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Editors' Suggestion

Time-dependent exchange-correlation potential in lieu of self-energy

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It is shown that the equation of motion of the one-particle Green function of an interacting many-electron system is governed by a multiplicative time-dependent exchange-correlation potential, which is the Coulomb potential of a time-dependent exchange-correlation hole. This exchange-correlation hole fulfills a sum rule, a generalization of the well-known sum rule of the static exchange-correlation hole. It is envisaged that the proposed formalism may provide an alternative route for calculating the Green function by finding a suitable approximation for the exchange-correlation hole or potential based on, e.g., a local-density approximation.

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I. INTRODUCTION

The one-particle Green function of an interacting many-particle system is of utmost importance in condensed-matter physics and other branches of physics such as molecular physics and nuclear physics. Essential physical properties, notably the ground-state expectation value of a single-particle operator, the total energy, and the particle addition and removal spectra can be extracted from the one-particle Green function, hereafter referred to simply as the Green function. Experimental photoemission and inverse photoemission spectra, which provide invaluable information about the electronic structure of the system, can be directly compared with the spectra extracted from the Green function, under the so-called sudden approximation and neglecting the matrix-element effects. Experimental data from transport measurements and many other experimental observations can also be related to the Green function. Much effort has therefore been expended on developing methods and techniques for calculating the Green function, from many-body perturbation theory [1] to methods employing path-integral techniques [2].

The zero-temperature time-ordered Green function is defined according to [1]

$$iG(rt,r't') = \langle T[\hat{\psi}(rt)\hat{\psi}^{\dagger}(r't')]\rangle, \tag{1}$$

where $r = (\mathbf{r},\sigma)$ is a combined label of space and spin variables, $\hat{\psi}(rt)$ is the field operator in the Heisenberg picture, T is the time-ordering symbol, and the expectation value is taken with respect to the ground state. The many-electron Hamiltonian defining the Heisenberg operator is given by

$$\hat{H} = \int dr\,\hat{\psi}^{\dagger}(r)h_0(r)\hat{\psi}(r) + \frac{1}{2}\int dr dr'\,\hat{\psi}^{\dagger}(r)\hat{\psi}^{\dagger}(r')v(r-r')\hat{\psi}(r')\hat{\psi}(r), \tag{2}$$

where $h_0 = -\frac{1}{2}\nabla^2 + V_{\text{ext}}(r)$ and $v(r-r') = 1/|\mathbf{r}-\mathbf{r}'|$. In our notation, $\int dr = \sum_{\sigma}\int d^3r$ and atomic units are used throughout, in which the Bohr radius a_0, the electron mass m_e, the electronic charge e, and $\hbar$ are set to unity.

Since the Hamiltonian is time independent it is convenient to set $t' = 0$. The Green function fulfills the following equation of motion,

$$\left(i\frac{\partial}{\partial t} - h_0(r)\right)G(r,r';t) + i\int dr''v(r-r'')\langle T[\hat{\rho}(r''t)\hat{\psi}(rt)\hat{\psi}^{\dagger}(r')]\rangle = \delta(r-r')\delta(t), \tag{3}$$

where $\hat{\rho}$ is the density operator. The interaction term contains a special case of the two-particle Green function:

$$G^{(2)}(r,r',r'';t) = \langle T[\hat{\rho}(r''t)\hat{\psi}(rt)\hat{\psi}^{\dagger}(r')]\rangle. \tag{4}$$

The traditional approach is to introduce a self-energy Σ as follows,

$$-i\int dr''v(r-r'')G^{(2)}(r,r',r'';t) - V_H(r)G(r,r';t) = \int dr''dt''\Sigma(r,r'';t-t'')G(r'',r';t''), \tag{5}$$

where V_H is the Hartree potential subtracted from $G^{(2)}$. Thus, the self-energy embodies the effects of exchange and correlations and a central quantity in Green function theory. The self-energy is a well-established framework for calculating the Green function but it acts on the Green function as a convolution in space and time and as such it is difficult to visualize its meaning in a clear physical picture. Moreover, from the Dyson equation, $G = G_0 + G_0\Sigma G$, it can be seen that Σ is an auxiliary quantity since it depends on the choice of the starting reference Green function G_0.

In this paper, a completely different route is proposed to calculate the Green function. It is shown that the equation of motion of the Green function can be reformulated so that it is governed by a time-dependent exchange-correlation potential that acts multiplicatively on the Green function. This exchange-correlation potential arises naturally from

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the Coulomb potential of the time-dependent exchange-correlation hole, which fulfills a sum rule. The static and equal-space limit $r' \to r$ of this exchange-correlation hole reduces to the well-known static exchange-correlation hole in the formal expression for the exchange-correlation energy. The focus is then shifted to finding an accurate approximation for the exchange-correlation hole or potential, in the spirit of density functional theory [3–6].

II. THEORY

A. Time-dependent exchange-correlation hole

Writing out the time ordering of the two-particle Green function in Eq. (4) and using the commutation

$$[\hat{\psi}(rt), \hat{\rho}(r''t)] = \delta(r - r'')\hat{\psi}(rt) \tag{6}$$

yields

$$\begin{aligned} G^{(2)}(r, r', r''; t) = {}& \langle\hat{\rho}(r''t)\hat{\psi}(rt)\hat{\psi}^{\dagger}(r')\rangle\theta(t) \\ & - \langle\hat{\psi}^{\dagger}(r')\hat{\psi}(rt)\hat{\rho}(r''t)\rangle\theta(-t) \\ & + \delta(r - r'')\langle\hat{\psi}^{\dagger}(r')\hat{\psi}(rt)\rangle\theta(-t). \end{aligned} \tag{7}$$

Consider now integrating $G^{(2)}$ over the variable r''. It should first be noted that for any state Ψ containing N electrons,

$$\int dr''\hat{\rho}(r'')|\Psi\rangle = \hat{N}|\Psi\rangle = N|\Psi\rangle, \tag{8}$$

where $\hat{N}$ counts the number of electrons in the system. Using $G^{(2)}$ in Eq. (7) one finds for $t < 0$,

$$\int dr'' G^{(2)}(r, r', r''; t) = iG(r, r'; t)(N - 1). \tag{9}$$

$G^{(2)}$ can be naturally factorized as follows,

$$G^{(2)}(r, r', r''; t) = iG(r, r'; t)g(r, r', r''; t)\rho(r''), \tag{10}$$

which defines the correlation function $g(r, r', r''; t)$, and after substitution into Eq. (9) one arrives at the sum rule

$$\int dr''[g(r, r', r''; t) - 1]\rho(r'') = -1. \tag{11}$$

This sum rule is valid for any r, r', and $t < 0$ and the integrand may be interpreted as the time-dependent exchange-correlation hole,

$$\rho_{\mathrm{xc}}(r, r', r''; t) = [g(r, r', r''; t) - 1]\rho(r''), \tag{12}$$

a generalization of the static exchange-correlation hole, first introduced by Slater for the exchange part [7]. Since $\rho_{\mathrm{xc}}(r, r', r''; t)$ is in general complex, the sum rule implies that the imaginary part integrates to zero.

It is interesting to observe that for $t > 0$ (the addition of an electron), the exchange-correlation hole integrates to zero, as can be seen from Eq. (7). This result may be understood by recognizing that the added electron is not part of the electron density that generates the Hartree potential so that there is no self-interaction corresponding to the last term of $G^{(2)}$ in Eq. (7). For $\sigma'' \neq \sigma$, the exchange-correlation hole integrates to zero, as may be seen from the presence of $\delta(r - r'') = \delta(\mathbf{r} - \mathbf{r}')\delta_{\sigma\sigma''}$ in Eq. (7). If one were to decompose ρ_{xc} into the exchange and the correlation holes, it is the exchange hole that would integrate to -1 whereas the correlation hole would integrate to zero. The sum rule can then be summarized as follows:

$$\int d^3r''\rho_{\mathrm{xc}}(r, r', r''; t < 0) = -\delta_{\sigma\sigma''}, \tag{13}$$

$$\int dr''\rho_{\mathrm{xc}}(r, r', r''; t < 0) = -1, \tag{14}$$

$$\int dr''\rho_{\mathrm{xc}}(r, r', r''; t > 0) = 0. \tag{15}$$

This sum rule may be viewed as the generalization of the well-known sum rule for the static exchange-correlation hole appearing in the formally exact expression for the exchange-correlation energy [5,6], originating from Slater's sum rule for the exchange hole only [7]. The static exchange-correlation hole corresponds to the limit $t \to 0^-$ and $r' \to r$.

B. Time-dependent exchange-correlation potential

Rearranging Eq. (10) yields

$$G^{(2)}(r, r', r''; t) = iG(r, r'; t)\rho(r'') + iG(r, r'; t)\rho_{\mathrm{xc}}(r, r', r''; t), \tag{16}$$

in which the first term on the right-hand side generates the Hartree term. When the above $G^{(2)}$ is substituted into the equation of motion of G in Eq. (3), it generates the time-dependent exchange-correlation potential as a function of r, r', and t,

$$V_{\mathrm{xc}}(r, r'; t) = \int dr'' v(r - r'')\rho_{\mathrm{xc}}(r, r', r''; t), \tag{17}$$

acting on G in a multiplicative fashion, in contrast to the self-energy which acts on G as a convolution in space-time as in Eq. (5). The equation of motion for G becomes

$$\left(i\frac{\partial}{\partial t} - h(r) - V_{\mathrm{xc}}(r, r'; t)\right)G(r, r'; t) = \delta(r - r')\delta(t), \tag{18}$$

where $h = h_0 + V_H$. This equation has a local character in the sense that the potential is multiplicative in both space and time. Apart from the source term on the right-hand side, for a given r' it is just as a one-particle time-dependent Schrödinger equation in the presence of a time-dependent field V_{xc}. The effects of exchange and correlations are now embodied in the time-dependent exchange-correlation potential V_{xc}, which is in general non-Hermitian. Equation (18) furnishes us with a different picture from that of the conventional self-energy formulation and offers a simple physical interpretation for the propagation of an added electron or hole, which is governed by, in addition to the external field and the Hartree potential, the time-dependent exchange-correlation potential. This exchange-correlation potential is simply the Coulomb potential of the time-dependent exchange-correlation hole.

The corresponding Dyson-like equation for G can be readily written down,

$$\begin{aligned} G(r, r'; t) = {}& G_H(r, r'; t) + \int dr''dt' G_H(r, r''; t - t') \\ & \times V_{\mathrm{xc}}(r'', r'; t')G(r'', r'; t'), \end{aligned} \tag{19}$$

where G_H is the Hartree Green function, and the relationship between $V_{\rm xc}$ and Σ in space-time is given by

$$V_{\rm xc}(r,r';t)G(r,r';t)=\int dr''dt'\Sigma(r,r'';t-t')G(r'',r';t'). \tag{20}$$

Expressed in a set of base orbitals $\{\varphi_i\}$, the equation of motion in Eq. (18) takes the form

$$i\frac{\partial}{\partial t}G_{ij}(t)-\sum_k h_{ik}G_{kj}(t)-\sum_{kl}V^{\rm xc}_{ik,lj}(t)G_{kl}(t)=\delta_{ij}\delta(t), \tag{21}$$

where G_{ij} and h_{ik} are the matrix elements of G and h in the orbitals and

$$V^{\rm xc}_{ik,lj}(t)=\int d^3rd^3r'\,\varphi_i^*(r)\varphi_k(r)V_{\rm xc}(r,r';t)\varphi_l^*(r')\varphi_j(r'), \tag{22}$$

exhibiting the two-particle character of $V_{\rm xc}$, a bosonic quantity, in contrast to the self-energy which is fermionic.

Much is known about the static exchange-correlation hole [6], which may provide a starting point for finding a good approximation for the time-dependent one. Approximating $V_{\rm xc}$ via the exchange-correlation hole $\rho_{\rm xc}$, which is a physically motivated entity, may be more advantageous than following the arduous route of finding a good approximation for the self-energy by means of many-body perturbation theory or a path-integral approach. The proposed formalism has a certain proximity to time-dependent density functional theory [8,9]. It should be noted, however, that the time dependence of $V_{\rm xc}$ does not arise from the presence of a time-dependent external field, but rather due to the dynamics of the Green function. The addition or removal of an electron causes the system to evolve in a nontrivial way due to the Coulomb interaction among the electrons.

C. Local-density approximation

It can be anticipated that $V_{\rm xc}$ is a relatively smooth function since it is the Coulomb potential of a charge distribution that integrates to -1 or 0. Following Gunnarsson and Lundqvist [5,10], it is readily seen by making a change of variable $\mathbf{R}=\mathbf{r}-\mathbf{r}''$ that, due to the form of the Coulomb interaction, only the spherical average of the exchange-correlation hole in the variable $\mathbf{R}$ is needed to determine $V_{\rm xc}$,

$$V_{\rm xc}(r,r';t)=\sum_{\sigma_R}\int dRR\,\overline{\rho}_{\rm xc}(r,r',R;t), \tag{23}$$

where $\overline{\rho}_{\rm xc}(r,r',R;t)$ depends only on the radial distance R with respect to $\mathbf{r}$,

$$\overline{\rho}_{\rm xc}(r,r',R;t)=\int d\Omega_R\rho_{\rm xc}(r,r',\mathbf{r}-\mathbf{R};t), \tag{24}$$

implying that the fine spatial details of the exchange-correlation hole may not be important, as illustrated vividly for the case of the static exchange-correlation hole in some light atoms [5,11]. According to Eq. (23), $V_{\rm xc}$ is the first radial moment of the spherically averaged $\rho_{\rm xc}$.

It can also be seen that $\mathbf{r}$ may be thought of as the center of the exchange-correlation hole whereas r' may be treated as a parameter representing the spatial origin of the created electron. One could imagine that the exchange-correlation hole moves with the added hole or electron as a function of time. From Eq. (7) it is quite evident that when $r''=r$, $G^{(2)}=g=0$ and hence $\rho_{\rm xc}(r,r',r;t)=-\rho(r)$ for *any* r, r', and t. Following Slater's argument [12], it can be concluded that the exchange-correlation potential behaves approximately as $\rho^{1/3}$. It may be envisaged that a local-density approximation for $V_{\rm xc}$ as in density functional theory can be developed and its time dependence can be constructed from knowledge of the time-dependent exchange-correlation hole of the electron gas and some generic model systems, depending on the correlation strength.

The correlation function of the homogeneous electron gas with density $\bar{\rho}$ can be written as follows,

$$g^{\rm HEG}_{\sigma\sigma''}(\bar{\rho},R',R'',\theta;t), \tag{25}$$

where $R'=|\mathbf{r}-\mathbf{r}'|$, $R''=|\mathbf{r}-\mathbf{r}''|$, θ is the angle between $\mathbf{R}'$ and $\mathbf{R}''$, and the spin dependence has been written explicitly. A simple local-density approximation for the exchange-correlation hole could be

$$\rho^{\rm LDA}_{\rm xc}(r,r',r'';t)=\big[g^{\rm HEG}_{\sigma\sigma''}(\rho(r),R',R'',\theta;t)-1\big]\rho(r''). \tag{26}$$

A more sophisticated approximation would be to employ the weighted-density approximation [11,13], in which the density dependence associated with the variable r' is taken into account. On the other hand, applying the local-density approximation directly on $V_{\rm xc}$,

$$V^{\rm LDA}_{\rm xc}(r,r';t)=V^{\rm HEG}_{\rm xc}(\rho(r),R;t), \tag{27}$$

where $R=|\mathbf{r}-\mathbf{r}'|$, may be too crude since information encoded in $\rho(r'')$ is lost. It would be interesting to compare this approximation with the local-density approximation for the self-energy based on the homogeneous electron gas proposed by Sham and Kohn many years ago [14]. One may speculate that a local-density approximation on $V_{\rm xc}$ is more favorable than on Σ since $V_{\rm xc}$ acts locally on G. Also, in contrast to Σ, which is fermionic, $V_{\rm xc}$ is a bosonic object and as such it may be easier to approximate in terms of the density, which is a bosonic quantity.

D. Connection with Kohn-Sham $V_{\rm xc}$

If $V_{\rm xc}(r,r';t)$ is approximated by the static Kohn-Sham exchange-correlation potential $V^{\rm KS}_{\rm xc}(r)$, then the Green function reduces to the Kohn-Sham noninteracting Green function, whose diagonal component will by construction yield the exact density. However, $V^{\rm KS}_{\rm xc}(r)$ is not necessarily the same as $V_{\rm xc}(r,r;0^-)$. From the equations of motion of G and $G^{\rm KS}$ one finds

$$\left(i\frac{\partial}{\partial t}-h(r)-V_{\rm xc}(r,r';t)\right)[G(r,r';t)-G^{\rm KS}(r,r';t)] \\ =\big[V_{\rm xc}(r,r';t)-V^{\rm KS}_{\rm xc}(r)\big]G^{\rm KS}(r,r';t). \tag{28}$$

Evaluating the equation at $r'\to r$ and $t\to 0^-$ and making use of the fact that both G and $G^{\rm KS}$ give the same density yields the relationship between $V_{\rm xc}(r,r;0^-)$ and $V_{\rm xc}^{\rm KS}(r)$:

$$\lim_{r'\to r, t\to 0^-}\left(\frac{\partial}{\partial t}-\frac{i}{2}\nabla^2\right)[G(r,r';t)-G^{\rm KS}(r,r';t)] = \left[V_{\rm xc}(r,r;0^-)-V_{\rm xc}^{\rm KS}(r)\right]\rho(r). \qquad (29)$$

There is no obvious reason why the left-hand side vanishes so that in general $V_{\rm xc}(r,r;0^-)\neq V_{\rm xc}^{\rm KS}(r)$. When integrated over r, the first term on the left-hand side involving the time derivative is the difference in the first moment of the occupied densities of states, whereas the second term is the difference in the kinetic energies, which is contained in the Kohn-Sham $E_{\rm xc}$.

One also notes that

$$g(r,r,r'';t=0^-)\neq g^{\rm KS}(r,r''), \qquad (30)$$

since $g^{\rm KS}$ is defined as a coupling-constant integration of g_λ, which is the static correlation function corresponding to a scaled Coulomb interaction λv, yielding the exact ground-state density independent of λ [10,15].

E. Kohn-Sham scheme for unoccupied states

Since $V_{\rm xc}(0^-)\neq V_{\rm xc}(0^+)$, there will in general be a discontinuity at $t=0$. This suggests that in the Kohn-Sham scheme, two exchange-correlation potentials are needed, one for the occupied states and another for the unoccupied ones. For the occupied states, the standard Kohn-Sham equation applies, while for the unoccupied states one has

$$\left(-\tfrac{1}{2}\nabla^2+V_{\rm ext}+V_H+V_{\rm xc}^+\right)\phi_{kn}=\epsilon_k\phi_{kn}, \qquad (31)$$

where $V_{\rm xc}^+$ is the exchange-correlation potential corresponding to an exchange-correlation hole that integrates to zero rather than to one. After solving the standard Kohn-Sham equation, the unoccupied states are used to diagonalize Eq. (31), which ensures that all states will be orthogonal. A local-density approximation for the exchange-correlation hole corresponding to $V_{\rm xc}^+$ can be taken to be the one in Eq. (26) with $r'=r$ and $t=0^+$.

Since the exchange-correlation hole corresponding to $V_{\rm xc}^+$ integrates to zero, it should be weaker than the one for the occupied states for weakly or moderately correlated systems. This implies that the unoccupied states would be pushed up, correcting the well-known underestimation of band gaps in semiconductors and insulators. For metals, however, one may reason that since the band dispersion is smooth across the Fermi surface, the discontinuity should tend to vanish.

As an approximate $V_{\rm xc}^+$ it may be reasonable to use only the correlation part of the standard $V_{\rm xc}$. A simple correction would be to use first-order perturbation theory:

$$\varepsilon_{kn}^+=\varepsilon_{kn}+\langle\phi_{kn}|V_{\rm xc}^+-V_{\rm xc}|\phi_{kn}\rangle. \qquad (32)$$

An even simpler correction would be to ignore entirely $V_{\rm xc}^+$, which may lead, however, to an overestimation of the gap since $V_{\rm xc}^+$ is likely to be negative.

F. Extension to temperature-dependent Green function

The temperature-dependent Green function is defined in a similar way as for the zero-temperature one with the ground-state expectation value replaced by the thermal average,

$$iG_\beta(rt,r't')=\frac{1}{Z}{\rm Tr}\{e^{-\beta\hat{K}}T[\hat{\psi}(rt)\hat{\psi}^\dagger(r't')]\}, \qquad (33)$$

where $\hat{K}=\hat{H}-\mu\hat{N}$, μ is the chemical potential, $Z={\rm Tr}\,e^{-\beta\hat{K}}$ is the partition function, and $\beta=1/(k_BT)$ with k_B being the Boltzmann constant and T the temperature. The Heisenberg operators is defined as

$$\hat{\psi}(rt)=e^{i\hat{K}t}\hat{\psi}(r)e^{-i\hat{K}t}. \qquad (34)$$

At this stage, one traditionally goes over to imaginary time yielding the Matsubara Green function. The reason is that Wick's theorem is no longer convenient to use if one stays along the real-time axis due to the presence of the thermal factor $e^{-\beta\hat{K}}$. The proposed formalism, however, makes no use of Wick's theorem so that it is not necessary to work along the imaginary-time axis. The ill-defined problem of analytic continuation to the real-time axis when calculating spectral functions associated with the Matsubara Green function is circumvented.

The field operators are independent of temperature so that the equation of motion of G_β is the same as the one in Eq. (3) with the understanding that the ground-state expectation value is now to be understood as thermal average and h_0 is replaced with $h_0-\mu$. It is quite evident that the sum rule and the equation of motion in Eq. (18) still hold with h replaced by $h-\mu$ and all quantities carry the temperature label β. As in the zero-temperature case, the main task is to find a good approximation for the temperature-dependent $\rho_{\rm xc}$ or $V_{\rm xc}$.

III. EXAMPLE: THE HUBBARD DIMER

To illustrate how the time-dependent exchange-correlation potential looks like and as a proof of concept, the half-filled Hubbard dimer with total spin zero is considered. Although it is very simple, it contains some of the essential physics of correlated electrons and it has the great advantage of being analytically solvable. The Hamiltonian of the Hubbard dimer in standard notation is given by

$$\hat{H}=-\Delta\sum_{i\neq j}\hat{c}_{i\sigma}^\dagger\hat{c}_{j\sigma}+U\sum_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}. \qquad (35)$$

By calculating $G^{(2)}$ and using the relation in Eq. (16), $V_{\rm xc}$ can be deduced. The results, shown in Fig. 1, are given by

$$V_{11,11}^{\rm xc}(t>0)=\frac{U}{2}\frac{(1-x^2)\{1+\exp(-i2\Delta t)\}}{(1+x)^2+(1-x)^2\exp(-i2\Delta t)}, \qquad (36)$$

$$V_{11,22}^{\rm xc}(t>0)=\frac{U}{2}\frac{(1-x^2)\{1-\exp(-i2\Delta t)\}}{(1+x)^2-(1-x)^2\exp(-i2\Delta t)}, \qquad (37)$$

where

$$x=\frac{1}{4\Delta}(\sqrt{U^2+16\Delta^2}-U) \qquad (38)$$

is the relative weight of double-occupancy configurations in the ground state and

$$2\Delta=E_1^--E_0^-=E_1^+-E_0^+>0 \qquad (39)$$

are the excitation energies of the $(N\pm1)$ systems. From symmetry, $V_{22,22}^{\rm xc}=V_{11,11}^{\rm xc}$ and $V_{22,11}^{\rm xc}=V_{11,22}^{\rm xc}$, i.e., $V_{\rm xc}$ is symmetric

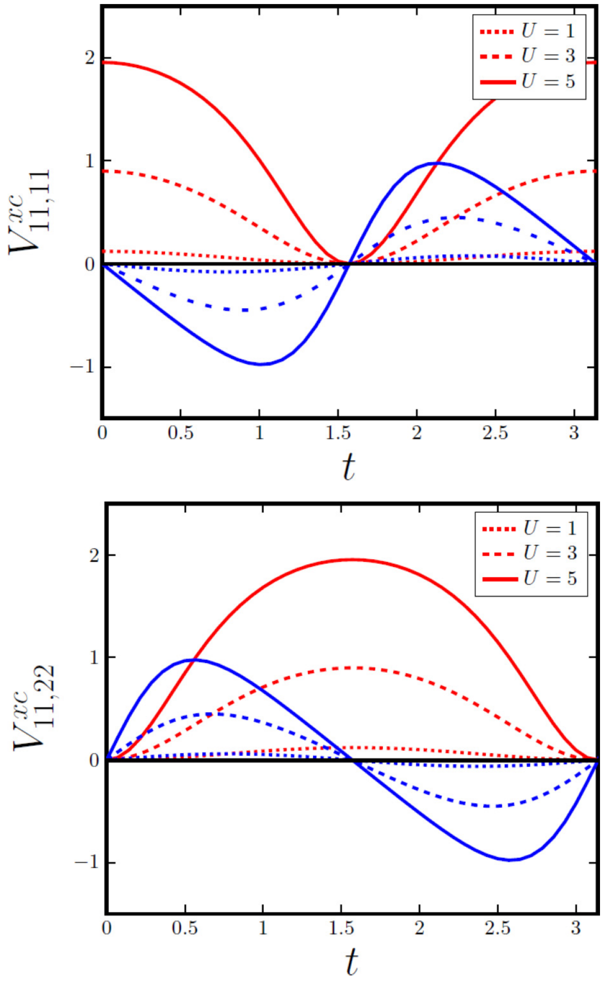

FIG. 1. The real (red) and imaginary (blue) parts of the exchange-correlation potentials $V^{\mathrm{xc}}_{11,11}$ and $V^{\mathrm{xc}}_{11,22}$ of the Hubbard dimer as a function of time for $U = 1, 3, 5$ with $\Delta = 1$. Due to the particle-hole symmetry, $V_{\mathrm{xc}}(-t) = -V_{\mathrm{xc}}(t)$.

but it is not Hermitian since it is complex. Due to the particle-hole symmetry, $V_{\mathrm{xc}}(-t) = -V_{\mathrm{xc}}(t)$.

A number of generic conclusions can be drawn from this simple model. Since x depends on U, V_{xc} is not simply proportional to the interaction U. In the weakly correlated limit corresponding to small $(1-x)$, it can be seen that the dependence of V_{xc} on time becomes weak whereas in the strongly correlated limit corresponding to small x, it becomes more pronounced. This result may well be quite general and it is in accordance with expectation since in the weakly correlated regime, a static mean-field potential is expected to be a good approximation.

One also notices that the time dependence is dictated by the excitation energies of the $(N \pm 1)$ systems and in general, these excitations include collective ones. For example, for solids one expects a time-dependent term of the form $\exp(-i\omega_p t)$ where ω_p is the plasmon energy. V_{xc} acts then as an effective external field, exchanging an energy ω_p with the system. It is also interesting to observe that the same energy dependence appears in the denominator. When expanded in a power series it would generate multiple excitations such as multiple plasmons observed experimentally in the alkalis. This is precisely what the cumulant expansion [16,17] within the self-energy formulation accomplishes but in an *ad hoc* manner. In the strong-coupling limit, $x \to 0$, expanding the denominator in a power series of the time exponential is no longer viable, indicating a fundamental difference in V_{xc} between weakly and strongly correlated systems.

Another interesting feature is the discontinuity in the diagonal element of $V^{\mathrm{xc}}_{11,11}$ at $t=0$, which is the difference between the particle $(t=0^+)$ and the hole $(t=0^-)$ values, reminiscent of the discontinuity in the exchange-correlation potential in density functional theory [18].

IV. CONCLUSION

The problem of calculating the self-energy is recast into the problem of constructing the exchange-correlation potential arising from the exchange-correlation hole, which is a physically motivated entity fulfilling an exact sum rule and some limiting properties. The proposed formalism is in the spirit of density functional theory, in which the main task is to find an accurate approximation for the exchange-correlation functional.

There are many aspects to explore and consider. For example, it would be interesting to investigate the degree of locality of V_{xc}, i.e., how V_{xc} behaves as a function of $|\mathbf{r}' - \mathbf{r}|$ and to study the time dependence of V_{xc} for a number of model systems such as the electron gas and one-dimensional systems solvable by means of the Bethe ansatz in order to accumulate clues and guidelines for constructing an accurate and reliable V_{xc} or ρ_{xc}.

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