Time-Dependent Density-Functional Theory for Superconductors

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A density-functional theory is established for strongly correlated inhomogeneous superconductors subject to time-dependent external scalar, vector, and pairing potentials. Hohenberg-Kohn and Kohn-Sham type theorems are formulated for gauge-invariant densities. The central result is a set of time-dependent Bogoliubov–de Gennes equations which include exchange-correlation effects.

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Dynamic charge transport phenomena observed in conventional [1–5] and strongly correlated inhomogeneous superconductors [6–8] have been interpreted theoretically using results from time-dependent mean-field theories [9–14]. Among these theories the time-dependent Bogoliubov–de Gennes equations have been especially useful in clarifying effects due to Andreev scattering [12–15]. However, they do not include exchange-correlation effects. Thus, there has remained some uncertainty so far whether considerations based on their solutions are pertinent to high-temperature and heavy-fermion [16] superconductors.

The purpose of this Letter is the presentation of a time-dependent density-functional theory for superconductors. The resulting time-dependent Bogoliubov–de Gennes equations, which take into account exchange-correlation effects, are suitable for the description of dynamic processes in strongly correlated inhomogeneous superconductors.

Our approach is based on methods from the time-dependent density-functional theory for nonsuperconducting systems [17–20] combined with ideas from time-independent density-functional theory for superconductors [21–24]. The central result of the latter is a set of stationary Bogoliubov–de Gennes equations that formally include all correlation effects via an exchange-correlation functional. They have recently been solved numerically with a phenomenological approximation for the exchange-correlation functional [25].

We consider superconductors described by the Hamiltonian

$$\hat{H}_{V,\mathbf{A},D}(t) = \hat{H}_K(t) + \hat{V}(t) + \hat{D}(t) + \hat{D}^\dagger(t) + \hat{W}(t), \tag{1}$$

where

$$\hat{H}_K(t) = \frac{1}{2m}\int d^3r\, \psi_\sigma^\dagger(\mathbf{r},t)\left(\hat{\mathbf{p}} + \frac{e}{c}\mathbf{A}(\mathbf{r},t)\right)^2 \psi_\sigma(\mathbf{r},t), \tag{2}$$

$$\hat{V}(t) = \int d^3r\, V(\mathbf{r},t)\psi_\sigma^\dagger(\mathbf{r},t)\psi_\sigma(\mathbf{r},t), \tag{3}$$

$$\hat{D}(t) = -\int d^3r\, D(\mathbf{r},t)\psi_\downarrow^\dagger(\mathbf{r},t)\psi_\uparrow^\dagger(\mathbf{r},t), \tag{4}$$

$$\hat{W}(t) = \frac{1}{2}\int\int d^3r_1\, d^3r_2\, \psi_\sigma^\dagger(\mathbf{r}_1,t)\psi_{\sigma'}^\dagger(\mathbf{r}_2,t)w(\mathbf{r}_1,\mathbf{r}_2) \times \psi_{\sigma'}(\mathbf{r}_2,t)\psi_\sigma(\mathbf{r}_1,t). \tag{5}$$

The $\psi_\sigma(\mathbf{r},t)$ are the usual electronic field operators in the Heisenberg picture. Summation over double spin indices σ is implied. The system is subject to three time-dependent external fields: the vector potential $\mathbf{A}(r,t)$, the scalar potential $V(\mathbf{r},t)$, and the pairing potential $D(\mathbf{r},t)$ [22], which can be viewed as being induced by an adjacent superconductor via the proximity effect [21]. The local interaction $w(\mathbf{r}_1,\mathbf{r}_2) = w_c(\mathbf{r}_1,\mathbf{r}_2) - \delta(\mathbf{r}_1 - \mathbf{r}_2)w_g(\mathbf{r}_1)$ is assumed to consist of a repulsive, e.g., Coulomb, term $w_c(\mathbf{r}_1,\mathbf{r}_2)$ and the spatially varying attractive Gorkov point contact interaction $w_g(\mathbf{r}_1)$ [26,27]. The time-independent many-body state of the system (in the Heisenberg picture) which does not have to be the ground state is given by the initial state $|\Psi_0\rangle$ at the initial time t_0. The dynamics of the system is determined by the Heisenberg equation of motion $i(\partial/\partial t)\psi_\sigma(\mathbf{r},t) = [\psi_\sigma(\mathbf{r},t), \hat{H}_{V,\mathbf{A},D}(t)]_-$ for the field operators, which results in a unique mapping F of the potentials on the field operators:

$$F\colon (V(\mathbf{r},t), \mathbf{A}(\mathbf{r},t), D(\mathbf{r},t)) \to \psi_\sigma^{(\dagger)}(\mathbf{r},t). \tag{6}$$

The crucial step in the formulation of any density-functional theory is in the identification of the appropriate densities for which a Hohenberg-Kohn-like theorem can be proved. For this purpose we employ the current density $\mathbf{j}(\mathbf{r},t) \equiv \langle\Psi_0|\hat{\mathbf{j}}(\mathbf{r},t)|\Psi_0\rangle$, $\hat{\mathbf{j}}(\mathbf{r},t)$ being the usual current-density operator in the Heisenberg picture, and the anomalous density

$$\Delta_{IP}(\mathbf{r},t) = \langle\Psi_0|\psi_\uparrow(\mathbf{r},t)\psi_\downarrow(\mathbf{r},t)e^{2i\int_{t_0}^{t} dt'\, V(r,t')}|\Psi_0\rangle, \tag{7}$$

which are invariant under the gauge transformation $\psi_\sigma(\mathbf{r},t) \to \psi_\sigma(\mathbf{r},t)\exp[-ie\lambda(\mathbf{r},t)/c]$, and the corresponding transformations for V, $\mathbf{A}$, and D, so that the action involving $\hat{H}_{V,\mathbf{A},D}(t)$ of Eq. (1) is gauge invariant. For the gauge function $\lambda(\mathbf{r},t)$ we choose the initial value $\lambda(\mathbf{r},t_0) = 0 \bmod (2\pi c/e)$. This class of transformations leaves the Heisenberg field operators and thus all physical properties of the system unchanged at the initial time t_0. The choice of the anomalous density $\Delta_{\mathrm{IP}}(\mathbf{r},t)$ is partly motivated by the fact that gauge-invariant phases (IP)

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appear in the Josephson equations for superconducting weak links.

The central Hohenberg-Kohn-like statement to be proved subsequently is as follows.

Theorem I: The densities $(\mathbf{j}(\mathbf{r},t), \Delta_{\rm IP}(\mathbf{r},t))$ and $(\mathbf{j}'(\mathbf{r},t), \Delta'_{\rm IP}(\mathbf{r},t))$ which evolve from a common initial state $|\Psi_0\rangle$ under the influence of two sets of potentials $(V(\mathbf{r},t), \mathbf{A}(\mathbf{r},t), D(\mathbf{r},t))$ and $(V'(\mathbf{r},t), \mathbf{A}'(\mathbf{r},t), D'(\mathbf{r},t))$, differing by more than a gauge transformation with $\lambda(\mathbf{r},t_0) = 0$, are always different, provided the potentials can be expanded in Taylor series around the initial time t_0.

Since we are working with gauge-invariant densities, the proof of the theorem can be carried out in a particular gauge where the scalar potentials vanish. We indicate the potentials in this gauge by a tilde. Thus we have to show that

$$(0, \tilde{\mathbf{A}}(\mathbf{r},t), \tilde{D}(\mathbf{r},t)) \neq (0, \tilde{\mathbf{A}}'(\mathbf{r},t), \tilde{D}'(\mathbf{r},t)) \quad (8)$$

implies

$$(\mathbf{j}(\mathbf{r},t), \Delta_{\rm IP}(\mathbf{r},t)) \neq (\mathbf{j}'(\mathbf{r},t), \Delta'_{\rm IP}(\mathbf{r},t)). \quad (9)$$

If $\tilde{\mathbf{A}}(\mathbf{r},t_0) \neq \tilde{\mathbf{A}}'(\mathbf{r},t_0)$, then the statement of the theorem is trivially true since $\mathbf{j}(\mathbf{r},t_0) \neq \mathbf{j}'(\mathbf{r},t_0)$. Otherwise, following Runge and Gross [17], we observe that the potentials in Eq. (8) are different if their Taylor coefficients are not the same. Thus

$$(\partial^k/\partial t^k)[\tilde{\mathbf{A}}(\mathbf{r},t) - \tilde{\mathbf{A}}'(\mathbf{r},t)]|_{t=t_0} \begin{cases} = 0, & k < l \\ \neq 0, & 1 \leq k = l \end{cases} \quad (10)$$

and

$$(\partial^k/\partial t^k)[\tilde{D}(\mathbf{r},t) - \tilde{D}'(\mathbf{r},t)]|_{t=t_0} \begin{cases} = 0, & k < m \\ \neq 0, & 0 \leq k = m \end{cases} \quad (11)$$

must be satisfied with suitable integers l and m. If $l < \infty$, m may be infinite; if $m < \infty$, l may be infinite, i.e., it is sufficient that either the vector or the pair potentials are different. If (10) and (11) are satisfied with $m \geq l$, we calculate the lth time derivative of the current densities $\mathbf{j}(\mathbf{r},t)$ and $\mathbf{j}'(\mathbf{r},t)$ by applying the Heisenberg equation of motion l times. Taking the difference at the initial time t_0, we obtain with the help of Eqs. (10) and (11)

$$\left(i\frac{\partial}{\partial t}\right)^l [\mathbf{j}(\mathbf{r},t) - \mathbf{j}'(\mathbf{r},t)]|_{t=t_0} = \frac{e}{mc} n(\mathbf{r},t_0) \left(i\frac{\partial}{\partial t}\right)^l [\tilde{\mathbf{A}}(\mathbf{r},t) - \tilde{\mathbf{A}}'(\mathbf{r},t)]|_{t=t_0} \neq 0, \quad (12)$$

where $n(\mathbf{r},t_0)$ is the particle density at t_0. If (10) and (11) are satisfied with $m < l$, the same procedure applied to the anomalous densities $\Delta_{\rm IP}(\mathbf{r},t)$ and $\Delta'_{\rm IP}(\mathbf{r},t)$ results in

$$\left(i\frac{\partial}{\partial t}\right)^{m+1} [\Delta_{\rm IP}(\mathbf{r},t) - \Delta_{\rm IP}'(\mathbf{r},t)]|_{t=t_0} = \langle\Psi_0|\psi_\downarrow^\dagger(\mathbf{r},t_0)\psi_\downarrow(\mathbf{r},t_0) - \psi_\uparrow(\mathbf{r},t_0)\psi_\uparrow^\dagger(\mathbf{r},t_0)|\Psi_0\rangle \left(i\frac{\partial}{\partial t}\right)^m \times [\tilde{D}(\mathbf{r},t) - \tilde{D}'(\mathbf{r},t)]|_{t=t_0} \neq 0. \quad (13)$$

The prefactor of the mth time derivative can be expressed by the particle density and the Dirac δ function and is equal to $n(\mathbf{r},t) - \delta(0) \neq 0$. The occurrence of $\delta(0)$ is the usual consequence of assuming a local pair potential [28]. For the present purpose it is sufficient that the prefactor is nonzero in the distributional sense. As a consequence of Eqs. (12) and (13), the set of densities $(\mathbf{j}(\mathbf{r},t), \Delta_{\rm IP}(\mathbf{r},t))$ will differ from the set of densities $(\mathbf{j}'(\mathbf{r},t), \Delta'_{\rm IP}(\mathbf{r},t))$ at times infinitesimally later than t_0. Hence they are different. This proves Theorem I, i.e., in a given gauge, the potentials are unique functionals $V[\mathbf{j}, \Delta_{\rm IP}]$, $\mathbf{A}[\mathbf{j}, \Delta_{IP}]$, and $D[\mathbf{j}, \Delta_{\rm IP}]$ of the densities.

By virtue of the mapping (6), the field operators are functionals of the potentials $V(\mathbf{r},t)$, $\mathbf{A}(\mathbf{r},t)$, and $D(\mathbf{r},t)$. As a consequence of Theorem I they can, alternatively, be considered as functionals of the densities, too. Thus all observable quantities represented by the expectation values with respect to $|\Psi_0\rangle$ of gauge-invariant operators $\hat{O}(\mathbf{r},t)$ are unique functionals of the densities, $\langle\hat{O}(\mathbf{r},t)\rangle \equiv O[\mathbf{j}, \Delta_{\rm IP}](\mathbf{r},t)$. In particular, the particle density $n[\mathbf{j}, \Delta_{\rm IP}](\mathbf{r},t)$ is a unique functional.

On the basis of Theorem I we now derive a variational principle. To this end we consider the quantum mechanical action

$$Q \equiv \int_{t_0}^{t_1} dt \left\langle \frac{1}{2} \int d^3r \left\{ \psi_\sigma^\dagger(\mathbf{r},t) \left(i\frac{\partial}{\partial t} \psi_\sigma(\mathbf{r},t) \right) - \left(i\frac{\partial}{\partial t} \psi_\sigma^\dagger(\mathbf{r},t) \right) \psi_\sigma(\mathbf{r},t) \right\} - \hat{H}_{V_0,\mathbf{A}_0,D_0}(t) \right\rangle, \quad (14)$$

where V_0, $\mathbf{A}_0$, and D_0 are *given* potentials characterizing the time-dependent system at hand. V_0, $\mathbf{A}_0$, and D_0 are to be distinguished from the potentials $V[\mathbf{j}, \Delta_{\rm IP}]$, $\mathbf{A}[\mathbf{j}, \Delta_{\rm IP}]$, and $D[\mathbf{j}, \Delta_{\rm IP}]$, corresponding, by Theorem I, to an arbitrary pair of densities $(\mathbf{j}, \Delta_{\rm IP})$. With these preliminaries the variational principle can be stated as follows.

Theorem II: The action Q can be written as a unique functional $Q_{V_0,\mathbf{A}_0,D_0}[\mathbf{j}, \Delta_{\rm IP}]$ of the densities $\mathbf{j}$ and $\Delta_{\rm IP}$. In terms of the potentials $V[\mathbf{j}, \Delta_{\rm IP}]$, $\mathbf{A}[\mathbf{j}, \Delta_{\rm IP}]$, $D[\mathbf{j}, \Delta_{\rm IP}]$, and the density $n[\mathbf{j}, \Delta_{\rm IP}]$, the action functional is

$$Q_{V_0,\mathbf{A}_0,D_0}[\mathbf{j}, \Delta_{\rm IP}] = B[\mathbf{j}, \Delta_{\rm IP}] - P_{V_0,\mathbf{A}_0}[\mathbf{j}, \Delta_{\rm IP}] + \int_{t_0}^{t_1} dt \int d^3r \, [D_0(\mathbf{r},t) e^{2i\int_{t_0}^{t} dt' V_0(r,t')} \Delta_{\rm IP}^*(\mathbf{r},t) + \text{c.c.}], \quad (15)$$

with

$$P_{V_0,\mathbf{A}_0}[\mathbf{j},\Delta_{\rm IP}] \equiv \int_{t_0}^{t_1} dt \int d^3r \Big\{ \Big(V_0(\mathbf{r},t) + \frac{e^2}{2mc^2}\mathbf{A}_0^2(\mathbf{r},t)\Big) n[\mathbf{j},\Delta_{\rm IP}](\mathbf{r},t) + \frac{e}{c}\mathbf{A}_0(\mathbf{r},t)\cdot\Big(\mathbf{j}(r,t) - \frac{e}{mc} n[\mathbf{j},\Delta_{\rm IP}](\mathbf{r},t)\mathbf{A}[\mathbf{j},\Delta_{\rm IP}](\mathbf{r},t)\Big)\Big\}, \tag{16}$$

where the gauge has been chosen such that $V[\mathbf{j},\Delta_{\rm IP}](\mathbf{r},t)$ equals the given scalar potential $V_0(\mathbf{r},t)$. $B[\mathbf{j},\Delta_{\rm IP}]$ is a *universal* functional depending only on the interaction $\hat{W}$ but not on the external potentials V_0, $\mathbf{A}_0$, and D_0 of the particular system considered. $Q_{V_0,\mathbf{A}_0,D_0}[\mathbf{j},\Delta_{\rm IP}]$ is stationary for the actual densities $\mathbf{j}^0$ and $\Delta_{\rm IP}^0$, corresponding to the given potentials V_0, $\mathbf{A}_0$, and D_0, i.e., the actual densities can be computed from the Euler-Lagrange equations

$$\frac{\delta Q_{V_0,\mathbf{A}_0,D_0}[\mathbf{j},\Delta_{\rm IP}]}{\delta \mathbf{j}(\mathbf{r},t)}\bigg|_{j^0,\Delta_{\rm IP}^0} = 0, \quad \frac{\delta Q_{V_0,\mathbf{A}_0,D_0}[\mathbf{j},\Delta_{\rm IP}]}{\delta \Delta_{\rm IP}^*(\mathbf{r},t)}\bigg|_{j^0,\Delta_{\rm IP}^0} = 0. \tag{17}$$

The proof of the theorem, not reproduced here, follows the reasoning of Runge and Gross [17], with the universal functional $B[\mathbf{j},\Delta_{\rm IP}]$ defined as

$$B[\mathbf{j},\Delta_{\rm IP}] \equiv R[\mathbf{j},\Delta_{\rm IP}] - \int_{t_0}^{t_1} dt \,\langle \hat{W}[\mathbf{j},\Delta_{\rm IP}](t)\rangle \tag{18}$$

with

$$R[\mathbf{j},\Delta_{\rm IP}] \equiv \frac{1}{2}\int_{t_0}^{t_1} dt \int d^3r \,\langle \psi_\sigma^\dagger[\mathbf{j},\Delta_{\rm IP}]\Big(i\frac{\partial}{\partial t} - \frac{\hat{\mathbf{p}}^2}{2m}\Big)\psi_\sigma[\mathbf{j},\Delta_{\rm IP}]\rangle + \text{c.c.} \tag{19}$$

As usual in density-functional theory a particularly useful consequence of the variational Theorem II is the possibility of computing the densities of the interacting system as densities of a noninteracting system with appropriate single-particle potentials. This is stated by the following Kohn-Sham-like theorem.

Theorem III: There exist unique functionals $V_s[\mathbf{j},\Delta_{\rm IP}]$, $\mathbf{A}_s[\mathbf{j},\Delta_{\rm IP}]$, and $D_s[\mathbf{j},\Delta_{\rm IP}]$ such that the densities

$$\mathbf{j}(\mathbf{r},t) = \sum_n \Big[\frac{1}{mi} v_n(\mathbf{r},t)\nabla v_n^*(\mathbf{r},t) + \text{c.c.}\Big] + \frac{e}{mc}\mathbf{A}_{s,0}(\mathbf{r},t)\sum_n 2 v_n(\mathbf{r},t) v_n^*(\mathbf{r},t) \tag{20}$$

and

$$\Delta_{\rm IP}(\mathbf{r},t) = \sum_n u_n(\mathbf{r},t) v_n^*(\mathbf{r},t) e^{2i\int_{t_0}^{t} dt' V_{s,0}(r,t')}, \tag{21}$$

resulting from the solutions $u_n(\mathbf{r},t)$ and $v_n(\mathbf{r},t)$ of the time-dependent single-particle equations

$$i\frac{\partial}{\partial t}\begin{pmatrix} u_n(\mathbf{r},t) \\ v_n(\mathbf{r},t)\end{pmatrix} = \begin{pmatrix} \frac{1}{2m}[\hat{\mathbf{p}} + \frac{e}{c}\mathbf{A}_{s,0}(\mathbf{r},t)]^2 + V_{s,0}(\mathbf{r},t) & D_{s,0}(\mathbf{r},t) \\ D_{s,0}^*(\mathbf{r},t) & -\frac{1}{2m}[\hat{\mathbf{p}} - \frac{e}{c}\mathbf{A}_{s,0}(\mathbf{r},t)]^2 - V_{s,0}(\mathbf{r},t)\end{pmatrix}\begin{pmatrix} u_n(\mathbf{r},t) \\ v_n(\mathbf{r},t)\end{pmatrix}, \tag{22}$$

are identical with the densities $\mathbf{j}^0$ and $\Delta_{\rm IP}^0$ of the interacting system at $T = 0$ K. Here, $V_{s,0}$, $\mathbf{A}_{s,0}$, $D_{s,0}$ is a shorthand for $V_s[\mathbf{j}^0,\Delta_{\rm IP}^0]$, $\mathbf{A}_s[\mathbf{j}^0,\Delta_{\rm IP}^0]$, and $D_s[\mathbf{j}^0,\Delta_{\rm IP}^0]$, respectively.

In order to prove this theorem, we first consider a system of noninteracting particles ($\hat{W} = 0$) moving in external potentials $V_s(\mathbf{r},t)$, $\mathbf{A}_s(r,t)$, and $D_s(\mathbf{r},t)$. The action functional of this noninteracting system is given by

$$Q^s_{V_s,\mathbf{A}_s,D_s}[\mathbf{j},\Delta_{\rm IP}] = R^s[\mathbf{j},\Delta_{\rm IP}] - P^s_{V_s,\mathbf{A}_s}[\mathbf{j},\Delta_{\rm IP}] + \int_{t_0}^{t_1} dt \int d^3r \,[D_s(\mathbf{r},t)e^{2i\int_{t_0}^{t} dt' V_s(r,t')}\Delta_{\rm IP}^*(\mathbf{r},t) + \text{c.c.}], \tag{23}$$

where $R^s[\mathbf{j},\Delta_{\rm IP}]$ and $P^s_{V_s,\mathbf{A}_s}[\mathbf{j},\Delta_{\rm IP}]$ are the noninteracting analogs of the functionals (19) and (16). Theorem II is valid for any given particle-particle interaction $\hat{W}$, in particular also for the special case $\hat{W} \equiv 0$, i.e., for noninteracting particles. As a consequence, the potentials $V_{s,0}$, $\mathbf{A}_{s,0}$, and $D_{s,0}$ which reproduce the densities $\mathbf{j}^0$ and $\Delta_{\rm IP}^0$ of the interacting system must satisfy

$$\frac{\delta Q^s_{V_{s,0},\mathbf{A}_{s,0},D_{s,0}}[\mathbf{j},\Delta_{\rm IP}]}{\delta \mathbf{j}(\mathbf{r},t)}\bigg|_{j^0,\Delta_{\rm IP}^0} = 0, \quad \frac{\delta Q^s_{V_{s,0},\mathbf{A}_{s,0},D_{s,0}}[\mathbf{j},\Delta_{\rm IP}]}{\delta \Delta_{\rm IP}^*(\mathbf{r},t)}\bigg|_{j^0,\Delta_{\rm IP}^0} = 0. \tag{24}$$

Equations (23) and (24) are valid in any gauge. To make contact with the interacting functional (15) we now fix the gauge such that $V_{s,0} = V_0$. Defining a *universal* exchange-correlation functional by

$$Q_{xc}[\mathbf{j}, \Delta_{\mathrm{IP}}] \equiv R^s[\mathbf{j}, \Delta_{\mathrm{IP}}] - B[\mathbf{j}, \Delta_{\mathrm{IP}}] + \int_{t_0}^{t_1} dt \int d^3r\, \Delta_{\mathrm{IP}}(\mathbf{r}, t) w_g(\mathbf{r}) \Delta^*_{\mathrm{IP}}(\mathbf{r}, t), \tag{25}$$

the action functional (15) of the interacting system can be written as

$$Q_{V_0,\mathbf{A}_0,D_0}[\mathbf{j}, \Delta_{\mathrm{IP}}] \equiv R^s[\mathbf{j}, \Delta_{\mathrm{IP}}] - P_{V_0,\mathbf{A}_0}[\mathbf{j}, \Delta_{\mathrm{IP}}] - Q_{xc}[\mathbf{j}, \Delta_{\mathrm{IP}}]$$
$$+ \int_{t_0}^{t_1} dt \int d^3r\, \{[D_0(\mathbf{r}, t) e^{2i \int_{t_0}^{t} dt' V_0(r,t')} \Delta^*_{\mathrm{IP}}(\mathbf{r}, t) + \text{c.c.}] + \Delta_{\mathrm{IP}}(\mathbf{r}, t) w_g(r) \Delta^*_{\mathrm{IP}}(\mathbf{r}, t)\}. \tag{26}$$

The explicit form of $\mathbf{A}_{s,0}$ and $D_{s,0}$ is then determined by equating the variational equations (17) of the interacting system with those of the noninteracting system (24). By virtue of Eq. (26) one obtains

$$\frac{\delta P^s_{V_0,\mathbf{A}_{s,0}}[\mathbf{j}, \Delta_{\mathrm{IP}}]}{\delta \mathbf{j}(\mathbf{r}, t)}\bigg|_{j^0,\Delta^0_{\mathrm{IP}}} = \frac{\delta P_{V_0,\mathbf{A}_0}[\mathbf{j}, \Delta_{\mathrm{IP}}]}{\delta \mathbf{j}(\mathbf{r}, t)}\bigg|_{j^0,\Delta^0_{\mathrm{IP}}} + \frac{\delta Q_{xc}[\mathbf{j}, \Delta_{\mathrm{IP}}]}{\delta \mathbf{j}(\mathbf{r}, t)}\bigg|_{j^0,\Delta^0_{\mathrm{IP}}}, \tag{27}$$

$$D_{s,0}(\mathbf{r}, t) e^{2i \int_{t_0}^{t} dt' V_0(\mathbf{r},t')} - \frac{\delta P^s_{V_0,\mathbf{A}_{s,0}}[\mathbf{j}, \Delta_{\mathrm{IP}}]}{\delta \Delta^*_{\mathrm{IP}}(\mathbf{r}, t)}\bigg|_{j^0,\Delta^0_{\mathrm{IP}}} = w_g(\mathbf{r})\, \Delta^0_{\mathrm{IP}}(\mathbf{r}, t) + D_0(\mathbf{r}, t) e^{2i \int_{t_0}^{t} dt' V_0(r,t')}$$
$$- \frac{\delta P_{V_0,\mathbf{A}_0}[\mathbf{j}, \Delta_{\mathrm{IP}}]}{\delta \Delta^*_{\mathrm{IP}}(\mathbf{r}, t)}\bigg|_{j^0,\Delta^0_{\mathrm{IP}}} - \frac{\delta Q_{xc}[\mathbf{j}, \Delta_{\mathrm{IP}}]}{\delta \Delta^*_{\mathrm{IP}}(\mathbf{r}, t)}\bigg|_{j^0,\Delta^0_{\mathrm{IP}}}. \tag{28}$$

Equations (27) and (28) are integral equations defining the potentials $\mathbf{A}_{s,0}$ and $D_{s,0}$. Together with Eq. (22) they constitute the time-dependent Bogoliubov–de Gennes Kohn-Sham scheme. The structure of the whole set of equations is evidently quite involved. However, one point should be emphasized: The mere fact that Eq. (22) can be derived rigorously for strongly correlated systems implies that the dynamic effects observed in inhomogeneous systems involving high-temperature superconductors can be related to Andreev scattering in a theoretically well founded way.

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