Frequency-dependent Linear Response of Superconducting Systems

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Abstract

We present a density-functional scheme for calculating the frequency-dependent linear response of superconductors. The central result is a set of integral equations determining the linear response of the normal and anomalous densities to external perturbations. Analytic solutions of these integral equations are obtained for homogeneous systems with separable effective interactions. For inhomogeneous superconductors, the formalism leads to a scheme for calculating the critical temperature without explicitly solving the gap equation.

1 Introduction

Many experimental data, such as the photoabsorption spectrum or the frequency-dependent conductivity, can be calculated from the linear response of a system to time-dependent external perturbations. The traditional density functional formalism of Hohenberg, Kohn and Sham [1, 2] is a ground-state theory. In principle, the response functions, being ground-state expectation values of the unperturbed system, are functionals of the ground-state density by virtue of the Hohenberg-Kohn (HK) theorem. However, due to the lack of reliable approximations, the frequency-dependent response is not readily accessible in ordinary (ground-state) density functional theory.

A suitable theoretical framework for the treatment of time-dependent situations is provided by the theory of Runge and Gross [3], which can be viewed as the time-dependent counterpart of the traditional Hohenberg-Kohn-Sham formalism. When applied to the linear-response regime [4, 5, 6], this formalism leads to an exact representation of the linear density response $n_1(\mathbf{r},t)$ in terms of the response function χ_s of the (unperturbed) Kohn-Sham (KS) system:

$$n_1(\mathbf{r},t) = \int\!\mathrm{d}^3r' \int\! dt'\, \chi_s(\mathbf{r},t;\mathbf{r}',t') \Bigg[v_1(\mathbf{r}',t') \; + \\ + \;\; \int\!\mathrm{d}^3r''\, \frac{n_1(\mathbf{r}'',t')}{|\mathbf{r}'-\mathbf{r}''|} + \int\!\mathrm{d}^3r'' \int\! dt''\, f_{xc}(\mathbf{r}',t';\mathbf{r}'',t'')\, n_1(\mathbf{r}'',t'') \Bigg]. \tag{1}$$

$v_1(\mathbf{r},t)$ denotes the *external* perturbation and $f_{xc}(\mathbf{r},t;\mathbf{r}',t')$ is an exchange-correlation (xc) kernel formally defined as the functional derivative of the time-dependent xc potential with respect to the time-dependent density,

$$f_{xc}[n_\circ](\mathbf{r},t;\mathbf{r}',t') = \left. \frac{\delta v_{xc}[n](\mathbf{r},t)}{\delta n(\mathbf{r}',t')} \right|_{n=n_\circ}, \tag{2}$$

to be evaluated at the unperturbed ground-state density $n_\circ$. Given an approximation of f_{xc}, the linear density response n_1 can be obtained from eq. (1) by iteration. This scheme has proven to be remarkably successful. Using either the static local-density approximation (LDA)

$$f_{xc}^{LDA}(\mathbf{r},t;\mathbf{r}',t') = \delta(t-t')\,\delta(\mathbf{r}-\mathbf{r}')\, \left. \frac{dv_{xc}^{LDA}(n)}{dn} \right|_{n=n_\circ(\mathbf{r})} \tag{3}$$

or an approximation of f_{xc} with memory [4, 5, 7], the scheme was applied to the photoresponse of atoms [8, 9, 10] and molecules [11, 12], metallic [13, 14, 15, 16, 17, 18, 19] and semiconductor surfaces [20], bulk semiconductors [21] and metal clusters [22, 23, 24, 25]. For a broad review of applications, the reader is referred to the textbook by Mahan and Subbaswamy [26].

The purpose of this paper is to generalize the above formalism to *superconducting systems at finite temperature.* After a short introduction to the time-independent density functional theory of superconductors in section 2, we shall develop the linear response-formalism in section 3. Subsequently, in section 4, the formalism will be applied to homogeneous superconductors, where the response equations can be solved analytically for a certain class of effective interactions. Finally, in section 5, the formalism is used to derive a scheme for calculating the transition temperature of inhomogeneous superconductors.

2 Density Functional Theory for Superconductors

Before investigating the linear response of superconducting systems to an external perturbation we shall, in this section, briefly review the density-functional description [27, 28, 29] of the unperturbed superconductor, which is decribed by the following Hamiltonian:

$$\begin{aligned}\hat{H} &= \sum_{\sigma=\uparrow\downarrow}\int \mathrm{d}^3r\,\hat{\psi}^\dagger_\sigma(\mathbf{r})\left(-\frac{\nabla^2}{2}+v(\mathbf{r})-\mu\right)\hat{\psi}_\sigma(\mathbf{r})+\hat{U}+\hat{W}\\ &- \int \mathrm{d}^3r\int \mathrm{d}^3r'\left(D^*(\mathbf{r},\mathbf{r}')\hat{\psi}_\uparrow(\mathbf{r})\hat{\psi}_\downarrow(\mathbf{r}')+D(\mathbf{r},\mathbf{r}')\hat{\psi}^\dagger_\downarrow(\mathbf{r}')\hat{\psi}^\dagger_\uparrow(\mathbf{r})\right). \qquad (4)\end{aligned}$$

Atomic (Hartree) units are used throughout. $\hat{U}$ is the mutual Coulomb repulsion of the electrons,

$$\hat{U}=\frac{1}{2}\sum_{\sigma\sigma'}\int \mathrm{d}^3r\int \mathrm{d}^3r'\,\hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}^\dagger_{\sigma'}(\mathbf{r}')\frac{1}{|\mathbf{r}-\mathbf{r}'|}\hat{\psi}_{\sigma'}(\mathbf{r}')\hat{\psi}_\sigma(\mathbf{r}), \qquad (5)$$

and $\hat{W}$ is a phonon-induced electron-electron interaction

$$\hat{W}=-\frac{1}{2}\sum_{\sigma,\sigma'}\int \mathrm{d}^3r\int \mathrm{d}^3r'\int \mathrm{d}^3x\int \mathrm{d}^3x'\,\hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}^\dagger_{\sigma'}(\mathbf{r}')w(\mathbf{r},\mathbf{r}';\mathbf{x},\mathbf{x}')\hat{\psi}_{\sigma'}(\mathbf{x})\hat{\psi}_\sigma(\mathbf{x}'). \qquad (6)$$

$v(\mathbf{r})$ is the Coulomb potential of the periodic lattice and $D(\mathbf{r},\mathbf{r}')$ is a nonlocal pairing field, which can be interpreted as being induced through the proximity effect.

Starting from this Hamiltonian, Oliveira, Gross and Kohn (OGK) [27] developed a density-functional formalism describing superconductors at finite temperature. The basic variables in this formalism are the normal density

$$n(\mathbf{r})=\sum_\sigma\langle\hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r})\rangle \qquad (7)$$

and the anomalous density

$$\Delta(\mathbf{r},\mathbf{r}')=\langle\hat{\psi}_\uparrow(\mathbf{r})\hat{\psi}_\downarrow(\mathbf{r}')\rangle \qquad (8)$$

which, in the appropriate limits, reduces to the Ginzburg-Landau order parameter. Following Mermin's [30] finite-temperature extension of ordinary density-functional theory, OGK established a 1-1 mapping between the pair of equilibrium densities $\{n(\mathbf{r}),\Delta(\mathbf{r},\mathbf{r}')\}$ and the pair of potentials $\{v(\mathbf{r})-\mu, D(\mathbf{r},\mathbf{r}')\}$. The grand-canonical potential is then a unique functional of the densities

$$\Omega[n,\Delta]=F[n,\Delta]+\int \mathrm{d}^3r\,v(\mathbf{r})\,n(\mathbf{r})+\int \mathrm{d}^3r\int \mathrm{d}^3r'\left(D^*(\mathbf{r},\mathbf{r}')\Delta(\mathbf{r},\mathbf{r}')+c.c.\right) \qquad (9)$$

where $F[n,\Delta]$ is a free-energy functional which depends only on the interactions $\hat{U}$ and $\hat{W}$, but not on the particular external potentials of the system considered. As a consequence of the Gibbs variational principle, the exact equilibrium densities minimize the grand-canonical potential (9). This fact can be exploited to establish a KS theorem for superconductors which ensures that the densities $n(\mathbf{r})$ and $\Delta(\mathbf{r},\mathbf{r}')$ of the interacting system can be calculated from the following single-particle equations:

$$\begin{aligned}
\left(-\frac{\nabla^2}{2}+v_s(\mathbf{r})-\mu\right)u_k(\mathbf{r})+\int\!\mathrm{d}^3r'\,D_s(\mathbf{r},\mathbf{r}')\,v_k(\mathbf{r}') &= E_k u_k(\mathbf{r}), &(10)\\
-\left(-\frac{\nabla^2}{2}+v_s(\mathbf{r})-\mu\right)v_k(\mathbf{r})+\int\!\mathrm{d}^3r'\,D_s^*(\mathbf{r},\mathbf{r}')\,u_k(\mathbf{r}') &= E_k v_k(\mathbf{r}). &(11)
\end{aligned}$$

In terms of the particle and hole amplitudes, $u_k(\mathbf{r})$ and $v_k(\mathbf{r})$, the densities are given by

$$\begin{aligned}
n(\mathbf{r}) &= 2\sum_k\Big(|u_k(\mathbf{r})|^2 f_\beta(E_k)+|v_k(r)|^2 f_\beta(-E_k)\Big) &(12)\\
\Delta(\mathbf{r},\mathbf{r}') &= \sum_k\left(v_k^*(\mathbf{r}')u_k(\mathbf{r})f_\beta(-E_k)-v_k^*(\mathbf{r})u_k(\mathbf{r}')f_\beta(E_k)\right) &(13)
\end{aligned}$$

where

$$f_\beta(E)=\frac{1}{1+e^{\beta E}} \qquad (14)$$

is the Fermi distribution function. Eqs. (10) and (11) have the same algebraic structure as the conventional Bogoliubov - de Gennes equations. However, in contrast to the latter, the effective potentials, given by

$$\begin{aligned}
v_s(\mathbf{r}) &= v(\mathbf{r})+\int\!\mathrm{d}^3r'\frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}+v_{xc}^\beta[n,\Delta](\mathbf{r}) &(15)\\
D_s(\mathbf{r},\mathbf{r}') &= D(\mathbf{r},\mathbf{r}')+\int\!\mathrm{d}^3x\int\!\mathrm{d}^3x'\,w(\mathbf{r},\mathbf{r}';\mathbf{x},\mathbf{x}')\,\Delta(\mathbf{x},\mathbf{x}')\\
&\quad +D_{xc}^\beta[n,\Delta](\mathbf{r},\mathbf{r}') &(16)
\end{aligned}$$

contain the xc contributions

$$\begin{aligned}
v_{xc}^\beta[n,\Delta](\mathbf{r}) &= \frac{\delta F_{xc}^\beta[n,\Delta]}{\delta n(\mathbf{r})}, &(17)\\
D_{xc}^\beta[n,\Delta](\mathbf{r},\mathbf{r}') &= -\frac{\delta F_{xc}^\beta[n,\Delta]}{\delta\Delta^*(\mathbf{r},\mathbf{r}')}, &(18)
\end{aligned}$$

which, in principle, include all superconducting correlations exactly. The exchange-correlation functional $F_{xc}^\beta[n,\Delta]$ is formally defined by

$$\begin{aligned}
F[n,\Delta] = T_s[n,\Delta]-\frac{1}{\beta}S_s[n,\Delta]+\frac{1}{2}\int\!\mathrm{d}^3r\int\!\mathrm{d}^3r'\,\frac{n(\mathbf{r})\,n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\\
-\int\!\mathrm{d}^3r\int\!\mathrm{d}^3r'\int\!\mathrm{d}^3x\int\!\mathrm{d}^3x'\,\Delta^*(\mathbf{r},\mathbf{r}')w(\mathbf{r},\mathbf{r}';\mathbf{x},\mathbf{x}')\Delta(\mathbf{x},\mathbf{x}')+F_{xc}^\beta[n,\Delta], \quad (19)
\end{aligned}$$

where T_s and S_s are the kinetic-energy and entropy functionals of the non interacting system. Equations (10) - (18) define the self-consistent KS scheme for superconductors. In practice, of course, the xc functional $F^{\beta}_{xc}[n, \Delta]$ has to be approximated. Most recently an LDA-type approximation has become available [28, 31].

3 Linear Response Formalism

The Hamiltonian (1) of the unperturbed system contains three real-valued external potentials: $v(\mathbf{r})$, $\mathrm{Re}[D(\mathbf{r}, \mathbf{r}')]$ and $\mathrm{Im}[D(\mathbf{r}, \mathbf{r}')]$. In the present context, however, it is more convenient to work, instead, with $v(\mathbf{r})$, $D(\mathbf{r}, \mathbf{r}')$ and $D^*(\mathbf{r}, \mathbf{r}')$, which couple to the following conjugate density operators:

$$\begin{array}{llll} v(\mathbf{r}) & : & \hat{n}(\mathbf{r}) & := \sum_\sigma \hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r}), \\ D^*(\mathbf{r}, \mathbf{r}') & : & \hat{\Delta}(\mathbf{r}, \mathbf{r}') & := \hat{\psi}_\uparrow(\mathbf{r})\hat{\psi}_\downarrow(\mathbf{r}'), \\ D(\mathbf{r}, \mathbf{r}') & : & \hat{\Delta}^\dagger(\mathbf{r}, \mathbf{r}') & := \hat{\psi}^\dagger_\downarrow(\mathbf{r}')\hat{\psi}^\dagger_\uparrow(\mathbf{r}). \end{array} \tag{20}$$

Since a perturbation added to any of these potentials can affect all three densities, we have to define nine response functions. The linear response of the normal density, for instance, is given by

$$\begin{aligned} n_1(\mathbf{r}; t) &= \int d^3x \int dt' \, \chi(\mathbf{r}, \mathbf{x}; t - t') \, v_1(\mathbf{x}; t') \\ &+ \int d^3x \int d^3x' \int dt' \Lambda^*(\mathbf{r}, \mathbf{x}, \mathbf{x}'; t - t') \, D_1(\mathbf{x}, \mathbf{x}'; t') \\ &+ \int d^3x \int d^3x' \int dt' \Lambda(\mathbf{r}, \mathbf{x}, \mathbf{x}'; t - t') \, D_1^*(\mathbf{x}, \mathbf{x}'; t'), \end{aligned} \tag{21}$$

where v_1 and D_1 are external time-dependent perturbations.

From now on we will use a formal operator notation where the symbol of each response function is to be interpreted as an integral operator such as the ones on the right hand side of eq. (21). With this convention the full system of response equations reads:

$$\begin{array}{lllll} n_1 & = \chi v_1 & + \Lambda^* D_1 & + \Lambda D_1^*, \\ \Delta_1 & = \Gamma v_1 & + \Xi D_1 & + \tilde{\Xi} D_1^*, \\ \Delta_1^* & = \Gamma^* v_1 & + \tilde{\Xi}^* D_1 & + \Xi^* D_1^*. \end{array} \tag{22}$$

To further simplify the notation we introduce a vector of density responses and a vector of external perturbations:

$$\vec{n}_1 := \begin{pmatrix} n_1 \\ \Delta_1 \\ \Delta_1^* \end{pmatrix}, \qquad \vec{v}_1 := \begin{pmatrix} v_1 \\ D_1 \\ D_1^* \end{pmatrix}. \tag{23}$$

With these conventions, the response equations can be written as

$$\vec{n}_1 = \hat{\chi}\vec{v}_1, \tag{24}$$

where $\hat{\chi}$ represents the 3×3 matrix

$$\hat{\chi} := \begin{pmatrix} \chi & \Lambda^* & \Lambda \\ \Gamma & \Xi & \tilde{\Xi} \\ \Gamma^* & \tilde{\Xi}^* & \Xi^* \end{pmatrix}. \tag{25}$$

The response functions are given by:

$$\chi(\mathbf{r}, \mathbf{x}; t - t') = -i\Big\langle \left[\hat{n}_H(\mathbf{r}, t), \hat{n}_H(\mathbf{x}, t')\right] \Big\rangle, \tag{26}$$

$$\Lambda(\mathbf{r}, \mathbf{x}, \mathbf{x}'; t - t') = -i\Big\langle \left[\hat{n}_H(\mathbf{r}, t), \hat{\Delta}_H(\mathbf{x}, \mathbf{x}', t')\right] \Big\rangle, \tag{27}$$

$$\Gamma(\mathbf{r}, \mathbf{r}', \mathbf{x}; t - t') = -i\Big\langle \left[\hat{\Delta}_H(\mathbf{r}, \mathbf{r}'; t), \hat{n}_H(\mathbf{x}; t')\right] \Big\rangle, \tag{28}$$

$$\Xi(\mathbf{r}, \mathbf{r}', \mathbf{x}, \mathbf{x}'; t - t') = -i\Big\langle \left[\hat{\Delta}_H(\mathbf{r}, \mathbf{r}'; t), \hat{\Delta}^\dagger_H(\mathbf{x}, \mathbf{x}'; t')\right] \Big\rangle, \tag{29}$$

$$\tilde{\Xi}(\mathbf{r}, \mathbf{r}', \mathbf{x}, \mathbf{x}'; t - t') = -i\Big\langle \left[\hat{\Delta}_H(\mathbf{r}, \mathbf{r}'; t), \hat{\Delta}_H(\mathbf{x}, \mathbf{x}'; t')\right] \Big\rangle, \tag{30}$$

where the index H denotes operators in the real-time Heisenberg picture.

The unperturbed superconducting system is assumed to be in thermal equilibrium, i.e. $\langle \cdots \rangle$ denotes a grand canonical ensemble average over the eigenstates of the full interacting Hamiltonian (1). The full response functions (26) - (30) of the interacting system are very hard to calculate. On the other hand, the corresponding response functions $\hat{\chi}_s$ of the (non-interacting) Kohn-Sham system are easily expressed in terms of the particle and hole amplitudes, $u_k(\mathbf{r})$ and $v_k(\mathbf{r})$, respectively. Explicit expressions for the nine KS response functions are given in the appendix.

We now define a 3×3 matrix of xc kernels $\hat{f}_{xc}$ by the Dyson-type equation

$$\hat{\chi} = \hat{\chi}_s + \hat{\chi}_s \left(\hat{w} + \hat{f}_{xc}\right) \hat{\chi}, \tag{31}$$

where $\hat{w}$ is given by

$$\hat{w} = \begin{pmatrix} u & 0 & 0 \\ 0 & w & 0 \\ 0 & 0 & w^* \end{pmatrix}. \tag{32}$$

u and w are shorthand notations for the bare Coulomb interaction and the phonon-induced interaction. Inserting (31) in the response equation (24), one obtains

$$\boxed{\vec{n}_1 = \hat{\chi}_s \left(\vec{v}_1 + (\hat{w} + \hat{f}_{xc})\vec{n}_1\right).} \tag{33}$$

Given an approximation for the xc kernels $\hat{f}_{xc}$, eq. (33) can be solved numerically by iteration. If the unperturbed system is homogeneous, eq. (33) can, under certain conditions, be solved analytically, as will be shown in the next section.

In the case of static perturbations, the Hohenberg-Kohn-Sham formalism developed in section 2 implies that the xc kernels can be written as functional derivatives,

$$\hat{f}_{xc} = \left(\begin{array}{ccc} \frac{\delta v_{xc}}{\delta n} & \frac{\delta v_{xc}}{\delta \Delta} & \frac{\delta v_{xc}}{\delta \Delta^*} \\ \frac{\delta D_{xc}}{\delta n} & \frac{\delta D_{xc}}{\delta \Delta} & \frac{\delta D_{xc}}{\delta \Delta^*} \\ \frac{\delta D^*_{xc}}{\delta n} & \frac{\delta D^*_{xc}}{\delta \Delta} & \frac{\delta D^*_{xc}}{\delta \Delta^*} \end{array} \right) \Bigg|_{n_\circ, \Delta_\circ, \Delta^*_\circ} , \tag{34}$$

to be evaluated at the unperturbed equilibrium densities $n_\circ$, $\Delta_\circ$ and $\Delta^*_\circ$. For eq. (34) to be valid in the case of time-dependent perturbations, a time-dependent extension of the density functional theory for superconductors is required. In particular a Runge-Gross theorem [3], ensuring the fundamental 1-1 correspondence between time-dependent densities and potentials, has to be established for superconductors. A theorem of this kind was recently proposed by Wacker, Kümmel and Gross [32]. However, the densities used in that work are different from the ones employed in the response formalism developed here. At present, eq. (34) is to be regarded as a postulate in the time-dependent case.

Eq. (33) can be viewed as the superconducting version of the density-functional formulation of linear response theory described in the introduction. In view of the great success this method has had for normal systems, we expect eq. (33) to be a very efficient tool for calculating the linear response of superconductors. As a first shot, the xc kernel $\hat{f}_{xc}$ can be approximated by eq. (34) using the static LDA-type xc potentials derived in [28, 31].

4 Homogeneous system

In this section we will consider a case where eq. (33) can be solved analytically, namely homogeneous superconductors with a model effective interaction $\hat{R} = \hat{w} + \hat{f}_{xc}$ which is assumed separable.

To keep the formulas readable we will present detailed calculations only for the RPA-limit, i.e. for $\hat{f}_{xc} \equiv 0$. Generalizations are given without explicit calculations.

In homogeneous systems a Fourier transformation to momentum space greatly facilitates the calculation. The Fourier transforms of the response functions and the interactions are defined as follows:

$$\chi_s(\mathbf{r};\mathbf{x};\omega) = \int \frac{\mathrm{d}^3k}{(2\pi)^3} \int \frac{\mathrm{d}^3q}{(2\pi)^3} \, e^{i\mathbf{kr}} e^{-i\mathbf{qx}} \, \chi_s(\mathbf{k};\mathbf{q};\omega), \tag{35}$$

$$
\begin{aligned}
\Lambda_s(\mathbf{r};\mathbf{x},\mathbf{x}';\omega) &= \int\frac{\mathrm{d}^3k}{(2\pi)^3}\int\frac{\mathrm{d}^3q}{(2\pi)^3}\int\frac{\mathrm{d}^3q'}{(2\pi)^3}\,e^{i\mathbf{kr}}e^{-i\mathbf{qx}}\times\\
&\quad\times e^{-i\mathbf{q}'\mathbf{x}'}\,\Lambda_s(\mathbf{k};\mathbf{q},\mathbf{q}';\omega), \qquad (36)\\
\Xi_s(\mathbf{r},\mathbf{r}';\mathbf{x},\mathbf{x}';\omega) &= \int\frac{\mathrm{d}^3k}{(2\pi)^3}\int\frac{\mathrm{d}^3k'}{(2\pi)^3}\int\frac{\mathrm{d}^3q}{(2\pi)^3}\int\frac{\mathrm{d}^3q'}{(2\pi)^3}\,e^{i\mathbf{kr}}e^{i\mathbf{k}'\mathbf{r}'}\times\\
&\quad\times e^{-i\mathbf{qx}}e^{-i\mathbf{q}'\mathbf{x}'}\,\Xi_s(\mathbf{k},\mathbf{k}';\mathbf{q},\mathbf{q}';\omega), \qquad (37)\\
&\vdots
\end{aligned}
$$

$$
\begin{aligned}
w(\mathbf{r},\mathbf{r}';\mathbf{x},\mathbf{x}') &= \int\frac{\mathrm{d}^3k}{(2\pi)^3}\int\frac{\mathrm{d}^3k'}{(2\pi)^3}\int\frac{\mathrm{d}^3q}{(2\pi)^3}\int\frac{\mathrm{d}^3q'}{(2\pi)^3}\,e^{i\mathbf{kr}}e^{i\mathbf{k}'\mathbf{r}'}\times \qquad (38)\\
&\quad\times e^{-i\mathbf{qx}}e^{-i\mathbf{q}'\mathbf{x}'}\,w(\mathbf{k},\mathbf{k}';\mathbf{q},\mathbf{q}'), \qquad (39)\\
u(\mathbf{r};\mathbf{x}) &= \int\frac{\mathrm{d}^3k}{(2\pi)^3}\int\frac{\mathrm{d}^3q}{(2\pi)^3}\,e^{i\mathbf{kr}}e^{-i\mathbf{qx}}u(\mathbf{k};\mathbf{q}). \qquad (40)
\end{aligned}
$$

Using the fact, that

$$
\begin{aligned}
\chi_s(\mathbf{k};\mathbf{q};\omega) &= \frac{(2\pi)^3}{\mathcal{V}}\,\delta(\mathbf{k}-\mathbf{q})\;\chi_s(\mathbf{k};\omega), \qquad (41)\\
\Lambda_s(\mathbf{k};\mathbf{q},\mathbf{q}';\omega) &= \frac{(2\pi)^3}{\mathcal{V}}\,\delta(\mathbf{k}-\mathbf{q}-\mathbf{q}')\;\Lambda_s(\mathbf{q},\mathbf{q}';\omega), \qquad (42)\\
\Gamma_s(\mathbf{k},\mathbf{k}';\mathbf{q};\omega) &= \frac{(2\pi)^3}{\mathcal{V}}\,\delta(\mathbf{k}+\mathbf{k}'-\mathbf{q})\;\Gamma_s(\mathbf{k},\mathbf{k}';\omega), \qquad (43)\\
\Xi_s(\mathbf{k},\mathbf{k}';\mathbf{q},\mathbf{q}';\omega) &= \frac{(2\pi)^3}{\mathcal{V}}\,\delta(\mathbf{k}-\mathbf{q})\;\frac{(2\pi)^3}{\mathcal{V}}\,\delta(\mathbf{k}'-\mathbf{q}')\;\Xi_s(\mathbf{k},\mathbf{k}';\omega), \qquad (44)\\
&\vdots
\end{aligned}
$$

and

$$
\begin{aligned}
u(\mathbf{k};\mathbf{q}) &= \frac{(2\pi)^3}{\mathcal{V}}\,\delta(\mathbf{k}-\mathbf{q})\;u(\mathbf{k}), \qquad (45)\\
w(\mathbf{k},\mathbf{k}';\mathbf{q},\mathbf{q}') &= \frac{(2\pi)^3}{\mathcal{V}}\,\delta(\mathbf{k}+\mathbf{k}'-\mathbf{q}-\mathbf{q}')\;V(\mathbf{k},\mathbf{k}';\mathbf{q}'), \qquad (46)
\end{aligned}
$$

with

$$
u(\mathbf{k}) = \frac{4\pi}{\mathbf{k}^2}, \qquad (47)
$$

the response equations (33) take the form:

$$
\begin{aligned}
& n_1(\mathbf{k};\omega) = n_1^{\circ}(\mathbf{k};\omega) \qquad (48)\\
&\quad+\;\chi_s(\mathbf{k};\omega)\,u(\mathbf{k})\,n_1(\mathbf{k};\omega)\\
&\quad+\;\int\frac{\mathrm{d}^3q}{(2\pi)^3}\int\frac{\mathrm{d}^3b}{(2\pi)^3}\,\Lambda_s^*(-\mathbf{q},\mathbf{q}-\mathbf{k};-\omega)\,V(\mathbf{q},\mathbf{k}-\mathbf{q};\mathbf{b})\,\Delta_1(\mathbf{b},\mathbf{k}-\mathbf{b};\omega)
\end{aligned}
$$

$$+ \int\frac{\mathrm{d}^3q}{(2\pi)^3}\int\frac{\mathrm{d}^3b}{(2\pi)^3}\,\Lambda_s(\mathbf{q},\mathbf{k}-\mathbf{q};\omega)\,V^*(-\mathbf{q},\mathbf{q}-\mathbf{k};-\mathbf{b})\,\Delta_1^*(-\mathbf{b},\mathbf{b}-\mathbf{k};-\omega),$$

$$\begin{aligned}\Delta_1(\mathbf{k},\mathbf{k}';\omega) &= \Delta_1^\circ(\mathbf{k},\mathbf{k}';\omega)\\ &+ \Gamma_s(\mathbf{k},\mathbf{k}';\omega)\,u(\mathbf{k}+\mathbf{k}')\,n_1(\mathbf{k}+\mathbf{k}';\omega)\\ &+ \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,\Xi_s(\mathbf{k},\mathbf{k}';\omega)\,V(\mathbf{k},\mathbf{k}';\mathbf{b})\,\Delta_1(\mathbf{b},\mathbf{k}+\mathbf{k}'-\mathbf{b};\omega)\\ &+ \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,\tilde{\Xi}_s(\mathbf{k},\mathbf{k}';\omega)\,V^*(-\mathbf{k},-\mathbf{k}';-\mathbf{b})\,\Delta_1^*(-\mathbf{b},\mathbf{b}-\mathbf{k}-\mathbf{k}';-\omega),\end{aligned} \tag{49}$$

$$\begin{aligned}\Delta_1^*(-\mathbf{k},-\mathbf{k}';-\omega) &= \Delta_1^{*\circ}(-\mathbf{k},-\mathbf{k}';-\omega)\\ &+ \Gamma_s^*(-\mathbf{k},-\mathbf{k}';-\omega)\,u(\mathbf{k}+\mathbf{k}')\,n_1(\mathbf{k}+\mathbf{k}';\omega)\\ &+ \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,\tilde{\Xi}_s^*(-\mathbf{k},-\mathbf{k}';-\omega)\,V(\mathbf{k},\mathbf{k}';\mathbf{b})\,\Delta_1(\mathbf{b},\mathbf{k}+\mathbf{k}'-\mathbf{b};-\omega)\\ &+ \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,\Xi_s^*(-\mathbf{k},-\mathbf{k}';-\omega)\,V^*(-\mathbf{k},-\mathbf{k}';-\mathbf{b})\,\Delta_1^*(-\mathbf{b},\mathbf{b}-\mathbf{k}-\mathbf{k}';-\omega).\end{aligned} \tag{50}$$

n_1°, Δ_1° and $\Delta_1^{*\circ}$ are the density responses of the non-interacting system:

$$\begin{aligned}n_1^\circ(\mathbf{k};\omega) &= \chi_s(\mathbf{k};\omega)\,v_1(\mathbf{k};\omega)\\ &+ \int\frac{\mathrm{d}^3q}{(2\pi)^3}\,\Lambda_s^*(-\mathbf{q},\mathbf{q}-\mathbf{k};-\omega)\,D_1(\mathbf{q},\mathbf{k}-\mathbf{q};\omega)\\ &+ \int\frac{\mathrm{d}^3q}{(2\pi)^3}\,\Lambda_s(\mathbf{q},\mathbf{k}-\mathbf{q};\omega)\,D_1^*(-\mathbf{q},\mathbf{q}-\mathbf{k};-\omega), \qquad (51)\\ \Delta_1^\circ(\mathbf{k},\mathbf{k}';\omega) &= \Gamma_s(\mathbf{k},\mathbf{k}';\omega)\,v_1(\mathbf{k}+\mathbf{k}';\omega)\\ &+ \Xi_s(\mathbf{k},\mathbf{k}';\omega)\,D_1(\mathbf{k},\mathbf{k}';\omega)\\ &+ \tilde{\Xi}_s(\mathbf{k},\mathbf{k}';\omega)\,D_1^*(-\mathbf{k},-\mathbf{k}';-\omega), \qquad (52)\\ \Delta_1^{*\circ}(-\mathbf{k},-\mathbf{k}';-\omega) &= \Gamma_s^*(-\mathbf{k},-\mathbf{k}';-\omega)\,D_1(\mathbf{k},\mathbf{k}';\omega)\\ &+ \tilde{\Xi}_s^*(\mathbf{k},-\mathbf{k}';-\omega)\,D_1(\mathbf{k},\mathbf{k}';\omega)\\ &+ \Xi_s^*(-\mathbf{k},-\mathbf{k};-\omega)\,D_1^*(-\mathbf{k},-\mathbf{k}';-\omega). \qquad (53)\end{aligned}$$

We now consider systems with a separable phonon-induced interaction, i.e.

$$V(\mathbf{k},\mathbf{k}';\mathbf{q}) = V\,g(\mathbf{k},\mathbf{k}')\,h(\mathbf{k}+\mathbf{k}';\mathbf{q}), \tag{54}$$

where the functions $g(\mathbf{k},\mathbf{k}')$ and $h(\mathbf{k};\mathbf{q})$ are arbitrary. A prominent example is the traditional BCS interaction [33],

$$V_{BCS}(\mathbf{k},\mathbf{k}';\mathbf{q}) = V_\circ\,\Theta(\omega_D-|\frac{\mathbf{k}^2}{2}-\mu|)\,\Theta(\omega_D-|\frac{\mathbf{k}'^2}{2}-\mu|)\,\delta_{\mathbf{k}+\mathbf{k}',0}, \tag{55}$$

where ω_D is the Debye-frequency. With interactions of the form (54) the response equations (48)-(50) can be written as:

$$\begin{aligned} n_1(\mathbf{k};\omega) = n_1^\circ(\mathbf{k};\omega) \;&+\; \chi_s(\mathbf{k};\omega)\,u(\mathbf{k})\,n_1(\mathbf{k};\omega) \\ &+\; V\,\hat{\Lambda}^\dagger(\mathbf{k};\omega)\,z(\mathbf{k};\omega) \\ &+\; V^*\,\hat{\Lambda}(\mathbf{k};\omega)\,z^\dagger(\mathbf{k};\omega), \end{aligned} \tag{56}$$

$$\begin{aligned} z(\mathbf{k};\omega) = z^\circ(\mathbf{k};\omega) \;&+\; \hat{\Gamma}(\mathbf{k};\omega)\,u(\mathbf{k})\,n_1(\mathbf{k};\omega) \\ &+\; V\,\hat{\Xi}(\mathbf{k};\omega)\,z(\mathbf{k};\omega) \\ &+\; V^*\,\hat{\hat{\Xi}}(\mathbf{k};\omega)\,z^\dagger(\mathbf{k};\omega), \end{aligned} \tag{57}$$

$$\begin{aligned} z^\dagger(\mathbf{k};\omega) = z^{\dagger\circ}(\mathbf{k};\omega) \;&+\; \hat{\Gamma}^\dagger(\mathbf{k};\omega)\,u(\mathbf{k})\,n_1(\mathbf{k};\omega) \\ &+\; V\,\hat{\hat{\Xi}}^\dagger(\mathbf{k};\omega)\,z(\mathbf{k};\omega) \\ &+\; V^*\,\hat{\Xi}^\dagger(\mathbf{k};\omega)\,z^\dagger(\mathbf{k};\omega), \end{aligned} \tag{58}$$

where the following definitions have been used:

$$z(\mathbf{k};\omega) \;=\; \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,h(\mathbf{k};\mathbf{b})\,\Delta_1(\mathbf{b},\mathbf{k}-\mathbf{b};\omega), \tag{59}$$

$$z^\dagger(\mathbf{k};\omega) \;=\; \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,h^*(-\mathbf{k};-\mathbf{b})\,\Delta_1^*(-\mathbf{b},\mathbf{b}-\mathbf{k};-\omega) \tag{60}$$

$$\hat{\Gamma}(\mathbf{k};\omega) \;:=\; \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,h(\mathbf{k};\mathbf{b})\,\Gamma_s(\mathbf{b},\mathbf{k}-\mathbf{b};\omega), \tag{61}$$

$$\hat{\Gamma}^\dagger(\mathbf{k};\omega) \;:=\; \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,h^*(-\mathbf{k};-\mathbf{b})\,\Gamma_s^*(-\mathbf{b},\mathbf{b}-\mathbf{k};-\omega), \tag{62}$$

$$\hat{\Lambda}(\mathbf{k};\omega) \;:=\; \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,\Lambda_s(\mathbf{b},\mathbf{k}-\mathbf{b};\omega)\,g^*(-\mathbf{b},\mathbf{b}-\mathbf{k}), \tag{63}$$

$$\hat{\Lambda}^\dagger(\mathbf{k};\omega) \;:=\; \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,\Lambda_s^*(-\mathbf{b},\mathbf{b}-\mathbf{k};-\omega)\,g(\mathbf{b},\mathbf{k}-\mathbf{b}), \tag{64}$$

$$\hat{\Xi}(\mathbf{k};\omega) \;:=\; \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,h(\mathbf{k};\mathbf{b})\,\Xi_s(\mathbf{b},\mathbf{k}-\mathbf{b};\omega)\,g(\mathbf{b},\mathbf{k}-\mathbf{b}), \tag{65}$$

$$\hat{\Xi}^\dagger(\mathbf{k};\omega) \;:=\; \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,h^*(-\mathbf{k};-\mathbf{b})\,\Xi_s^*(-\mathbf{b},\mathbf{b}-\mathbf{k};-\omega)\,g^*(-\mathbf{b},\mathbf{b}-\mathbf{k}). \tag{66}$$

Omitting the momentum and frequency variables, eqs. (56)-(58) can be written in matrix notation:

$$\underbrace{\begin{pmatrix} n_1 \\ z \\ z^\dagger \end{pmatrix}}_{=:\vec{z}_1} = \underbrace{\begin{pmatrix} n_1^\circ \\ z^\circ \\ z^{\dagger\circ} \end{pmatrix}}_{=:\vec{z}_1^\circ} + \underbrace{\begin{pmatrix} u\chi_s & V\hat{\Lambda}^\dagger & V\hat{\Lambda} \\ u\hat{\Gamma} & V\hat{\Xi} & V\hat{\hat{\Xi}} \\ u\hat{\Gamma}^\dagger & V^*\hat{\hat{\Xi}}^\dagger & V^*\hat{\Xi}^\dagger \end{pmatrix}}_{=:\hat{X}} \begin{pmatrix} n_1 \\ z \\ z^\dagger \end{pmatrix} \tag{67}$$

or simply

$$\vec{z}_1 = \vec{z}_1^\circ + \hat{X}\vec{z}_1. \tag{68}$$

This equation can be solved for $\vec{z}_1$ by inversion of $(\hat{1} - \hat{X})$:

$$\vec{z}_1 = \underbrace{(\hat{1} - \hat{X})^{-1}}_{=:\hat{M}} \vec{z}_1^\circ. \tag{69}$$

Inserting this result back into the response equations (56)-(58) and collecting those terms which contain the external perturbation v_1 and give a contribution to the change of the normal density n_1 we can identify the density-density response function of the interacting system as

$$\chi^{RPA}(\mathbf{k};\omega) = M_{11}(\mathbf{k};\omega)\chi_s(\mathbf{k};\omega) + M_{12}(\mathbf{k};\omega)\hat{\Gamma}(\mathbf{k};\omega) + M_{13}(\mathbf{k};\omega)\hat{\Gamma}^\dagger(\mathbf{k};\omega). \tag{70}$$

This result can be generalized in two ways. First we will go beyond the RPA by explicitly taking into account the matrix $\hat{f}_{xc}$. Since $\hat{f}_{xc}$ is not diagonal, each of the eqs. (48), (49), (50) gains six additional terms. Similar to the ansatz (54) we will now consider systems where the effective interaction $\hat{R} = \hat{w} + \hat{f}_{xc}$ is separable, i.e. the elements of the matrix

$$\hat{R} = \begin{pmatrix} R_{vn} & R_{v\Delta} & R_{v\Delta^*} \\ R_{Dn} & R_{D\Delta} & R_{D\Delta^*} \\ R_{D^*n} & R_{D^*\Delta} & R_{D^*\Delta^*} \end{pmatrix} \tag{71}$$

are assumed to have the form:

$$\begin{aligned} R_{vn}(\mathbf{k},\mathbf{q};\omega) &= (2\pi)^3\,\delta(\mathbf{k}-\mathbf{q})\,R_{vn}(\mathbf{k};\omega), & (72)\\ R_{v\Delta}(\mathbf{k};\mathbf{q},\mathbf{q}';\omega) &= (2\pi)^3\,\delta(\mathbf{k}-\mathbf{q}-\mathbf{q}')\,R_{v\Delta}(\mathbf{q},\mathbf{q}';\omega), & (73)\\ R_{Dn}(\mathbf{k},\mathbf{k}';\mathbf{q};\omega) &= (2\pi)^3\,\delta(\mathbf{k}+\mathbf{k}'-\mathbf{q})\,\tilde{R}_{Dn}(\mathbf{k},\mathbf{k}';\omega), & (74)\\ R_{D\Delta}(\mathbf{k},\mathbf{k}';\mathbf{q},\mathbf{q}';\omega) &= (2\pi)^3\,\delta(\mathbf{k}+\mathbf{k}'-\mathbf{q}-\mathbf{q}')\times \\ &\quad \tilde{R}_{D\Delta}(\mathbf{k},\mathbf{k}';\omega)\,R_{D\Delta}(\mathbf{q},\mathbf{k}+\mathbf{k}'-\mathbf{q};\omega). & (75) \end{aligned}$$

With this effective interaction the calculation can be carried out in analogy to the RPA case. Defining

$$z_\alpha(\mathbf{k};\omega) := \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,R_{\alpha\Delta}(\mathbf{b},\mathbf{k}-\mathbf{b};\omega)\,\Delta_1(\mathbf{b},\mathbf{k}-\mathbf{b};\omega) \tag{76}$$

$$z_\alpha^\dagger(\mathbf{k};\omega) := \int\frac{\mathrm{d}^3b}{(2\pi)^3}\,R_{\alpha\Delta^*}(\mathbf{b},\mathbf{k}-\mathbf{b};\omega)\,\Delta_1^*(-\mathbf{b},\mathbf{b}-\mathbf{k};-\omega) \tag{77}$$

where $\alpha = \{v, D, D^*\}$, the set of response equations again reduces to a set of linear equations for the $z_\alpha(\mathbf{k};\omega)$, $z^\dagger_\alpha(\mathbf{k};\omega)$ and $n_1(\mathbf{k};\omega)$. This set of linear equations can be written as a 7×7 matrix equation which has to be solved by matrix inversion. The matrix elements are generalized in the same way as the $z(\mathbf{k})$:

$$\hat{X} = \begin{pmatrix} X_\circ & \chi_s & \hat{\Lambda}^\dagger_\Delta & \hat{\Lambda}_\Delta & \chi_s & \hat{\Lambda}^\dagger_{\Delta^*} & \hat{\Lambda}_{\Delta^*} \\ X_v & \hat{\Gamma}_v & \hat{\Xi}_{v\Delta} & \hat{\hat{\Xi}}_{v\Delta} & \hat{\Gamma}_v & \hat{\Xi}_{v\Delta^*} & \hat{\hat{\Xi}}_{v\Delta^*} \\ X_D & \hat{\Gamma}_D & \hat{\Xi}_{D\Delta} & \hat{\hat{\Xi}}_{D\Delta} & \hat{\Gamma}_D & \hat{\Xi}_{D\Delta^*} & \hat{\hat{\Xi}}_{D\Delta^*} \\ X_{D^*} & \hat{\Gamma}_{D^*} & \hat{\Xi}_{D^*\Delta} & \hat{\hat{\Xi}}_{D^*\Delta} & \hat{\Gamma}_{D^*} & \hat{\Xi}_{D^*\Delta^*} & \hat{\hat{\Xi}}_{D^*\Delta^*} \\ X^\dagger_v & \hat{\Gamma}^\dagger_v & \hat{\Xi}^\dagger_{v\Delta} & \hat{\hat{\Xi}}^\dagger_{v\Delta} & \hat{\Gamma}^\dagger_v & \hat{\Xi}^\dagger_{v\Delta^*} & \hat{\hat{\Xi}}^\dagger_{v\Delta^*} \\ X^\dagger_D & \hat{\Gamma}^\dagger_D & \hat{\Xi}^\dagger_{D\Delta} & \hat{\hat{\Xi}}^\dagger_{D\Delta} & \hat{\Gamma}^\dagger_D & \hat{\Xi}^\dagger_{D\Delta^*} & \hat{\hat{\Xi}}^\dagger_{D\Delta^*} \\ X^\dagger_{D^*} & \hat{\Gamma}^\dagger_{D^*} & \hat{\Xi}^\dagger_{D^*\Delta} & \hat{\hat{\Xi}}^\dagger_{D^*\Delta} & \hat{\Gamma}^\dagger_{D^*} & \hat{\Xi}^\dagger_{D^*\Delta^*} & \hat{\hat{\Xi}}^\dagger_{D^*\Delta^*} \end{pmatrix}, \quad \vec{z} = \begin{pmatrix} n_1 \\ z_v \\ z_D \\ z_{D^*} \\ z^\dagger_v \\ z^\dagger_D \\ z^\dagger_{D^*} \end{pmatrix}. \quad (78)$$

The definitions of some representative matrix elements are:

$$\hat{X}_\circ(\mathbf{k};\omega) = \chi_s(\mathbf{k};\omega)\, R_{vn}(\mathbf{k};\omega) + \hat{\Lambda}_n(\mathbf{k};\omega) + \hat{\Lambda}^\dagger_n(\mathbf{k};\omega) \quad (79)$$

$$\hat{\Lambda}^\dagger_\beta(\mathbf{k};\omega) = \int\frac{\mathrm{d}^3q}{(2\pi)^3}\, \Lambda^*_s(-\mathbf{q},\mathbf{q}-\mathbf{k};-\omega)\, \tilde{R}_{D\beta}(\mathbf{q},\mathbf{k}-\mathbf{q};\omega) \quad (80)$$

$$\hat{\Lambda}_\beta(\mathbf{k};\omega) = \int\frac{\mathrm{d}^3q}{(2\pi)^3}\, \Lambda_s(\mathbf{q},\mathbf{k}-\mathbf{q};\omega)\, \tilde{R}_{D^*\beta}(\mathbf{q},\mathbf{k}-\mathbf{q};\omega) \quad (81)$$

$$X_\alpha(\mathbf{k};\omega) = \hat{\Gamma}_\alpha(\mathbf{k};\omega)R_{vn}(\mathbf{k};\omega) + \hat{\Xi}_{\alpha n}(\mathbf{k};\omega) + \hat{\hat{\Xi}}_{\alpha n}(\mathbf{k};\omega) \quad (82)$$

$$\hat{\Gamma}_\alpha(\mathbf{k};\omega) = \int\frac{\mathrm{d}^3q}{(2\pi)^3}\, R_{\alpha\Delta}(\mathbf{q},\mathbf{k}-\mathbf{q};\omega)\Gamma_s(\mathbf{q},\mathbf{k}-\mathbf{q};\omega) \quad (83)$$

$$\hat{\Xi}_{\alpha\beta}(\mathbf{k};\omega) = \int\frac{\mathrm{d}^3q}{(2\pi)^3}\, R_{\alpha\Delta}(\mathbf{q},\mathbf{k}-\mathbf{q};\omega)\, \Xi_s(\mathbf{q},\mathbf{k}-\mathbf{q};\omega)\, \tilde{R}_{D\beta}(\mathbf{q},\mathbf{k}-\mathbf{q};\omega) \quad (84)$$

where $\alpha = \{v, D, D^*\}$ and $\beta = \{n, \Delta, \Delta^*\}$. The result for the density-density response function is again obtained by applying $\hat{M} = (1-\hat{X})^{-1}$ to $\vec{z}^\circ$:

$$\begin{aligned} \chi(\mathbf{k};\omega) &= M_{11}(\mathbf{k};\omega)\chi_s(\mathbf{k};\omega) + M_{12}(\mathbf{k};\omega)\hat{\Gamma}_v(\mathbf{k};\omega) + M_{13}(\mathbf{k};\omega)\hat{\Gamma}_D(\mathbf{k};\omega) \\ &+ M_{14}(\mathbf{k};\omega)\hat{\Gamma}_{D^*}(\mathbf{k};\omega) + M_{15}(\mathbf{k};\omega)\hat{\Gamma}^\dagger_v(\mathbf{k};\omega) + M_{16}(\mathbf{k};\omega)\hat{\Gamma}^\dagger_D(\mathbf{k};\omega) \\ &+ M_{17}(\mathbf{k};\omega)\hat{\Gamma}^\dagger_{D^*}(\mathbf{k};\omega) \end{aligned} \quad (85)$$

A further generalization is to allow effective interactions which are given by a finite sum over separable terms:

$$\begin{aligned} R_{D\Delta}(\mathbf{k},\mathbf{k}';\mathbf{q},\mathbf{q};\omega) &= (2\pi)^3\delta(\mathbf{k}+\mathbf{k}'-\mathbf{q}-\mathbf{q}') \times \\ &\sum_{i=1}^{N} \tilde{R}^i_{D\Delta}(\mathbf{k},\mathbf{k}';\omega)\, R^i_{D\Delta}(\mathbf{q},\mathbf{k}+\mathbf{k}'-\mathbf{q};\omega). \end{aligned} \quad (86)$$

The calculation is analogous to the one presented above, but all quantities have to be supplemented by the index i of the corresponding part of the interaction. This leads to a $7N\times 7N$ matrix equation which has to be solved by inversion.

5 Determination of the critical temperature

As a possible application of the above formalism we now present a method of calculating the critical temperature of superconductors without explicitly solving the gap equation. For this purpose we consider the system to be in the normal phase, i.e. $T > T_c$ and thus $D(\mathbf{r}, \mathbf{r}') \equiv 0$. If the system is now cooled slowly below T_c an infinitesimal pairing field $D_{ext}(\mathbf{r}, \mathbf{r}')$ will immediately take the system into the superconducting phase. In other words, the response of the system in the *normal* phase to an external pairing field must diverge for temperatures below T_c.

In the normal phase the off-diagonal elements of the KS response matrix vanish, i.e.

$$\hat{\chi}_s^{D=0} = \begin{pmatrix} \chi_s & 0 & 0 \\ 0 & \Xi_s & 0 \\ 0 & 0 & \Xi_s^* \end{pmatrix}. \tag{87}$$

To simplify the discussion we will restrict ourselves to the RPA in this section, i.e. we set $\hat{f}_{xc} \equiv 0$. Since the matrix $\hat{w}$ is diagonal too, the set of response equations (33) decouples into one equation per density. The equation of interest is

$$\begin{aligned} \Delta_1(\mathbf{r}, \mathbf{r}') &= \Delta_1^\circ(\mathbf{r}, \mathbf{r}') \\ &+ \int d^3x \int d^3x' \int d^3y \int d^3y' \, \Xi_s(\mathbf{r}, \mathbf{r}'; \mathbf{x}, \mathbf{x}'; \omega = 0) \, w(\mathbf{x}, \mathbf{x}'; \mathbf{y}, \mathbf{y}') \, \Delta_1(\mathbf{y}, \mathbf{y}'). \end{aligned} \tag{88}$$

The anomalous density can be expanded in the Bloch orbitals of the unperturbed periodic system:

$$\Delta(\mathbf{r}, \mathbf{r}') = \sum_{kk'} \Delta(k, k') \varphi_k(\mathbf{r}) \varphi_{k'}(\mathbf{r}'). \tag{89}$$

The indices k, q denote the complete set of quantum numbers for the system. The response function (see appendix) has the form:

$$\Xi_s^\circ(\mathbf{r}, \mathbf{r}', \mathbf{x}, \mathbf{x}', \omega) = \sum_{kq} \frac{(1 - f_\beta(E_k) - f_\beta(E_q))}{\omega + (E_k + E_q) + i0^+} \varphi_k(\mathbf{r}) \varphi_q(\mathbf{r}') \varphi_k^*(\mathbf{x}) \varphi_q^*(\mathbf{x}') \tag{90}$$

$$=: \sum_{kq} \Xi(k, q) \, \varphi_k(\mathbf{r}) \varphi_q(\mathbf{r}') \varphi_k^*(\mathbf{x}) \varphi_q^*(\mathbf{x}'). \tag{91}$$

With the phonon-induced interaction transformed as

$$w(\mathbf{r}, \mathbf{r}'; \mathbf{x}, \mathbf{x}') = \sum_{kk'qq'} w(k, k'; q, q') \, \varphi_k(\mathbf{r}) \, \varphi_{k'}(\mathbf{r}') \, \varphi_q^*(\mathbf{x}) \, \varphi_{q'}^*(\mathbf{x}') \tag{92}$$

equation (88) reads:

$$\Delta_1(k, k') = \Delta_1^\circ(k, k') + \Xi(k, k'; \omega = 0) \sum_{q,q'} w(k, k'; q, q') \, \Delta_1(q, q') \tag{93}$$

where the orthonormality of the Bloch-functions $\varphi_k(\mathbf{r})$ has been used.

In the vicinity of the critical temperature, the matrix $\Delta_1(k,k')$ is dominated [34] by the elements with $k+k'=0$, i.e. we can approximately set

$$\Delta_1(k,k') = \Delta_1(k)\,\delta_{k+k',0}. \tag{94}$$

Insertion of (94) in (93) then leads to

$$\Delta_1(k) = \Delta_1^\circ(k) + \Xi(k,-k)\sum_q w(k,-k,q,-q)\Delta_1(q). \tag{95}$$

Assuming a separable interaction of the form

$$w(k,k',q,q') = \sum_{i=1}^{N} V_i\, g_i(k,k')\, h_i(q,q') \tag{96}$$

equation (95) can be solved by defining the quantities

$$z_i := \sum_{i=1}^{N} h_i(q,-q)\,\Delta_1(q). \tag{97}$$

which satisfy the following set of linear equations:

$$z_i = z_i^\circ + \sum_q h_i(q,-q)\,\Xi(q,-q)\sum_{j=1}^{N} V_j g_j(q,-q)\, z_j(q) \tag{98}$$

with

$$z_i^\circ = \sum_q h_i(q,-q)\,\Xi(q,-q)\,D_1(q). \tag{99}$$

This set of equations can be rewritten in matrix form:

$$\underline{z} = \underline{z}^\circ + \underline{\underline{Y}}\,\underline{z}, \tag{100}$$

where the matrix $\underline{\underline{Y}}$ is defined by

$$Y_{ij} = V_j\sum_q h_i(q,-q)\,\Xi(q,-q)\,g_j(q,-q). \tag{101}$$

$\underline{z}$ is obtained by inverting $(\underline{\underline{1}}-\underline{\underline{Y}})$:

$$\underline{z} = (\underline{\underline{1}}-\underline{\underline{Y}})^{-1}\,\underline{z}^\circ. \tag{102}$$

Inserting this in eq. (95) one ends up with

$$\begin{aligned}\Delta_1(k) &= \Xi(k,-k)\,D_1(k) \qquad (103)\\ &+ \Xi(k,-k)\sum_{i=1}^{N} V_i g_i(k,-k)\sum_{j=1}^{N}\left((\underline{\underline{1}}-\underline{\underline{Y}})^{-1}\right)_{ij}\sum_q h_j(q,-q)\,\Xi(q,-q)\,D_1(q)\end{aligned}$$

and the response function in RPA is readily identified as:

$$\begin{aligned} \Xi^{RPA}(k,q) &= \Xi(k,-k)\,\delta_{k,q} \\ &+ \Xi(k,-k) \sum_{i,j=1}^{N} V_i g_i(k,-k) \left((\underline{\underline{1}} - \underline{\underline{Y}})^{-1} \right)_{ij} \sum_q h_j(q,-q)\,\Xi(q,-q). \end{aligned} \tag{104}$$

Since the response function of the non-interacting system has no singularities as a function of temperature, Ξ^{RPA} diverges when the matrix $(\underline{\underline{1}} - \underline{\underline{Y}})$ is not invertible. Thus the equation to determine the critical temperature is:

$$\boxed{\det(\,\underline{\underline{1}} - \underline{\underline{Y}}\,) = 0 \qquad \Longrightarrow \qquad T = T_c} \tag{105}$$

As a test for this formalism we apply it to the BCS interaction, as obtained by insertion of eq. (55) in eq. (46),

$$w_{BCS}(k,k';q,q') = V_\circ\,\Theta(\omega_D - |\epsilon_k - \mu|)\,\Theta(\omega_D - |\epsilon_{k'} - \mu|)\,\delta_{k+k',0}\,\delta_{k+k',q+q'}. \tag{106}$$

In this case eq.(105) reduces to the scalar equation

$$1 - \Xi = 0 \tag{107}$$

with

$$\Xi = \sum_{\mathbf{q}} V_\circ \frac{1}{2} \frac{\tanh(\frac{\beta_c}{2} E_{\mathbf{q}})}{E_{\mathbf{q}}}\,\Theta(\omega_D - |\epsilon_{\mathbf{q}} - \mu|) \qquad \text{and} \qquad E_q = \epsilon_q - \mu. \tag{108}$$

This is exactly the BCS equation for T_c:

$$1 = V_\circ \sum_{\substack{k \\ |\epsilon_k - \mu| < w_D}} \frac{1}{2} \frac{\tanh(\frac{\beta_c}{2} E_k)}{E_k}. \tag{109}$$

Appendix

In order to calculate the response functions of the Kohn-Sham system we first define the spectral densities $S_{AB}(\omega)$ by

$$S_{AB}(\omega) = \int d(t-t') e^{i\omega(t-t')} \left\langle [\hat{A}(t)_H, \hat{B}(t')_H] \right\rangle_S \tag{A 1}$$

where $\langle \cdots \rangle_S$ denotes a grand canonical ensemble average over the eigenstates of the (non-interacting) Kohn-Sham system (10)-(18). In terms of these spectral densities, the KS response functions can be written as

$$\chi_s(\mathbf{r},\mathbf{x};\omega) = \lim_{\delta\to 0^+}\int d\omega' \,\frac{S_{nn}(\mathbf{r},\mathbf{x};\omega')}{\omega-\omega'+i\delta} \tag{A 2}$$

$$\Lambda_s(\mathbf{r},\mathbf{x},\mathbf{x}';\omega) = \lim_{\delta\to 0^+}\int d\omega' \,\frac{S_{n\Delta}(\mathbf{r},\mathbf{x},\mathbf{x}';\omega')}{\omega-\omega'+i\delta} \tag{A 3}$$

$$\Lambda_s^*(\mathbf{r},\mathbf{x},\mathbf{x}';-\omega) = \lim_{\delta\to 0^+}\int d\omega' \,\frac{S_{n\Delta^\dagger}(\mathbf{r},\mathbf{x},\mathbf{x}';\omega')}{\omega-\omega'+i\delta} \tag{A 4}$$

$$\Gamma_s(\mathbf{r},\mathbf{r}',\mathbf{x};\omega) = \lim_{\delta\to 0^+}\int d\omega' \,\frac{S_{\Delta n}(\mathbf{r},\mathbf{r}',\mathbf{x};\omega')}{\omega-\omega'+i\delta} \tag{A 5}$$

$$\Gamma_s^*(\mathbf{r},\mathbf{r}',\mathbf{x},-\omega) = \lim_{\delta\to 0^+}\int d\omega' \,\frac{S_{\Delta^\dagger n}(\mathbf{r},\mathbf{r}',\mathbf{x};\omega')}{\omega-\omega'+i\delta} \tag{A 6}$$

$$\Xi_s(\mathbf{r},\mathbf{r}',\mathbf{x},\mathbf{x}';\omega) = \lim_{\delta\to 0^+}\int d\omega' \,\frac{S_{\Delta\Delta^\dagger}(\mathbf{r},\mathbf{r}',\mathbf{x},\mathbf{x}';\omega')}{\omega-\omega'+i\delta} \tag{A 7}$$

$$\tilde{\Xi}_s(\mathbf{r},\mathbf{r}',\mathbf{x},\mathbf{x}';\omega) = \lim_{\delta\to 0^+}\int d\omega' \,\frac{S_{\Delta\Delta}(\mathbf{r},\mathbf{r}',\mathbf{x},\mathbf{x}';\omega')}{\omega-\omega'+i\delta} \tag{A 8}$$

$$\Xi_s^*(\mathbf{r},\mathbf{r}',\mathbf{x},\mathbf{x}';-\omega) = \lim_{\delta\to 0^+}\int d\omega' \,\frac{S_{\Delta^\dagger\Delta}(\mathbf{r},\mathbf{r}',\mathbf{x},\mathbf{x}';\omega')}{\omega-\omega'+i\delta} \tag{A 9}$$

$$\tilde{\Xi}_s^*(\mathbf{r},\mathbf{r}',\mathbf{x},\mathbf{x}';-\omega) = \lim_{\delta\to 0^+}\int d\omega' \,\frac{S_{\Delta^\dagger\Delta^\dagger}(\mathbf{r},\mathbf{r}',\mathbf{x},\mathbf{x}';\omega')}{\omega-\omega'+i\delta} \tag{A 10}$$

The spectral densities, in turn, are calculated by substituting the Bogoliubov-Valatin transformation [35]

$$\hat{\psi}_\uparrow(\mathbf{r}) = \sum_k (u_k(\mathbf{r})\hat{\gamma}_{k\uparrow} - v_k^*(\mathbf{r})\hat{\gamma}_{k\downarrow}^\dagger) \tag{A 11}$$

$$\hat{\psi}_\downarrow(\mathbf{r}) = \sum_k (u_k(\mathbf{r})\hat{\gamma}_{k\downarrow} + v_k^*(\mathbf{r})\hat{\gamma}_{k\uparrow}^\dagger) \tag{A 12}$$

for the field operators $\hat{\psi}_\sigma(\mathbf{r})$ appearing in the density operators (20). Hence one is left with matrix elements involving four quasi-particle operators $\hat{\gamma}_{k\sigma}$. Employing the fermionic anticommutation relations of these operators one obtains after a lengthy but straightforward calculation

$$
\begin{aligned}
&S_{n,n}(\mathbf{r},\mathbf{x},\omega) = \\
&\sum_{k,q}\Big\{\Big(f(E_k)+f(E_q)-1\Big)\times \\
&\qquad\Big[\ \delta\Big(\omega-(E_k+E_q)\Big)\Big(u_k^*(\mathbf{r})v_q^*(\mathbf{r})+u_q^*(\mathbf{r})v_k^*(\mathbf{r})\Big) \\
&\qquad\qquad\times\Big(u_k(\mathbf{x})v_q(\mathbf{x})+u_q(\mathbf{x})v_k(\mathbf{x})\Big) \\
&\qquad-\delta\Big(\omega+(E_k+E_q)\Big)\Big(u_k(\mathbf{r})v_q(\mathbf{r})+u_q(\mathbf{r})v_k(\mathbf{r})\Big) \\
&\qquad\qquad\times\Big(u_k^*(\mathbf{x})v_q^*(\mathbf{x})+u_q^*(\mathbf{x})v_k^*(\mathbf{x})\Big)\Big] \\
&+\Big(f(E_k)-f(E_q)\Big)\times \\
&\qquad\Big[\ \delta\Big(\omega-(E_k-E_q)\Big)\Big(v_k^*(\mathbf{r})v_q(\mathbf{r})-u_k^*(\mathbf{r})u_q(\mathbf{r})\Big) \\
&\qquad\qquad\times\Big(v_q^*(\mathbf{x})v_k(\mathbf{x})-u_q^*(\mathbf{x})u_k(\mathbf{x})\Big) \\
&\qquad-\delta\Big(\omega+(E_k-E_q)\Big)\Big(v_k^*(\mathbf{r})v_q(\mathbf{r})-u_k^*(\mathbf{r})u_q(\mathbf{r})\Big) \\
&\qquad\qquad\times\Big(v_q^*(\mathbf{x})v_k(\mathbf{x})-u_q^*(\mathbf{x})u_k(\mathbf{x})\Big)\Big]\Big\} \qquad \text{(A 13)}
\end{aligned}
$$

$$
\begin{aligned}
&S_{n,\Delta}(\mathbf{r},\mathbf{x},\mathbf{x}',\omega) = \\
&\sum_{k,q}\Big\{\Big(f(E_k)+f(E_q)-1\Big)\times \\
&\qquad\Big[\ \delta\Big(\omega-(E_k+E_q)\Big)\Big(u_k^*(\mathbf{r})v_q^*(\mathbf{r})+u_q^*(\mathbf{r})v_k^*(\mathbf{r})\Big)\,u_k(\mathbf{x}')u_q(\mathbf{x}) \\
&\qquad-\delta\Big(\omega+(E_k+E_q)\Big)\Big(u_k(\mathbf{r})v_q(\mathbf{r})+u_q(\mathbf{r})v_k(\mathbf{r})\Big)\,v_k^*(\mathbf{x}')v_q^*(\mathbf{x})\Big] \\
&+\Big(f(E_k)-f(E_q)\Big)\times \\
&\qquad\Big[\ \delta\Big(\omega-(E_k-E_q)\Big)\Big(v_k^*(\mathbf{r})v_q(\mathbf{r})-u_k^*(\mathbf{r})u_q(\mathbf{r})\Big)\,v_q^*(\mathbf{x})u_k(\mathbf{x}') \\
&\qquad-\delta\Big(\omega+(E_k-E_q)\Big)\Big(v_k^*(\mathbf{r})v_q(\mathbf{r})-u_k^*(\mathbf{r})u_q(\mathbf{r})\Big)\,v_q^*(\mathbf{x}')u_k(\mathbf{x})\Big]\Big\} \qquad \text{(A 14)}
\end{aligned}
$$

$$
\begin{aligned}
&S_{n,\Delta^\dagger}(\mathbf{r},\mathbf{x},\mathbf{x}',\omega) = \\
&\sum_{k,q}\Big\{\Big(f(E_k)+f(E_q)-1\Big)\times \\
&\qquad\Big[\ \delta\Big(\omega-(E_k+E_q)\Big)\Big(u_k^*(\mathbf{r})v_q^*(\mathbf{r})+u_q^*(\mathbf{r})v_k^*(\mathbf{r})\Big)\,v_k(\mathbf{x})v_q(\mathbf{x}') \\
&\qquad-\delta\Big(\omega+(E_k+E_q)\Big)\Big(u_k(\mathbf{r})v_q(\mathbf{r})+u_q(\mathbf{r})v_k(\mathbf{r})\Big)\,u_k^*(\mathbf{x})u_q^*(\mathbf{x}') \\
&+\Big(f(E_k)-f(E_q)\Big)\times \\
&\qquad\Big[\ \delta\Big(\omega+(E_k-E_q)\Big)\Big(v_k^*(\mathbf{r})v_q(\mathbf{r})-u_k^*(\mathbf{r})u_q(\mathbf{r})\Big)\,u_q^*(\mathbf{x})v_k(\mathbf{x}') \\
&\qquad+\delta\Big(\omega-(E_k-E_q)\Big)\Big(v_k^*(\mathbf{r})v_q(\mathbf{r})-u_k^*(\mathbf{r})u_q(\mathbf{r})\Big)\,u_q^*(\mathbf{x}')v_k(\mathbf{x})\Big]\Big\}
\end{aligned}
\quad \text{(A 15)}
$$

$$
\begin{aligned}
&S_{\Delta,n}(\mathbf{r},\mathbf{r}',\mathbf{x},\omega) = \\
&\sum_{k,q}\Big\{\Big(f(E_k)+f(E_q)-1\Big)\times \\
&\qquad\Big[\ \delta\Big(\omega-(E_k+E_q)\Big)\,v_k^*(\mathbf{r})v_q^*(\mathbf{r}')\Big(u_k(\mathbf{x})v_q(\mathbf{x})+u_q(\mathbf{x})v_k(\mathbf{x})\Big) \\
&\qquad-\delta\Big(\omega+(E_k+E_q)\Big)\,u_k(\mathbf{r})u_q(\mathbf{r}')\Big(u_k^*(\mathbf{x})v_q^*(\mathbf{x})+u_q^*(\mathbf{x})v_k^*(\mathbf{x})\Big)\Big] \\
&+\Big(f(E_k)-f(E_q)\Big)\times \\
&\qquad\Big[\ \delta\Big(\omega+(E_k-E_q)\Big)\,v_k^*(\mathbf{r}')u_q(\mathbf{r})\Big(v_q^*(\mathbf{x})v_k(\mathbf{x})-u_q^*(\mathbf{x})u_k(\mathbf{x})\Big) \\
&\qquad-\delta\Big(\omega-(E_k-E_q)\Big)\,v_k^*(\mathbf{r})u_q(\mathbf{r}')\Big(v_q^*(\mathbf{x})v_k(\mathbf{x})-u_q^*(\mathbf{x})u_k(\mathbf{x})\Big)\Big]\Big\}
\end{aligned}
\quad \text{(A 16)}
$$

$$
\begin{aligned}
&S_{\Delta^\dagger,n}(\mathbf{r},\mathbf{r}',\mathbf{x},\omega) = \\
&\sum_{k,q}\Big\{\Big(f(E_k)+f(E_q)-1\Big) \\
&\qquad\Big[\ \delta\Big(\omega-(E_k+E_q)\Big)\,u_k^*(\mathbf{r}')u_q^*(\mathbf{r})\Big(u_k(\mathbf{x})v_q(\mathbf{x})+u_q(\mathbf{x})v_k(\mathbf{x})\Big) \\
&\qquad-\delta\Big(\omega+(E_k+E_q)\Big)\,v_k(\mathbf{r}')v_q(\mathbf{r})\Big(u_k^*(\mathbf{x})v_q^*(\mathbf{x})+u_q^*(\mathbf{x})v_k^*(\mathbf{x})\Big)\Big] \\
&-\Big(f(E_k)-f(E_q)\Big)\times \\
&\qquad\Big[\ \delta\Big(\omega-(E_k-E_q)\Big)\,u_k^*(\mathbf{r}')v_q(\mathbf{r})\Big(v_q^*(\mathbf{x})v_k(\mathbf{x})-u_q^*(\mathbf{x})u_k(\mathbf{x}) \\
&\qquad-\delta\Big(\omega+(E_k-E_q)\Big)\,u_k^*(\mathbf{r})v_q(\mathbf{r}')\Big(v_q^*(\mathbf{x})v_k(\mathbf{x})-u_q^*(\mathbf{x})u_k(\mathbf{x})\Big)\Big]\Big\}
\end{aligned}
\quad \text{(A 17)}
$$

$$
\begin{aligned}
&S_{\Delta,\Delta}(\mathbf{r},\mathbf{r}',\mathbf{x},\mathbf{x}',\omega) = \\
&\sum_{k,q}\Big\{\Big(f(E_k)+f(E_q)-1\Big)\times \\
&\qquad\qquad \Big[\ \delta\Big(\omega-(E_k+E_q)\Big)\, v_k^*(\mathbf{r})v_q^*(\mathbf{r}')u_k(\mathbf{x}')u_q(\mathbf{x}) \\
&\qquad\qquad -\delta\Big(\omega+(E_k+E_q)\Big)\, v_k^*(\mathbf{x}')v_q^*(\mathbf{x})u_k(\mathbf{r})u_q(\mathbf{r}')\Big] \\
&+\Big(f(E_k)-f(E_q)\Big)\times \\
&\qquad\qquad \Big[\ \delta\Big(\omega+(E_k-E_q)\Big)\, v_k^*(\mathbf{r}')v_q^*(\mathbf{x}')u_k(\mathbf{x})u_q(\mathbf{r}) \\
&\qquad\qquad -\delta\Big(\omega-(E_k-E_q)\Big)\, v_k^*(\mathbf{r})v_q^*(\mathbf{x})u_k(\mathbf{x}')u_q(\mathbf{r}')\Big]\Big\}
\end{aligned}
\tag{A 18}
$$

$$
\begin{aligned}
&S_{\Delta^\dagger,\Delta^\dagger}(\mathbf{r},\mathbf{r}',\mathbf{x},\mathbf{x}',\omega) = \\
&\sum_{k,q}\Big\{\Big(f(E_k)+f(E_q)-1\Big)\times \\
&\qquad\qquad \Big[\ \delta\Big(\omega-(E_k+E_q)\Big)\, u_k^*(\mathbf{r}')u_q^*(\mathbf{r})v_k(\mathbf{x})v_q(\mathbf{x}') \\
&\qquad\qquad -\delta\Big(\omega+(E_k+E_q))\, u_k^*(\mathbf{x})u_q^*(\mathbf{x}')v_k(\mathbf{r}')v_q(\mathbf{r})\Big] \\
&+\Big(f(E_k)-f(E_q)\Big)\times \\
&\qquad\qquad \Big[\ \delta\Big(\omega+(E_k-E_q)\Big)\, u_k^*(\mathbf{r})u_q^*(\mathbf{x})v_k(\mathbf{x}')v_q(\mathbf{r}') \\
&\qquad\qquad -\delta\Big(\omega-(E_k-E_q)\Big)\, u_k^*(\mathbf{r}')u_q^*(\mathbf{x}')v_k(\mathbf{x})v_q(\mathbf{r})\Big]\Big\}
\end{aligned}
\tag{A 19}
$$

$$
\begin{aligned}
&S_{\Delta,\Delta^\dagger}(\mathbf{r},\mathbf{r}',\mathbf{x},\mathbf{x}',\omega) = \\
&\sum_{k,q}\Big\{\Big(f(E_k)+f(E_q)-1\Big)\times \\
&\qquad\qquad \Big[\ \delta\Big(\omega-(E_k+E_q)\Big)\, v_k(\mathbf{x})v_k^*(\mathbf{r})v_q(\mathbf{x}')v_q^*(\mathbf{r}') \\
&\qquad\qquad -\delta\Big(\omega+(E_k+E_q)\Big)\, u_k(\mathbf{r})u_k^*(\mathbf{x})u_q(\mathbf{r}')u_q^*(\mathbf{x}')\Big] \\
&+\Big(f(E_k)-f(E_q)\Big)\times \\
&\qquad\qquad \Big[\ \delta\Big(\omega+(E_k-E_q)\Big)\, u_q(\mathbf{r})u_q^*(\mathbf{x})v_k(\mathbf{x}')v_k^*(\mathbf{r}') \\
&\qquad\qquad -\delta\Big(\omega-(E_k-E_q)\Big)\, u_q(\mathbf{r}')u_q^*(\mathbf{x}')v_k(\mathbf{x})v_k^*(\mathbf{r})\Big]\Big\}
\end{aligned}
\tag{A 20}
$$

$$
\begin{aligned}
&S_{\Delta^\dagger,\Delta}(\mathbf{r},\mathbf{r}',\mathbf{x},\mathbf{x}',\omega) = \\
&\sum_{k,q}\Big\{\Big(f(E_k)+f(E_q)-1\Big)\times \\
&\qquad\qquad\Big[\,\delta\Big(\omega-(E_k+E_q)\Big)\,u_k(\mathbf{x}')u_k^*(\mathbf{r}')u_q(\mathbf{x})u_q^*(\mathbf{r}) \\
&\qquad\qquad-\delta\Big(\omega+(E_k+E_q)\Big)\,v_k(\mathbf{r}')v_k^*(\mathbf{x}')v_q(\mathbf{r})v_q^*(\mathbf{x})\Big] \\
&+\Big(f(E_k)-f(E_q)\Big)\times \\
&\qquad\qquad\Big[\,\delta\Big(\omega+(E_k-E_q)\Big)\,u_k(\mathbf{x})u_k^*(\mathbf{r})v_q(\mathbf{r}')v_q^*(\mathbf{x}') \\
&\qquad\qquad-\delta\Big(\omega-(E_k-E_q)\Big)\,u_k(\mathbf{x}')u_k^*(\mathbf{r}')v_q(\mathbf{r})v_q^*(\mathbf{x})\Big]\Big\}
\end{aligned} \tag{A 21}
$$

These formulas were generated with MATHEMATICA [36].

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