepsilon_0(t_*)] + \delta E(t_*). \tag{21}$$

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. (21); and then uses the minimum of the resulting set of $\Delta(t_*)$ to upper bound Δ. Because the KS dynamics is non-interacting, it has been possible to treat KS systems with $N \sim 10^3$ KS fermions [9–11]. This would allow evaluation of the minimum gap $\Delta(N)$ for the QAE algorithm for $N \sim 10^3$.

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

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to a specific lattice site. Consequently, anti-symmetrization of the fermion wavefunction 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. [21]. 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. (7)] has no self-interaction terms. Finally, because the fermions are pinned, it will be necessary to test the gap for sensitivity to derivative discontinuities [22] in $\xi_c[n]$.

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