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Starting from the recently proposed dynamical exchange-correlation field framework, the equation of motion of the diagonal part of the many-electron Green function is derived, from which the spectral function can be obtained. The resulting equation of motion takes the form of the continuity equation of charge and current densities in electrodynamics with a source. An unknown quantity in this equation is the divergence of the temporal current density, corresponding to the kinetic energy. A procedure *à la* Kohn-Sham scheme is then proposed, in which the difference between the kinetic potential of the interacting system and the noninteracting Kohn-Sham system is shifted into the exchange-correlation field. The task of finding a good approximation for the exchange-correlation field should be greatly simplified since only the diagonal part is needed. A formal solution to the continuity equation provides an explicit expression for calculating the spectral function, given an approximate exchange-correlation field.

DOI: [10.1103/PhysRevB.108.115110](https://doi.org/10.1103/PhysRevB.108.115110)**I. INTRODUCTION**

The total spectral function of a many-electron system, hereafter referred to simply as the spectral function, is given by the trace of the Green function. This implies that to calculate the spectral function only the diagonal components of the Green function are required. Although for solids, the momentum-resolved spectral function contains more detailed information about the electronic structure of the system, it often suffices for many purposes to know the integrated spectral function. It is therefore an attractive proposition to determine the spectral function from the diagonal part of the Green function since it is presumably much simpler to calculate than the full Green function. A relevant work along this direction is the work by Gatti *et al.* [1] who proposed using an effective potential, local in space but energy dependent, from which the spectral function can be calculated directly. It is quite feasible that for a given system an effective potential that reproduces the exact diagonal part of the Green function exists. It is, however, not evident how to construct such an effective potential. Another work of relevance is that of Savrasov and Kotliar [2], who introduced the concept of spectral density-functional theory. In their work, the key variable is given by the local Green function rather than the electron density.

In this paper a different approach is taken. Starting from the recently derived equation of motion of the Green function within the dynamical exchange-correlation field framework [3,4], the equation of motion for the diagonal part of the

Green function, referred to as temporal density, is obtained. The derivation takes advantage of the fact that the exchange-correlation field acts locally on the Green function. It should be noted that a similar derivation cannot be carried out in a natural way within the self-energy formalism. The resulting equation has the form of the continuity equation of charge and current densities in electrodynamics with a source/sink term. An unknown quantity in the equation is the divergence of the temporal current density, which is associated with the kinetic energy. By defining the divergence of the temporal current density of the Kohn-Sham system and transferring the difference in kinetic energy between the interacting system and the noninteracting Kohn-Sham system into the exchange-correlation field, a formally exact continuity equation for the diagonal part of the Green function is obtained. For practical calculations, a local-density approximation for the modified exchange-correlation field based on the homogeneous electron gas is proposed. An example from a model of the interacting electron gas is considered to illustrate the exchange-correlation field and the kinetic potential.

The paper continues with a theory section, where the continuity equation is derived, followed by an illustration from the model electron gas. It closes with a summary and conclusions.

II. THEORY**A. The exchange-correlation field framework**

The zero-temperature time-ordered Green function in equilibrium is defined as [5]

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

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

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Hamiltonian defining the Heisenberg operator is given by

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

where $h_0 = -\frac{1}{2}\nabla^2 + V_{\text{ext}}(r)$, $v(r-r') = 1/|\mathbf{r}-\mathbf{r}'|$, and $\int dr = \sum_\sigma \int d^3r$. $V_{\text{ext}}(r)$ is the external potential arising from the nuclei and other externally applied fields. Atomic unit is 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, the Green function depends only on the time difference $t-t'$ and it is convenient to set $t'=0$. The equation of motion of the Green function in the dynamical exchange-correlation (xc) field framework is given by [3]

$$[i\partial_t - h(r) - V_{\text{xc}}(r, r'; t)]G(r, r'; t) = \delta(r-r')\delta(t), \quad (3)$$

where

$$h(r) = -\frac{1}{2}\nabla^2 + V_{\text{MF}}(r), \quad V_{\text{MF}} = V_{\text{ext}} + V_{\text{H}}. \quad (4)$$

V_{MF} is the mean field consisting of the external field V_{ext} and the Hartree field V_{H} . The exchange-correlation field has a simple physical interpretation as the Coulomb potential of the exchange-correlation hole ρ_{xc} :

$$V_{\text{xc}}(r, r'; t) = \int dr'' v(r-r'')\rho_{\text{xc}}(r, r'', t). \quad (5)$$

As in Slater's static exchange hole, the exchange-correlation hole fulfils a sum rule

$$\int d^3r'' \rho_{\text{xc}}(r, r', r''; t) = -\delta_{\sigma\sigma'}\theta(-t) \quad (6)$$

and an exact constraint

$$\rho_{\text{xc}}(r, r', r'' = r; t) = -\rho(r) \quad (7)$$

for any r, r' , and t . $\rho(r)$ is the ground-state electron density. It can also be shown [6] that the exchange-correlation hole can be expressed as the linear response of the logarithmic of G :

$$\rho_{\text{xc}}(1, 2, 3) = i\frac{\delta}{\delta\varphi(3)} \ln G(1, 2), \quad (8)$$

where $1 = (r_1 t_1)$, etc., and φ is a time-dependent probing field.

Comparison with the equation of motion in the conventional self-energy approach yields a formal relationship between the exchange-correlation field V_{xc} and the self-energy Σ :

$$V_{\text{xc}}(r, r'; t) = \frac{1}{G(r, r'; t)} \int dr'' dt' \times \Sigma(r, r''; t-t')G(r'', r'; t'). \quad (9)$$

This relation provides a means for calculating V_{xc} when an approximate self-energy is known.

A prominent feature that distinguishes the exchange-correlation field from the self-energy is its local character. Unlike the self-energy, it acts on the Green function locally in both space and time so that the equation of motion of the Green function is equivalent to the Schrödinger equation. The

Green function can be propagated pointwise in time since $G(t+\delta t)$ at an infinitesimal time later can be calculated from $G(t)$ without knowledge of its previous values at earlier times. In other words, in contrast to the self-energy approach, the equation of motion has no memory.

B. Temporal density

The temporal density proportional to the diagonal part of the Green function is defined as

$$\rho(r, t) = -iG(r, r; t). \quad (10)$$

For $t=0^-$ the temporal density reduces to the electron density

$$\rho(r, 0^-) = -iG(r, r; 0^-) = \rho(r). \quad (11)$$

When $\rho(r, t)$ is integrated over r and Fourier transformed in t , it yields the spectral function or density of states

$$\rho(\omega) = \frac{1}{\Omega} \int dr \int dt e^{i\omega t} \rho(r, t). \quad (12)$$

The temporal density is not the same as the time-dependent density associated with density fluctuations upon addition of a hole or an electron. For example, for electron addition ($t > 0$) at r , the latter is the density corresponding to the time-evolved state

$$|\Psi(r, t)\rangle = e^{-i\hat{H}t} \hat{\psi}^\dagger(r)|\Psi_0\rangle, \quad (13)$$

yielding

$$\begin{aligned} \rho_{\text{nuc}}(r, t) &= \langle \Psi(r, t) | \hat{\rho}(r) | \Psi(r, t) \rangle \\ &= \langle \Psi_0 | \hat{\psi}(r) e^{i\hat{H}t} \hat{\rho}(r) e^{-i\hat{H}t} \hat{\psi}^\dagger(r) | \Psi_0 \rangle, \end{aligned} \quad (14)$$

which is real and different from the temporal density, which is given by (for $t > 0$)

$$\begin{aligned} \rho(r, t) &= -\langle \Psi_0 | \hat{\psi}(rt) \hat{\psi}^\dagger(r) | \Psi_0 \rangle \\ &= -e^{itE_0} \langle \Psi_0 | \hat{\psi}(r) e^{-i\hat{H}t} \hat{\psi}^\dagger(r) | \Psi_0 \rangle. \end{aligned} \quad (15)$$

The temporal density is complex and proportional to the probability amplitude that a hole or an electron created at r is annihilated at the same position at a later time t . Hence the nomenclature ‘‘temporal density.’’ The temporal density is also different from the time-dependent density in time-dependent density-functional theory [7,8], which describes the dynamics of the density upon application of an external time-dependent field.

Considering the equation of motion for the Green function in Eq. (3) for $r' = r, t \neq 0$ and defining

$$V_{\text{xc}}(r, t) = V_{\text{xc}}(r, r; t), \quad (16)$$

one finds

$$[i\partial_t - V_{\text{MF}}(r) - V_{\text{xc}}(r, t)]\rho(r, t) - \frac{i}{2}\nabla^2 G(r, r'; t)|_{r'=r} = 0. \quad (17)$$

One may define the temporal current density for each r'

$$\mathbf{j}(r, r'; t) = -\frac{1}{2}\nabla G(r, r'; t), \quad (18)$$

and the equation of motion for $t \neq 0$ becomes

$$\partial_t \rho(r, t) + \nabla \cdot \mathbf{j}(r, t) = S(r, t), \quad (19)$$

in which

$$\nabla \cdot \mathbf{j}(r, t) = \nabla \cdot \mathbf{j}(r, r'; t)|_{r'=r} = -\frac{1}{2} \nabla^2 G(r, r'; t)|_{r'=r} \quad (20)$$

and

$$S(r, t) = -i[V_{\text{MF}}(r) + V_{\text{xc}}(r, t)]\rho(r, t). \quad (21)$$

More explicitly, $G(r, r'; t)$ can be expanded in a complete set of orbitals $\{\varphi_i\}$:

$$G(r, r'; t) = \sum_{ij} \varphi_i(r) G_{ij}(t) \varphi_j^*(r'), \quad (22)$$

and the divergence of the temporal current density for a given r is given by

$$\nabla \cdot \mathbf{j}(r, t) = -\frac{1}{2} \sum_i \nabla^2 \varphi_i(r) \psi_i^*(r, t), \quad (23)$$

where

$$\psi_i^*(r, t) = \sum_j G_{ij}(t) \varphi_j^*(r). \quad (24)$$

The equation of motion can be interpreted as a continuity equation with a source/sink term S on the right-hand side. Since the divergence of the temporal current density is the curvature of the Green function at $r' = r$, only knowledge of the diagonal components $G(r, r; t)$, and the neighboring points along the diagonal $G(r \pm \delta r, r; t)$, is needed. Substantially much less information than that of the full Green function is required to calculate the spectral function. There is no auxiliary system invoked in this derivation and all quantities are well defined and their existence is guaranteed.

C. Practical scheme

The continuity equation can be rewritten as

$$i\partial_t \ln \rho(r, t) = V_{\text{MF}}(r) + V_{\text{xc}}(r, t) + V_{\text{K}}(r, t), \quad (25)$$

where V_{K} is termed the kinetic potential

$$V_{\text{K}}(r, t) = -i \frac{\nabla \cdot \mathbf{j}(r, t)}{\rho(r, t)}. \quad (26)$$

The formal solution is given by

$$\rho(r, t) = \rho(r, 0^\pm) \exp[-iV_{\text{MF}}(r)t] \times \exp \left\{ -i \int_0^t dt' [V_{\text{xc}}(r, t') + V_{\text{K}}(r, t')] \right\}. \quad (27)$$

Assuming that a good approximation for V_{xc} is known, the remaining input required to solve for the temporal density is the divergence of the temporal current density, which is associated with the kinetic energy. The kinetic energy is known to be very difficult to approximate with an explicit functional of the electron density.

To construct a practical scheme for calculating the temporal density, one may follow the Kohn-Sham scheme of

density-functional theory [9–12] by defining ΔV_{K} according to

$$\Delta V_{\text{K}} = -i \left\{ \frac{\nabla \cdot \mathbf{j}}{\rho} - \frac{\nabla \cdot \mathbf{j}^{\text{KS}}}{\rho^{\text{KS}}} \right\} = V_{\text{K}} - V_{\text{K}}^{\text{KS}}, \quad (28)$$

where ρ^{KS} and \mathbf{j}^{KS} are, respectively, the temporal density and the temporal current density obtained from the Kohn-Sham Green function. ΔV_{K} is the difference in kinetic potential between the interacting system and the noninteracting Kohn-Sham system. The continuity equation becomes

$$\partial_t \rho(r, t) + \frac{\nabla \cdot \mathbf{j}^{\text{KS}}(r, t)}{\rho^{\text{KS}}(r, t)} \rho(r, t) = \tilde{S}(r, t), \quad (29)$$

where

$$\tilde{S}(r, t) = -i[V_{\text{MF}}(r) + \tilde{V}_{\text{xc}}(r, t)]\rho(r, t), \quad (30)$$

$$\tilde{V}_{\text{xc}} = V_{\text{xc}} + \Delta V_{\text{K}}. \quad (31)$$

Alternatively, the equation of motion for the temporal density can be written as

$$i\partial_t \ln \rho(r, t) = V_{\text{MF}}(r) + \tilde{V}_{\text{xc}}(r, t) + V_{\text{K}}^{\text{KS}}(r, t). \quad (32)$$

The formal solution is given by

$$\rho(r, t) = \rho(r, 0^\pm) \exp[-iV_{\text{MF}}(r)t] \times \exp \left\{ -i \int_0^t dt' [\tilde{V}_{\text{xc}}(r, t') + V_{\text{K}}^{\text{KS}}(r, t')] \right\}. \quad (33)$$

This procedure is analogous to the Kohn-Sham scheme [9–12] in which the difference in kinetic energy between the interacting system and the auxiliary noninteracting system is shifted into the exchange-correlation energy. Here, the difference between the kinetic potentials of the interacting system and the noninteracting Kohn-Sham system is incorporated into the exchange-correlation field. It should, however, be emphasized that Eq. (29) describes the equation of motion of the true interacting temporal density. The Kohn-Sham temporal density and current density are only used as a means of taking into account part of the interacting kinetic potential. Unlike the Kohn-Sham scheme of density-functional theory, there is no auxiliary system introduced.

D. Local-density approximation and nearsightedness

The problem of calculating the spectral function amounts to finding a good approximation for \tilde{V}_{xc} , which should be simpler compared with the full exchange-correlation field that depends on two position variables. $\tilde{V}_{\text{xc}}(n, t)$ can be calculated for the homogeneous electron gas (HEG) as a function of the electron density n within, e.g., the *GW* approximation [13–15] or better approximations such as the cumulant expansion [16–21], and applied to real inhomogeneous systems within the local-density approximation (LDA)

$$\tilde{V}_{\text{xc}}^{\text{LDA}}(r, t) = \tilde{V}_{\text{xc}}^{\text{HEG}}(\rho(r), t). \quad (34)$$

To justify the use of the local-density approximation, it is instructive to return to the original concept of Slater's effective local exchange potential [22], which arises as the Coulomb potential of the exchange hole. Due to the sum rule that the exchange role must integrate to -1 and the constraint that the

exchange hole associated with a given electron is equal to the negative of the density $\rho(r)$ at the position of the electron, Slater argued that the exchange hole can be approximated by a uniform charge density enclosed in a sphere of radius r_0 such that

$$\frac{4\pi}{3}r_0^3\rho(r) = 1. \quad (35)$$

Since the Coulomb potential at the center of the uniformly charged sphere is proportional to $1/r_0$, the exchange potential is then proportional to $\rho^{1/3}(r)$, which leads to the local-density approximation. As pointed out later by Slater [23], this reasoning is based on the exact properties of the exchange hole and does not rely on the homogeneous electron gas. There is no assumption for the density to be slowly varying or close to being homogeneous. Slater's argument also applies to the exchange-correlation field since the associated exchange-correlation hole fulfils the same sum rule and exact constraint as for the exchange hole. This provides a justification for employing the local-density approximation for the dynamical exchange-correlation field.

The dependence of the exchange potential on the local density at the position of the electron in question may be seen as an example of Kohn's concept of nearsightedness [24–26]. A recent study by Wetherell *et al.* [27] on a one-dimensional double well offers an illustration of the nearsightedness of the effective orbital-dependent local exchange potential defined as

$$V_{x,m}^{\text{eff}}(r) = \frac{1}{\phi_m(r)} \int dr' F(r, r') \phi_m(r'), \quad (36)$$

where $F(r, r')$ is the Fock exchange operator and ϕ_m is an orbital. It is shown that this potential, which is the Coulomb potential of the exchange hole associated with an electron occupying orbital ϕ_m , is significant only in the region where the orbital is located and cancels the Hartree potential, which represents the spurious self-interaction. In contrast, the exact Kohn-Sham potential, which is orbital independent, contains a step at the interface of the two wells, deviating from the principle of nearsightedness.

The exchange-correlation field in Eq. (9) can be regarded as a generalization of the effective local exchange-potential in Eq. (36). Thus, $G(r, r'; t)$ is the time-dependent analog of $\phi_m(r)$ with r' playing the role of the orbital index m . Indeed, $V_{xc}(r, r'; t)$ is the Coulomb potential of the exchange-correlation hole $\rho_{xc}(r, r', r''; t)$ as expressed in Eq. (5). In contrast to the Kohn-Sham exchange-correlation potential, which is an auxiliary effective potential felt by all the electrons in the system and associated with the noninteracting Kohn-Sham Green function, the dynamical exchange-correlation field in the present formalism depends on the position of the electron or hole introduced into the system. Moreover, although it is a constructed quantity, it is associated with the true rather than an auxiliary Green function.

The validity of the local-density approximation is less evident for ΔV_K , which is the difference in the kinetic potential of the true and the Kohn-Sham systems. Unlike the exchange-correlation field, there is no known relationship between the exchange-correlation hole and the kinetic potential. Slater's

argument for the local exchange potential, which does not rely on the homogeneous electron gas, cannot be readily carried over to the kinetic potential. However, since the relevant quantity is the difference in the kinetic potential between the true and the Kohn-Sham systems, the error may be less severe compared with the error of the individual kinetic potential.

III. EXAMPLES

Two examples, the noninteracting homogeneous electron gas and a model for the interacting homogeneous electron gas, are considered to verify that the equation of motion for the temporal density reproduces the correct results. The model also provides illustrations for how the two essential quantities in the proposed formalism, namely, the exchange-correlation field and the kinetic potential, may look like in real systems. The given examples are not intended as a means of investigating how to construct reliable approximations for the two quantities.

A. Noninteracting homogeneous electron gas

As a simple example, consider the noninteracting homogeneous electron gas whose Green function is given by

$$iG_0(R; t) = \frac{1}{\Omega} \sum_{k > k_F} e^{i\mathbf{k}\cdot\mathbf{R}} e^{-i\varepsilon_k t} \theta(t) - \frac{1}{\Omega} \sum_{k \leq k_F} e^{i\mathbf{k}\cdot\mathbf{R}} e^{-i\varepsilon_k t} \theta(-t), \quad (37)$$

where $\varepsilon_k = \frac{1}{2}k^2$, k_F is the Fermi wave vector, and Ω is the space volume.

For a noninteracting electron gas $V_{xc} = 0$ and V_{ext} is a uniform positive background so that $V_{\text{MF}} = V_{\text{ext}} + V_{\text{H}} = 0$. Since the system is uniform, only the case of $R = 0$ is needed. The temporal density per spin is given by

$$\begin{aligned} \rho_0(t < 0) &= \frac{1}{\Omega} \sum_{k \leq k_F} e^{-i\varepsilon_k t} \\ &= \frac{1}{2\pi^2} \int_0^{k_F} dk k^2 e^{-itk^2/2} \end{aligned} \quad (38)$$

and the kinetic energy corresponding to the temporal current density is given by

$$\begin{aligned} \nabla \cdot \mathbf{j}_0(r, t) &= -\frac{1}{2} \nabla^2 G_0(R; t < 0)|_{R=0} \\ &= \frac{i}{\Omega} \sum_{k \leq k_F} \frac{k^2}{2} e^{-i\varepsilon_k t} \\ &= \frac{i}{4\pi^2} \int_0^{k_F} dk k^4 e^{-itk^2/2}, \end{aligned} \quad (39)$$

where

$$k_F^3 = 3\pi^2 n_0, \quad \rho_0(0) = \frac{1}{2} n_0, \quad (40)$$

and n_0 is the density of the homogeneous electron gas. Since for the noninteracting electron gas $S = 0$, the continuity equation in Eq. (19) is indeed fulfilled.

B. A model Green function for the interacting electron gas

To illustrate and study the behavior of the exchange-correlation field and the kinetic potential, a physically motivated model for the Green function of the interacting electron gas is considered. This model was proposed in a previous article [6] and given by the following:

$$G(R, t < 0) = \frac{i}{\Omega} \sum_{k \leq k_F} (C_1 + C_2) e^{i\mathbf{k} \cdot \mathbf{R}}, \quad (41)$$

$$G(R, t > 0) = -\frac{i}{\Omega} \sum_{k > k_F} (D_1 + D_2) e^{i\mathbf{k} \cdot \mathbf{R}}, \quad (42)$$

where

$$C_1 = Z e^{-iE_k t}, \quad (43)$$

$$C_2 = (1 - Z) e^{-i(E_k - \omega_p) t}, \quad (44)$$

$$D_1 = Z e^{-iE_k t}, \quad (45)$$

$$D_2 = (1 - Z) e^{-i(E_k + \omega_p) t}, \quad (46)$$

where E_k is the quasiparticle energy, Z_k is the quasiparticle renormalization factor, and ω_k is the plasmon energy. For simplicity, Z_k and ω_k are assumed to be independent of k and E_k is taken to be a renormalized free-electron gas dispersion

$$Z_k = Z, \quad \omega_k = \omega_p, \quad E_k = \alpha \varepsilon_k = \frac{\alpha}{2} k^2. \quad (47)$$

For an electron gas of density n_0 the plasmon energy is given by

$$\omega_p = \sqrt{4\pi n_0}. \quad (48)$$

In Fig. 1, the hole spectral function of the model for $r_s = 4$ is compared with that of the noninteracting electron gas. The model essentially accounts for the quasiparticle band narrowing and the transfer of the quasiparticle weight to the plasmon satellite, located at one plasmon energy below the main quasiparticle band. For simplicity, only one plasmon is taken into account and there is no weight arising from states above the Fermi level. The Fermi level of the interacting model has been adjusted to coincide with that of the noninteracting one.

For $t \neq 0$, the exchange-correlation field can be obtained from the equation of motion

$$V_{xc}(R, t) = \frac{1}{G(R, t)} [i\partial_t - h(R)] G(R, t). \quad (49)$$

Since

$$h(R) \exp(i\mathbf{k} \cdot \mathbf{R}) = \frac{k^2}{2} \exp(i\mathbf{k} \cdot \mathbf{R}), \quad (50)$$

one finds for $t < 0$

$$[i\partial_t - h(R)] G(R, t < 0) = \frac{i}{\Omega} \sum_{k \leq k_F} (A_1 + A_2) e^{i\mathbf{k} \cdot \mathbf{R}}, \quad (51)$$

where

$$A_1 = Z(E_k - \varepsilon_k) e^{-iE_k t}, \quad (52)$$

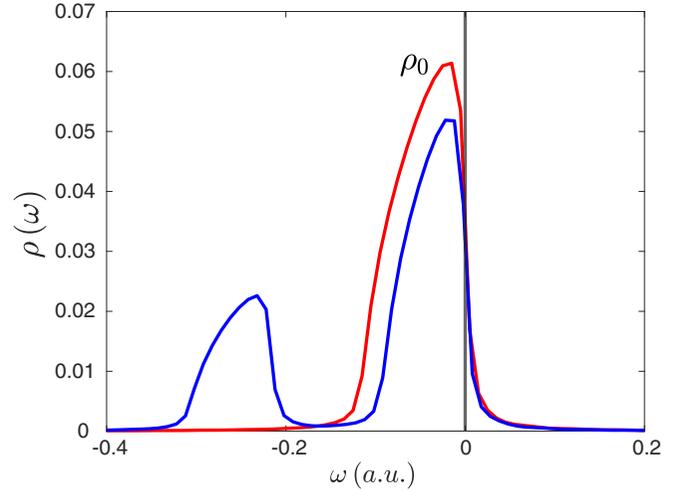


FIG. 1. The hole spectral functions of the model interacting electron gas (blue) and the noninteracting electron gas (red), labeled ρ_0 . The Fermi level is at the zero of the energy, indicated by a vertical line. The peak at around $\omega = -0.25$ is the plasmon satellite, located at one plasmon energy below the main quasiparticle peak. The model corresponds to $r_s = 4$, giving a plasmon frequency $\omega_p = 0.217$. A quasiparticle renormalization factor $Z = 0.7$, a band-narrowing $\alpha = 0.8$, and a broadening $\eta = 0.005$ have been used.

$$A_2 = (1 - Z)(E_k - \varepsilon_k - \omega_p) e^{-i(E_k - \omega_p) t}. \quad (53)$$

For $t > 0$

$$[i\partial_t - h(R)] G(R, t > 0) = -\frac{i}{\Omega} \sum_{k > k_F} (B_1 + B_2) e^{i\mathbf{k} \cdot \mathbf{R}}, \quad (54)$$

where

$$B_1 = Z(E_k - \varepsilon_k) e^{-iE_k t}, \quad (55)$$

$$B_2 = (1 - Z)(E_k - \varepsilon_k + \omega_p) e^{-i(E_k + \omega_p) t}. \quad (56)$$

1. The exchange-correlation field and the kinetic potential

Consider the case $t < 0$. Defining

$$I_n = \int_0^{k_F} dk k^{2n} e^{-i\alpha k^2 t/2}, \quad (57)$$

one obtains

$$\frac{1}{\Omega} \sum_{k \leq k_F} A_1 = \frac{1}{2\pi^2} Z \frac{\alpha - 1}{2} I_2, \quad (58)$$

$$\frac{1}{\Omega} \sum_{k \leq k_F} A_2 = \frac{1}{2\pi^2} (1 - Z) e^{i\omega_p t} \left(\frac{\alpha - 1}{2} I_2 - \omega_p I_1 \right), \quad (59)$$

$$\frac{1}{\Omega} \sum_{k \leq k_F} (C_1 + C_2) = \frac{1}{2\pi^2} [Z + (1 - Z) e^{i\omega_p t}] I_1. \quad (60)$$

Using the above results leads to

$$[i\partial_t - h(R)] G(R, t < 0)|_{R=0} = \frac{i}{2\pi^2} [a_2 I_2 - a_1 I_1], \quad (61)$$

$$G(0, t < 0) = \frac{i}{2\pi^2} c_1 I_1, \quad (62)$$

where

$$a_1 = \omega_p(1 - Z)e^{i\omega_p t}, \quad (63)$$

$$c_1 = Z + (1 - Z)e^{i\omega_p t}, \quad (64)$$

$$a_2 = \frac{\alpha - 1}{2}c_1. \quad (65)$$

The exchange-correlation field becomes

$$V_{xc}(t < 0) = \frac{1}{2}(\alpha - 1)\frac{I_2}{I_1} - \frac{a_1}{c_1}. \quad (66)$$

To calculate the difference in the kinetic potentials one needs

$$-i\nabla \cdot \mathbf{j} = \frac{1}{\Omega} \sum_{k \leq k_F} \frac{k^2}{2}(C_1 + C_2) = \frac{1}{4\pi^2}c_1 I_2, \quad (67)$$

$$-i\nabla \cdot \mathbf{j}^{KS} = \frac{1}{\Omega} \sum_{k \leq k_F} \frac{k^2}{2}e^{-ik^2/2} = \frac{1}{4\pi^2}I_2^0, \quad (68)$$

where

$$I_n^0 = \int_0^{k_F} dk k^{2n} e^{-ik^2/2}. \quad (69)$$

The temporal densities are given by

$$\rho_0(t < 0) = -iG_0(0, t < 0) = \frac{1}{2\pi^2}I_1^0, \quad (70)$$

$$\rho(t < 0) = -iG(0, t < 0) = \frac{1}{2\pi^2}c_1 I_1, \quad (71)$$

yielding

$$V_K(t < 0) = \frac{1}{2}\frac{I_2}{I_1}, \quad (72)$$

$$V_K^{KS}(t < 0) = \frac{1}{2}\frac{I_2^0}{I_1^0}. \quad (73)$$

It is interesting to note that the kinetic potential does not depend explicitly on the plasmon energy and it is counteracted by a term proportional to I_2/I_1 in the exchange-correlation field:

$$V_{xc} + V_K = \frac{\alpha}{2}\frac{I_2}{I_1} - \frac{a_1}{c_1}. \quad (74)$$

2. Physical interpretation

The roles of the exchange-correlation field and the kinetic potential in determining the spectral function may be understood as follows. Using the relation

$$\frac{\partial I_1}{\partial t} = -\frac{i\alpha}{2}I_2, \quad (75)$$

the exchange-correlation field and the kinetic potential can be rewritten as

$$V_{xc}(t < 0) = \frac{\alpha - 1}{\alpha}i\partial_t \ln I_1 - \frac{a_1}{c_1}, \quad (76)$$

and

$$V_K = \frac{i}{\alpha}\partial_t \ln I_1, \quad (77)$$

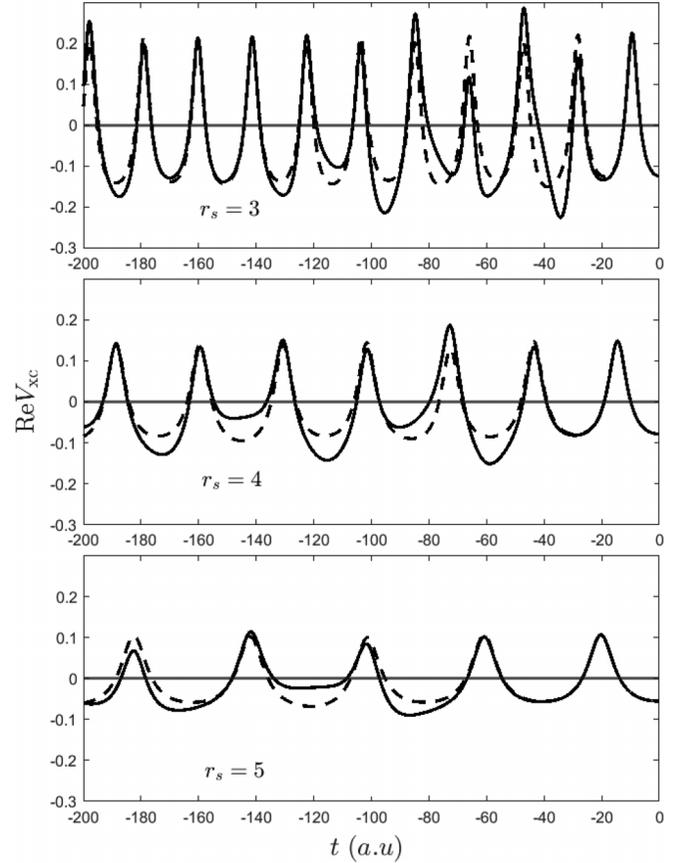


FIG. 2. The real part of the exchange-correlation potentials V_{xc} (dashed) and \tilde{V}_{xc} (solid) as defined in the text for $r_s = 3, 4, 5$. The difference $\Delta V_K = \tilde{V}_{xc} - V_{xc}$ is shown in Fig. 4.

so that

$$V_{xc} + V_K = i\partial_t \ln I_1 - \frac{a_1}{c_1}. \quad (78)$$

The first term of $V_{xc} + V_K$ when integrated over time from 0 to t is given by

$$-i \int_0^t dt' i \frac{\partial}{\partial t'} \ln I_1 = \ln \frac{I_1(t)}{I_1(0)} \quad (79)$$

and the second is given by

$$\begin{aligned} i \int_0^t dt' \frac{a_1}{c_1} &= i\omega_p \int_0^t dt' \frac{(1 - Z)e^{i\omega_p t'}}{Z + (1 - Z)e^{i\omega_p t'}} \\ &= \ln [Z + (1 - Z)e^{i\omega_p t}]. \end{aligned} \quad (80)$$

Collecting the above two terms leads to

$$e^{-i \int_0^t dt' [V_{xc}(t') + V_K(t')]} = [Z + (1 - Z)e^{i\omega_p t'}] \frac{I_1(t)}{I_1(0)}. \quad (81)$$

Since $I_1(0) = 2\pi^2\rho(r)$, the formal solution in Eq. (27) is then

$$\rho(r, t) = \frac{1}{2\pi^2} [Z + (1 - Z)e^{i\omega_p t}] I_1(t), \quad (82)$$

which reproduces the temporal density in Eq. (71).

Some general conclusions may be drawn from the electron gas model. From the above analysis, there are two essential terms which determine the temporal density. The first

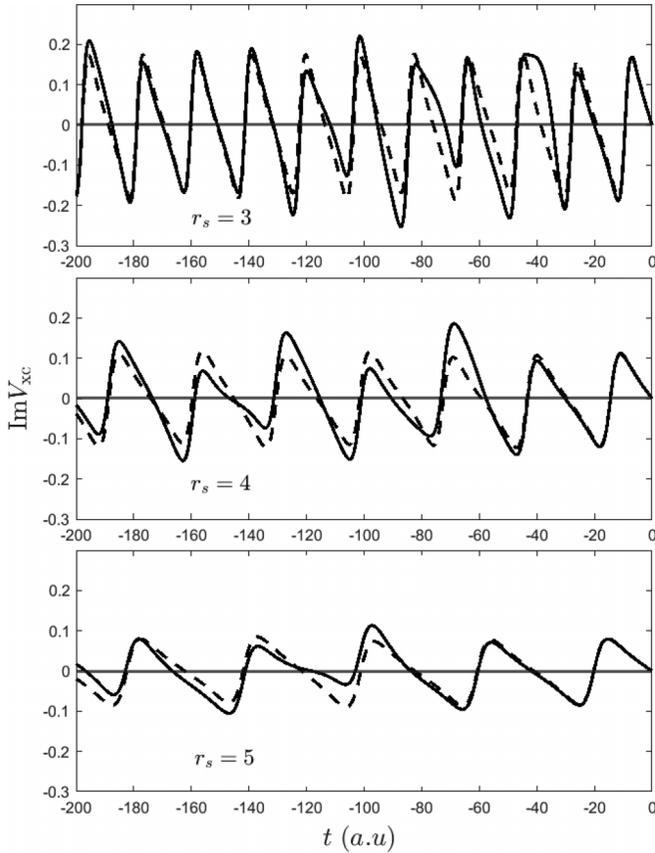


FIG. 3. The imaginary part of the exchange-correlation potentials V_{xc} (dashed) and \tilde{V}_{xc} (solid) as defined in the text for $r_s = 3, 4, 5$. The difference $\Delta V_K = \tilde{V}_{xc} - V_{xc}$ is shown in Fig. 4.

term in Eq. (78) yields $I_1(t)$ which when Fourier transformed results in the main quasiparticle peak whereas the second term $-a_1/c_1$ is responsible for the spectral weight redistribution between the quasiparticle and the plasmon excitations. The kinetic potential in Eq. (77) by itself would generate $I_1^{1/\alpha}(t)$ which yields a wrong quasiparticle bandwidth. A corresponding term in V_{xc} partially cancels the kinetic potential to give the correct bandwidth. Analogous to the self-energy, the exchange-correlation field has a twofold role of renormalizing the quasiparticle bandwidth and transferring weight from the quasiparticle to the satellite (plasmon).

C. Results

Atomic units are used throughout. A quasiparticle renormalization factor $Z = 0.7$, a band-narrowing parameter $\alpha = 0.8$, and a broadening $\eta = 0.005$ have been used for all values of r_s .

From the model Green function, the exchange-correlation fields can be extracted as detailed in the theory section. The results are shown in Figs. 2 and 3 for the real and imaginary parts of V_{xc} and \tilde{V}_{xc} . The former exhibits a more distinct periodicity whereas the latter appears to have a less well-defined periodicity. This can be understood from Fig. 4, which shows the difference between \tilde{V}_{xc} and V_{xc} . This difference, which is also the difference in kinetic potential between the interacting system and the noninteracting Kohn-Sham system, has a beat

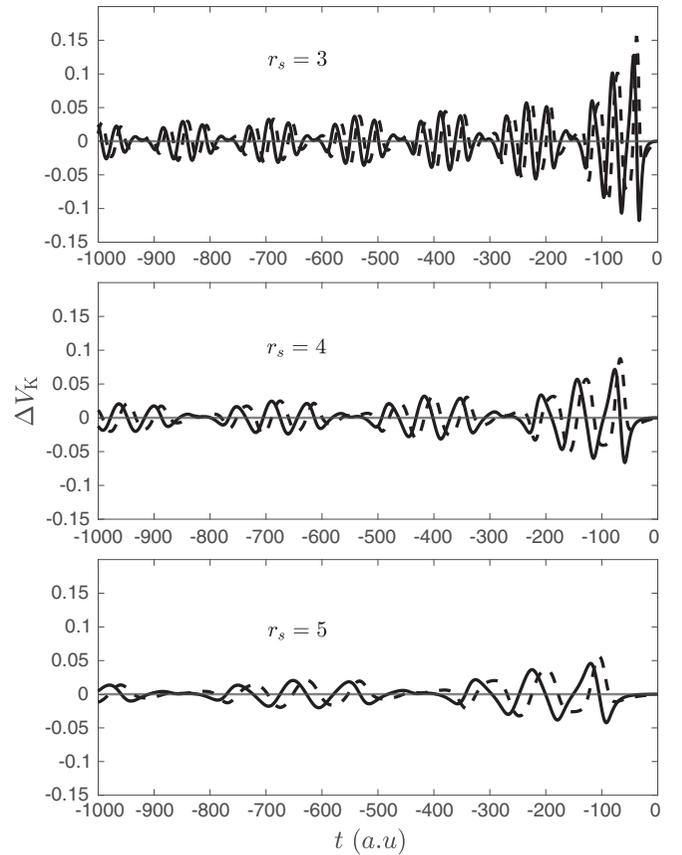


FIG. 4. The real part (solid) and the imaginary part (dashed) of the kinetic potential difference $\Delta V_K = V_K - V_K^{KS}$ for $r_s = 3, 4, 5$.

pattern which decreases in magnitude as $-t$ increases. The price of approximating the interacting kinetic potential by that of the Kohn-Sham system and transferring the difference into the exchange-correlation field is a more irregular behavior of the latter.

In Fig. 5 the kinetic potentials of the interacting system and the noninteracting Kohn-Sham system are shown, both displaying well-defined oscillations. The interacting kinetic potential mimics the behavior of the Kohn-Sham kinetic potential but with a shifted phase, which appears to be time dependent. This suggests that rather than approximating the interacting kinetic potential by that of the Kohn-Sham system and shifting the difference into the exchange-correlation field, it could be more favorable to model directly the interacting kinetic potential by the Kohn-Sham one but with a time-dependent shifted phase. The phase shift between the two kinetic potentials increases as the density is lowered, indicating that at high density the Kohn-Sham kinetic potential better approximates the interacting kinetic potential. This is as anticipated as correlations are expected to be less important as the density increases.

There is a general trend of the exchange-correlation field and the kinetic potential as functions of r_s . The smaller r_s or the higher the density the more oscillatory the quantities become. This is understandable since the oscillatory behavior of the exchange-correlation field is determined to a large

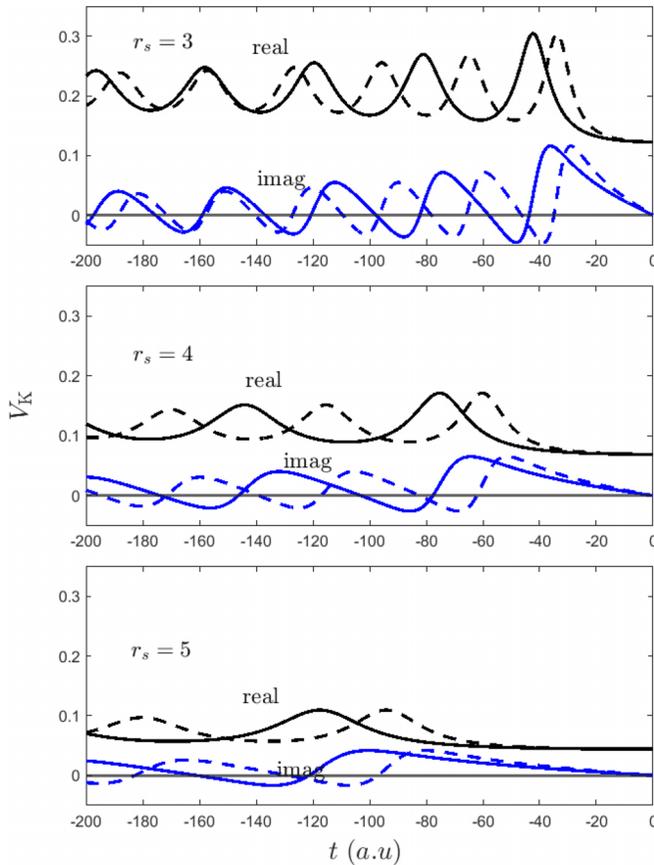


FIG. 5. The real (black) and imaginary (blue) parts of the kinetic potentials V_K (solid) and V_K^{KS} (dashed) as defined in the text for $r_s = 3, 4, 5$.

extent by the plasmon energy, which increases with the density. The kinetic potential, on the other hand, does not follow the same oscillatory behavior of the exchange-correlation field since it does not depend explicitly on the plasmon energy, as can be seen in Eq. (73). In the case of the kinetic potential, it is the Fermi wavevector that determines the oscillatory behavior, which increases as the density increases or as r_s decreases.

IV. SUMMARY AND CONCLUSIONS

The continuity equation for the temporal density has been derived, starting from the recently proposed dynamical exchange-correlation field framework. The divergence of the temporal current density, which is an unknown quantity in this equation, is approximated by that of the Kohn-Sham system and the difference is transferred into the exchange-correlation field. There remains the task of finding a good approximation for the exchange-correlation field, which should be substantially simplified since only the diagonal part is needed. If a good approximation for the exchange-correlation field can be constructed, the spectral function can be readily calculated from an explicit solution to the continuity equation. A model Green function of the interacting electron gas is used to illustrate the key quantities in the proposed formulation.

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