Strong-coupling equations for superconductivity with a radial-momentum dependent potential

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Strong-coupling equations for superconductivity with a radial-momentum dependent potential

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Abstract: We consider the strong coupling equations for superconductivity induced by some "instantaneous" momentum-dependent potentials. Such potentials may arise from non-local corrections to the Local Density Approximation (LDA). The set of potentials and solutions is richer in comparison with the retarded "local" interactions, as in the latter case, the causality imposes constraints on the frequency dependent analytic properties of the normal and anomalous Green functions. Our main purpose is to study the momentum renormalization, and to show why it must be kept in a generalized Hartree-Fock scheme for superconductivity. While the frequency renormalization always lowers the electronic group velocity, the momentum renormalization can increase it. The superconducting gap is considerably larger for a momentum dependent interaction than for a frequency-dependent (i.e. retarded) one.

1 Introduction

BCS theory [1] for weak-coupling superconductivity is based on the gap equation (at $T = 0$):

$$\Delta(\vec{k}) = -\frac{1}{2} \sum_{\vec{k'}} V_{\vec{k}\vec{k'}} \frac{\Delta(\vec{k'})}{\sqrt{\xi(\vec{k'})^2 + \Delta(\vec{k'})^2}} \tag{1.1}$$

where

$$\xi(\vec{k}) = v_F |\vec{k} - \vec{k}_F|$$

is the energy measured from the Fermi Surface (FS). The potential $V_{\vec{k}\vec{k}'}$ is negative for an attractive interaction (providing a solution $\Delta(\vec{k})$) and positive for a repulsive interaction. In BCS theory, the potential is a function of the momenta $\vec{k}$, $\vec{k}'$.

Using the Green's function method for superconductivity [2], Eliashberg [3] generalized this theory to the case of strong coupling, for a phonon-mediated interaction, for $T = 0$ and finite temperature, and obtained a set of equations after his name. Those equations were solved for Pb by Scalapino et al. [4] and for Nb by Peter et al. [5] (with the equations extended to the anisotropic case for $T = T_c$), and by Bergmann and Rainer [6] for several values of the electron-phonon coupling.

The main feature of the electron-phonon mediated interaction [7] is its retardation, which is reflected in the frequency dependence of the effective interaction. When we consider an interaction different from the electron-phonon one, for example an interaction mediated by electrons, such as an excitonic interaction [8, 9, 10], or interactions via paramagnons [11, 12, 13] or just the Coulomb interaction in complex systems, the interaction can depend strongly on the momentum as well as on the frequency.

In the present paper we consider an "instantaneous" interaction that depends on the momentum. If the interaction is more attractive in higher angular momentum channels [14], one has to consider the generalization of the s-wave pairing in superconductors to p-wave pairing, d-wave pairing, etc. [15]. Instead of angular dependence, we study radial dependence of the s-wave singlet pairing. For very strong attractive coupling, the gap may become isotropic even when the interaction is rather anisotropic [16]. In this isotropic case the summation over $\vec{k}'$ can be replaced by an integration over energies $\int N(\xi')d\xi'$.

The Eliashberg equations [3] along the imaginary frequency axis, can be written:

$$
\begin{aligned}
(X(\xi,\omega) - 1)\xi &= \frac{1}{2\pi} \int d\xi' \int d\omega' \frac{N(\xi')V(\xi,\xi',\omega-\omega')X(\xi',\omega')\xi'}{\Omega} \\
(Z(\xi,\omega) - 1)\omega &= -\frac{1}{2\pi} \int d\xi' \int d\omega' \frac{N(\xi')V(\xi,\xi',\omega-\omega')Z(\xi',\omega')\omega'}{\Omega} \\
\phi(\xi,\omega) &= -\frac{1}{2\pi} \int d\xi' \int d\omega' \frac{N(\xi')V(\xi,\xi',\omega-\omega')\phi(\xi',\omega')}{\Omega} \\
\Omega &= (Z(\xi',\omega')\omega')^2 + (X(\xi',\omega')\xi')^2 + \phi(\xi',\omega')^2
\end{aligned}
\tag{1.2}
$$

X and Z are related to the self-energy:

$$
\begin{aligned}
X(\xi,\omega) &= 1 + \frac{1}{2}(\Sigma_1(\xi,\omega) + \Sigma_1(\xi,-\omega))/\xi \\
Z(\xi,\omega) &= 1 - \frac{1}{2}(\Sigma_1(\xi,\omega) - \Sigma_1(\xi,-\omega))/\omega.
\end{aligned}
\tag{1.3}
$$

In the standard calculations the self-energy Σ_1 is lumped with the energy [17], therefore $X = 1$. This approximation is valid when the renormalization X is not much affected by the superconducting state, and therefore, by considering it as a normal-state effect, it can be absorbed in a renormalized band [18]. In the present work, we will show some cases where this condition breaks down and where it is necessary to consider the ϕ dependence of X.

As special cases, this formalism reduces to the Hartree-Fock equations in jellium, if $\xi(\vec{k})$ is the free electron band and V is the Coulomb potential and to the standard BCS theory if V is the Cooper potential [17]. A density-functional theory for superconductors which also incorporates exchange correlation effects has been proposed in ref.[19].

2   Momentum dependent interaction

Since we consider a potential V that does not depend on frequency, we can integrate-out the variable ω using the residue theorem and obtain the following equations:

$$
\begin{aligned}
(X(\xi) - 1)\xi &= \frac{1}{2} \int d\xi' \frac{N(\xi')V(\xi,\xi')\xi'}{R} \\
\Delta(\xi) &= -\frac{1}{2}\frac{1}{X(\xi)} \int d\xi' \frac{N(\xi')V(\xi,\xi')\Delta(\xi')}{R} \\
R &= \sqrt{(\xi')^2 + \Delta(\xi')^2},
\end{aligned}
\tag{2.1}
$$

where $\Delta = \phi/X$. These equations can be viewed as a generalized Hartree-Fock scheme [17]. X is the renormalization function appropriate for the momentum-dependent interaction. The quasiparticle energy is given by $X(\xi)\xi$. Therefore X renormalizes the DOS, the group velocity and the specific-heat effective mass as

$$
N^*(\xi) = N(\xi)/X(\xi) \quad v^*(\xi) = v(\xi)X(\xi) \quad \text{and} \quad m^*(\xi) = m/X(\xi) \tag{2.2}
$$

(provided one can neglect $dX/d\xi$). Independence of ω means $Z = 1$ (no wavefunction renormalization). We see immediately that for a repulsive interaction, $X > 1$, and for an attractive one, $X < 1$. When $X = 0$, we obtain an instability.

We start by studying a *strip potential* with a cut-off ξ_1:

$$
V(\xi,\xi') = \begin{cases} V_0 & \text{if } |\xi - \xi'| < \xi_1 \\ 0 & \text{otherwise} \end{cases} \tag{2.3}
$$

The DOS that we employ is given by:

$$
N(\xi) = \begin{cases} N_0 & |\xi| < \Gamma \\ 0 & \text{otherwise} \end{cases} \tag{2.4}
$$

The coupling constant is given by N_0V_0. Usually, the symbol λ is used for coupling due to electron-phonon interaction: it is positive for an attractive interaction. We use the symbol μ for coupling due to electron-electron interactions and it can be either positive (repulsion) or negative (attraction). In Fig. 1 and Fig. 2, we show $X(\xi)$ and the renormalized DOS for a repulsive, as well as for an attractive strip potential in the normal state ($\Delta = 0$).

We may note that Hedin and Lundquist [20] considered the momentum-renormalization $X(k)$ as well as the standard frequency renormalization $Z(\omega)$ caused by the Coulomb interaction for realistic metals, such as alkalis, and estimated that $X(k) \approx 1.3$, $Z(\omega) \approx 1.3$;
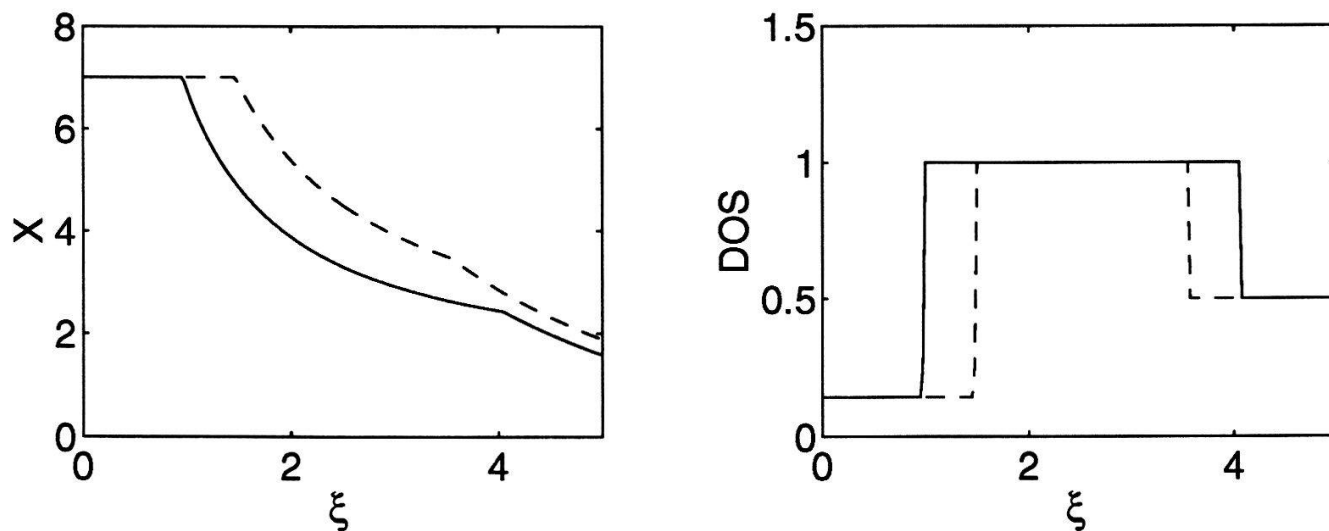
Figure 1: Momentum renormalization X and DOS in the normal state for a repulsive strip potential with $\mu = 6$ as a function of ξ. The full line represents a case $\xi_1 = 1 < \Gamma/2 = 2.5$ and the dashed line represents a case $\xi_1 = 3.5 > \Gamma/2 = 2.5$. A Coulomb quasigap is clearly seen in the DOS.
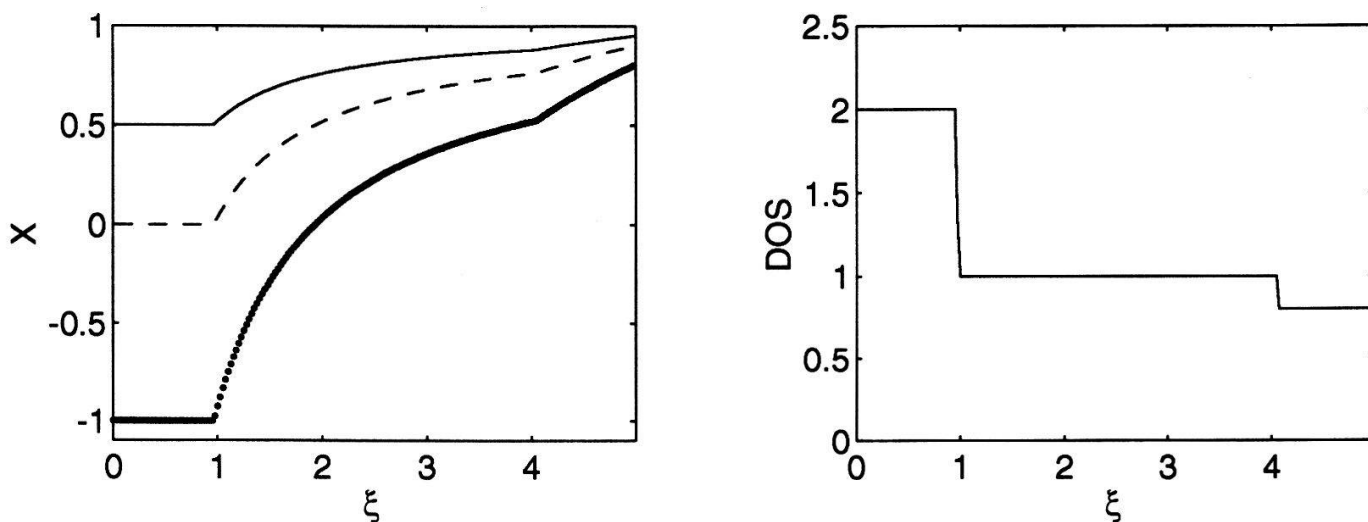

Figure 2: Momentum renormalization X in the normal state for attractive strip potentials as a function of ξ (in ξ_1 units) for $\mu = -0.5$ (full line) and $\mu = -1$ (dashed line) and $\mu = -2$ (bold dotted line). For $\mu = -0.5$ we give the DOS, the other two cases give instabilities $X < 0$.
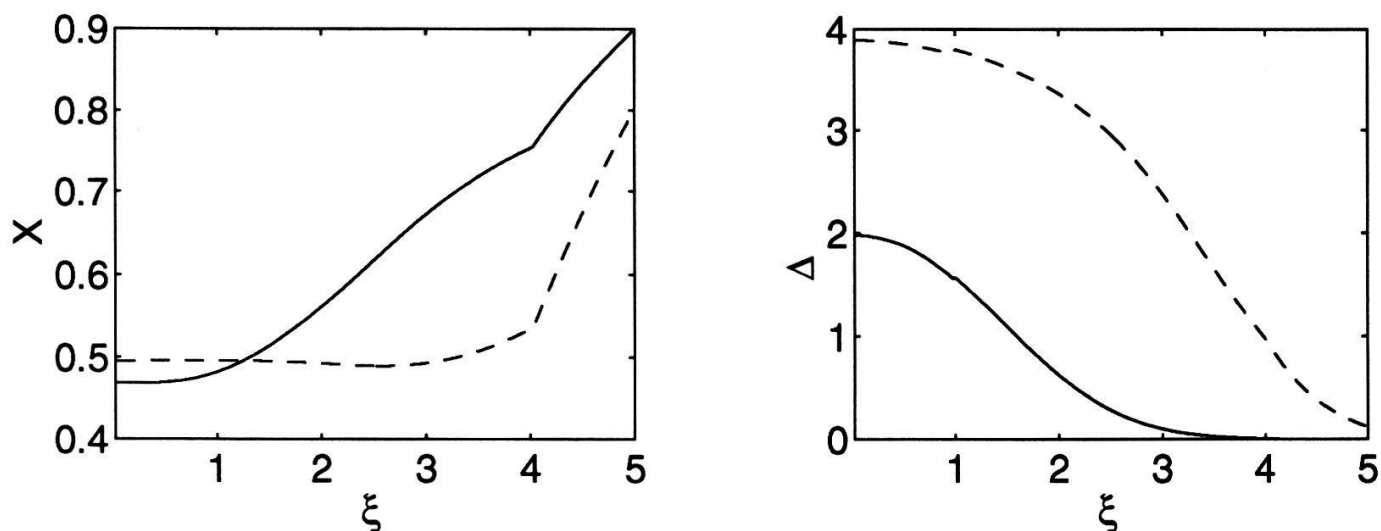
Figure 3: Momentum renormalization X and the gap parameter Δ (in ξ_1 units) at $T = 0$ for attractive strip potentials: $\mu = -1$ (full line) and $\mu = -2$ (dashed line).

thus the increase in velocity (decrease in mass) caused by X, and the decrease in velocity (increase in mass) caused by Z, nearly cancel each other, leaving a residual effect of order 5%, which is thus negligible. Therefore, renormalization effects caused by the Coulomb interaction are usually neglected. However, for "exotic" metals, such as the high-T_c cuprates, these estimates no longer apply, and X may be large, and not necessarily compensated by Z.

We see that $X(k_F) = 1 + \mu$. This result is somewhat analogous to McMillan's result [21] $Z(0) = 1 + \lambda$ (where λ is the electron-phonon coupling constant); but here, for the momentum dependent interaction, μ may be negative (attractive interaction) as well as positive (repulsive interaction). $X(\xi)$ is constant up to $\xi = \xi_1$. When ξ_1 is larger than $\Gamma/2$, the form of $X(\xi)$ changes somewhat, and $X(\xi)$ is constant only up to $\Gamma - \xi_1$. Thus the average of X over the interval $0 < \xi < \xi_1$ decreases.

An increase in velocity due to a repulsive k-dependent interaction was found by Lindhard [22] (for an unscreened Coulomb interaction in the Hartree-Fock approximation) and by Galitski [23] (for a short-range, hard core interaction).

3   The superconducting state

In the superconducting state, we show, in Fig. 3, $\Delta(\xi)$ and $X(\xi)$ at $T = 0$ for $\mu = -1$, $\mu = -2$ (attractive interaction). The $\Delta(\xi)$ curve is broader for $\mu = -2$ than for $\mu = -1$, i.e. there is substantial pairing at energies larger than the cutoff ξ_1 for a large coupling constant. We call this *deep pairing* [24]. This broadening is not present for a separable potential, such as the Cooper potential. Note that here X is regular (positive) in contrast with the situation $T > T_c$ (Fig. 2). We have thus some explicit examples, where X renormalization

in the normal state and in the superconducting state are very different. In these cases, it is *essential* to solve X and Δ at the same level using the generalized Hartree-Fock scheme.

Our set of equations for Δ and X is mathematically similar to the standard Eliashberg equations for Δ and Z, with Z replaced by X and the electron-phonon coupling constant λ replaced by μ. Consequently, for weak to moderate coupling, the gap Δ is given by a McMillan-like equation. For an attractive interaction (negative μ)

$$\Delta = 2\xi_1 \exp(\frac{-X}{|\mu|}) = 2\xi_1 \exp(-\frac{1-|\mu|}{|\mu|}) \tag{3.1}$$

because of the $1 - |\mu|$ factor, Δ is a factor of e larger than the BCS value $2\xi_1 \exp(-1/|\mu|)$, and a factor e^2 larger than the value given by the McMillan expression $2\omega_{ph} \exp(-\frac{1+\lambda}{\lambda})$. For very strong attractive coupling $X \to 1/2$ and $\Delta \approx \xi_1/\sinh(1/2|\mu|) \approx 2|\mu|\xi_1$ which is near the BCS value, and substantially larger than the Eliashberg value for the case of a phonon Einstein spectrum with $\omega_{ph} = \xi_1 = 1$ (Fig. 4). However for momentum renormalization, the parameter $\Delta = \phi/X$ does not give the lowest excitation energy. This value is given by $\phi = X\Delta$ (Fig. 4), because the quasi-particle energy is $\sqrt{(X\xi)^2 + \phi^2}$. Consequently, the gap is given at weak and moderate coupling by

$$\phi = 2\xi_1(1 - |\mu|) \exp(-\frac{1-|\mu|}{\mu}) \tag{3.2}$$

and for very strong coupling by the original BCS expression $\phi = |\mu|\xi_1$.

Non-trivial solutions for Δ exist in principle for a repulsive interaction, as pointed out by Englman, Halperin and Weger [25]. For these solutions, $\Delta(\xi)$ oscillates as function of ξ with a period of $(4/3)\xi_1$. Antisymmetric solutions (in ξ) exist as well as symmetric ones [24]. For these solutions a constant repulsive potential μ has no effect however strong it is, since the product of Δ and μ oscillates and its integral vanishes [26]. If we ignore renormalization, i.e. arbitrarily set $X(\xi) = 1$, the solution is obtained immediately for a coupling constant $\mu > 2$ (Fig. 5). However, when we introduce $X(\xi)$, then for a strip potential with $\xi_1 < \Gamma/2$, the solutions disappear and there is no solution however large μ is. We can obtain a solution nevertheless if $\xi_1 > \Gamma/2$ and thus the renormalization is reduced. An extreme limit is when $\xi_1 >> \Gamma$, and then $X \approx 1$. Alternatively, a solution is obtained if the renormalization is for some reason smaller than $X(\xi)$. The elimination of the solution by the renormalization is a property of the square-barrier potential. For other forms of the potential, a solution may be present even when the renormalization $X(\xi)$ is properly introduced, as for a Bardeen-Pines potential:

$$V(\xi, \xi') = \frac{-V_0\xi_1^2}{(\xi - \xi')^2 - \xi_1^2} \tag{3.3}$$

For such a potential, a solution exists even for very small $|\mu|$. The solutions for the attractive and the repulsive case are shown in Fig. 6 (we have assumed that the Bardeen-Pines has a small factor $i\delta$ in the denominator, without it, the gap could be considerably larger [25]). We can notice a resemblance between Fig. 5 and Fig. 6, regarding the oscillating behaviour.

An antisymmetric solution in ξ for antisymmetric, separable, model potential was considered by Cohen [27] and Nakajima [28]. Antisymmetric solutions in ω where proposed by
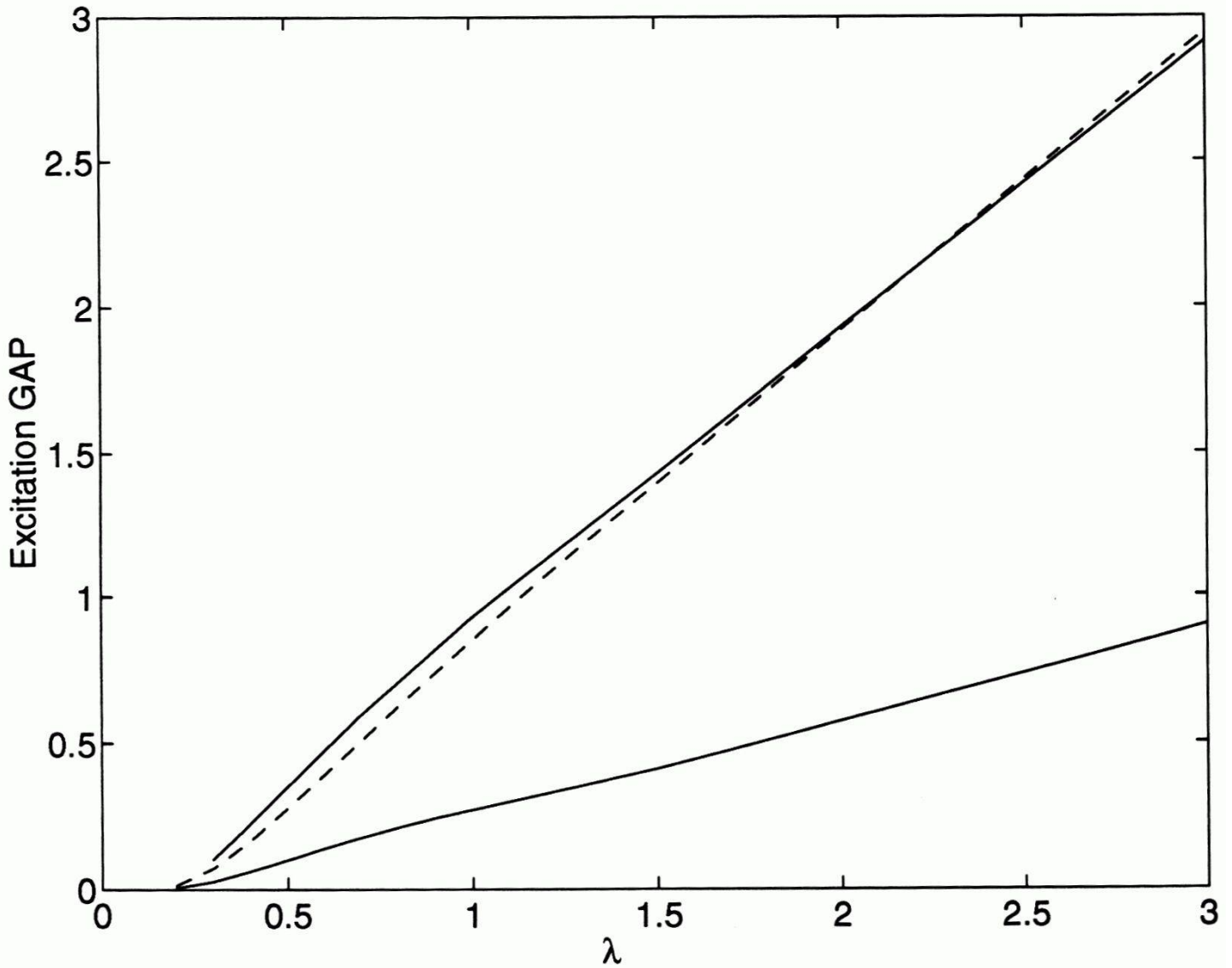
Figure 4: The excitation gap in units of the cutoff as a function of the coupling λ, for the original BCS model (dashed line), Eliashberg theory for an Einstein spectrum (lower full line) and for the attractive momentum dependent strip potential (upper full line) ($\omega_{ph} = \xi_1 = 1$).

Figure 5: Δ and excitation energy E (in ξ_1 units) at $T = 0$ for a repulsive strip potentials with $\mu = 6$: (A) and (B) symmetric solution; (C) and (D) antisymmetric solution. The renormalization is neglected: $X = 1$.

Figure 6: Momentum renormalization X and Δ (in ξ_1 units) at $T = 0$ for Bardeen-Pines potentials: $\mu = -0.3$ (attractive) and $\mu = +0.5$ (repulsive).
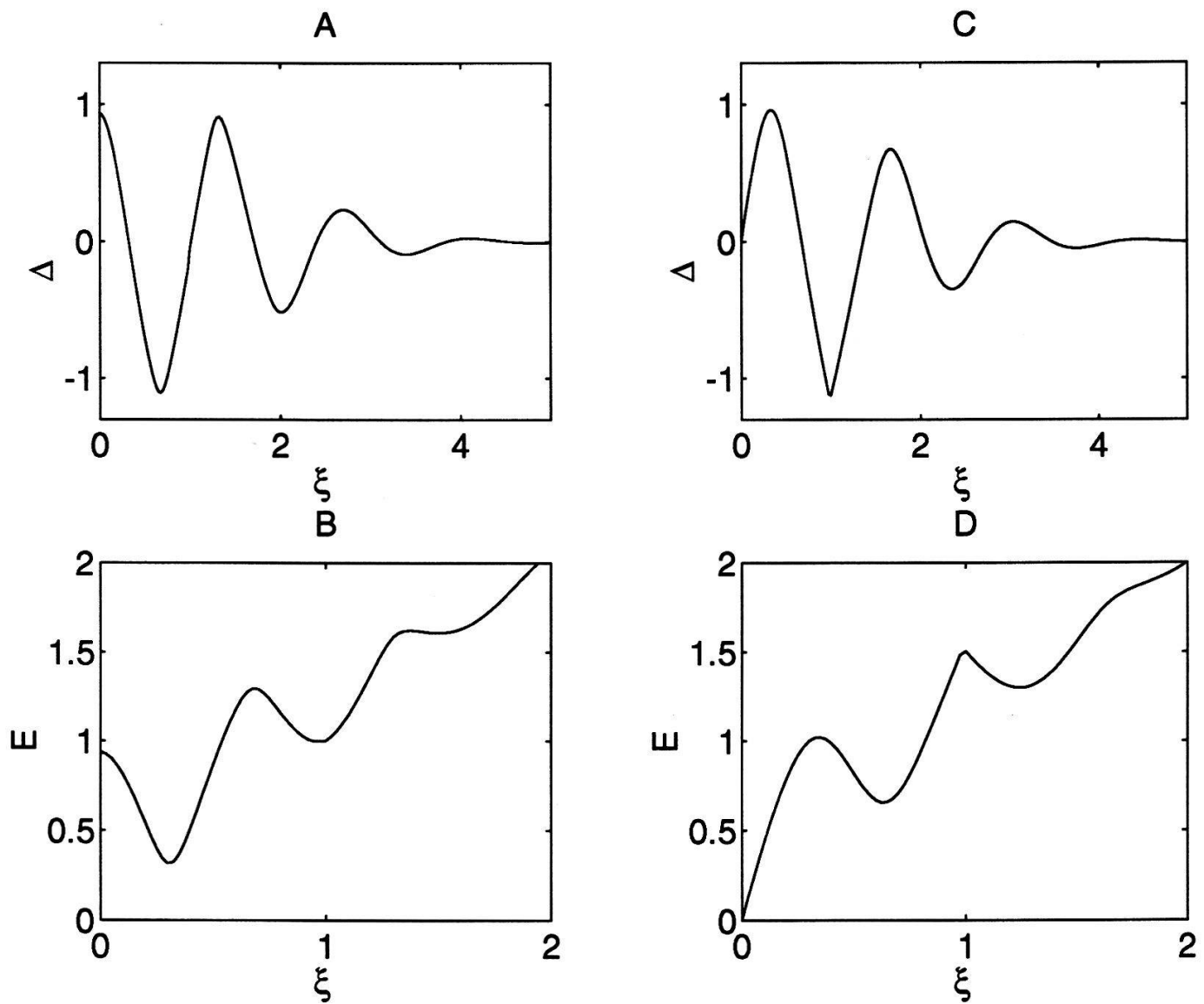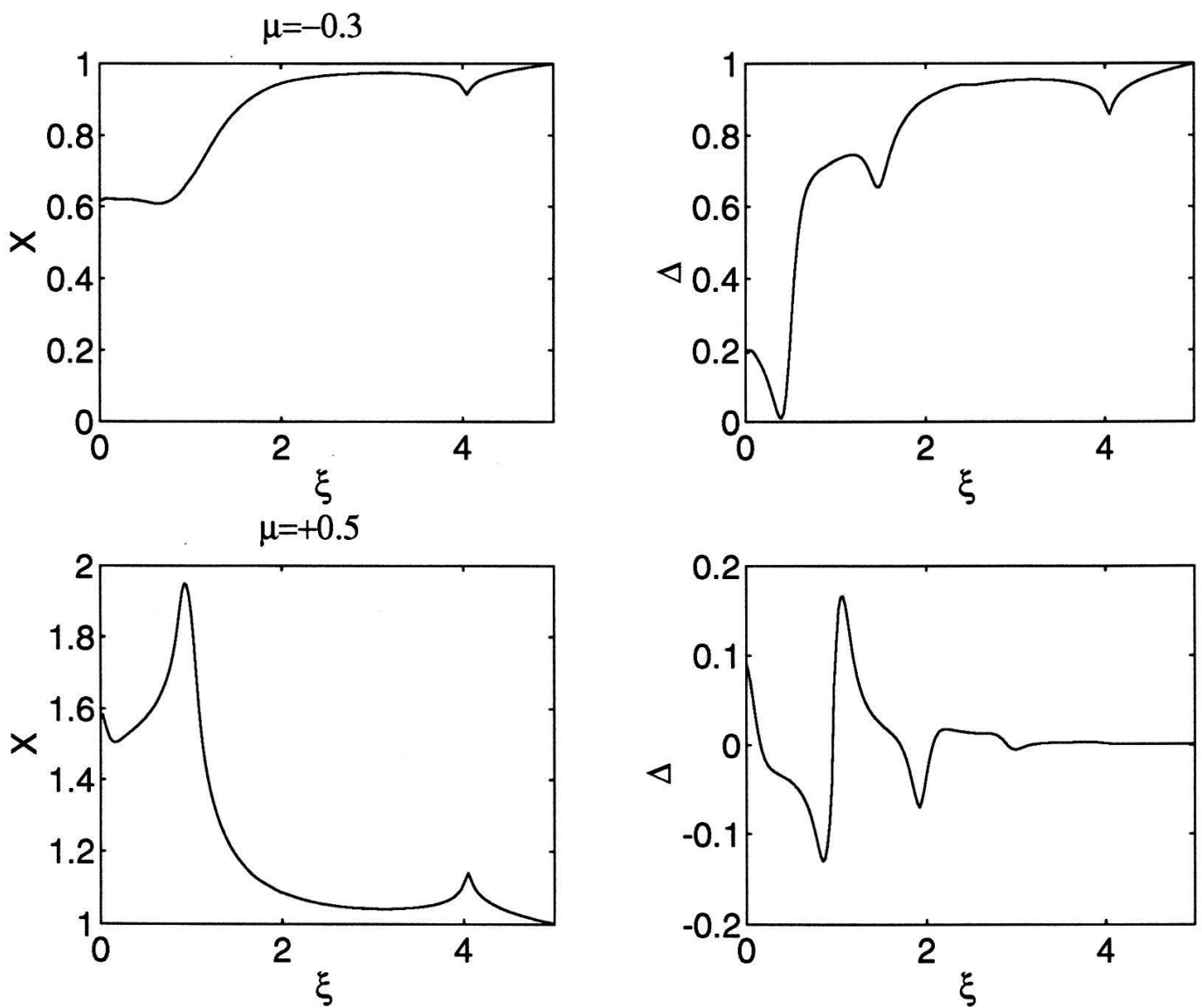
Berezinskii [29] for the spin-triplet pairing and extended on a spin-singlet pairing by other authors [30]. The antisymmetric solutions in ξ, were also considered by Mila and Abrahams within a weak-coupling theory [31]. These authors consider a sum of a repulsion with a large ξ cutoff (short range potential) and an attractive strip potential (i.e. square well potential) with a short ξ cut-off. For the attractive momentum-dependent potential, the solution persists in the presence of the renormalization X. The constant Coulomb potential drops out as had been pointed out previously [26].

For an attractive interaction (negative μ in our notation), there is an instability for a square-well potential, in the normal state, when $|\mu| > 1$, X becoming negative (when $X = 0$ the DOS diverges). An instability of this kind could occur in the formation of a bound state such as lattice-distortion bipolarons [32], or spin bipolarons [33]. Moreover, a recent study using Monte Carlo simulations on the 2D attractive Hubbard model [34] shows that singlet pairing correlations develop above T_c. Therefore, for an attractive momentum-dependent interaction, there is a bound state even at temperatures higher than T_c, for the case of strong coupling. This is in the spirit of the Schafroth model [35], where there are bosons above T_c, which undergo a Bose-Einstein condensation below T_c. The formation of bound pairs above T_c is also discussed by Nozières and Schmitt-Rink [36].

4   Comparison with Eliashberg theory

For a frequency-dependent interaction, we do not encounter the instability of the renormalization function of the momentum-dependent interaction. A frequency-dependent interaction must be an analytic function of ω, as are the solutions $Z(\omega)$, $\Delta(\omega)$, and the normal and anomalous Green's functions $G(k,\omega)$ and $F(k,\omega)$ [3]. Causality implies the well-known singularity along the real ω-axis and analyticity elsewhere in the complex plane [37]. Therefore the path of integration can be deformed in the complex-ω plane and consequently the solution of these equations is straightforward. The Eliashberg equations (at $T = 0$) for the ω-dependent interaction $D(\omega - \omega')$, along the imaginary ω-axis, may also be obtained using the residue theorem

$$
\begin{aligned}
(Z(i\omega) - 1)\omega &= -\int d\omega' \frac{D(i\omega - i\omega')\omega'}{R} \\
\Delta(i\omega) &= -\frac{1}{Z(\omega)} \int d\omega' \frac{D(i\omega - i\omega')\Delta(i\omega')}{R} \\
R &= \sqrt{(\omega')^2 + \Delta(i\omega')^2},
\end{aligned}
\tag{4.1}
$$

where $\Delta = \phi/Z$. The structure of these equations is similar to generalized Hartree-Fock scheme that we considered before, however the physics is very different because the causality imposes some constraints. Since the Green (or kernel) functions must be analytic functions of ω away from the real axis (causality), the retarded part of an effective interaction due to phonons with an Einstein spectrum with frequency ω_0,

$$
\frac{2\omega_0}{(\omega - \omega')^2 + \omega_0^2}
\tag{4.2}
$$

Interaction	Coupling strength	Instantaneous momentum dependent	Retarded local
Attractrive	weak	BCS solution	Eliashberg BCS-like solution
	strong	Schafroth-like solution	Eliashberg solution
Repulsive		Oscillatory solution (under special conditions)	No bound-pair solution

Table 1: Nature of the superconductivity for momentum and frequency dependent, attractive and repulsive interactions.

is a smooth function of the imaginary frequency and no solution exists for negative λ [25]. A frequency-dependent strip potential similar to the one we used before for the momentum dependence cannot be obtained as a superposition of phonon kernels and, in addition, violates the causality as it is not analytical away from the real ω axis.

In conclusion, the momentum-dependent potentials give a richer set of solutions in comparison with the retarded interaction (see table 1), as the severe constraint of the analyticity away from the real axis for the kernels is no longer required for the momentum dependent interaction.

5   Experimental considerations

Let us discuss now some physical considerations relating to the question whether this model bears any relevance to the high-T_c cuprates. The increase in velocity by the momentum renormalization: $v \rightarrow Xv$ is associated with a decrease in the DOS: $N \rightarrow N/X$ (Fig. 1). Thus, there is a minimum in the DOS at the Fermi level. This minimum can be regarded as a Coulomb quasigap. Coulomb gaps and quasigaps were considered by Altshuler and Aronov [38] and by Efros [39]. They considered disordered systems, while here we consider an ordered system. Therefore, our Coulomb quasigap differs in some essential respects from those of the Altshuler Aronov and Efros theories. In those theories, the decrease in the DOS in not associated with an increase in the velocity, as is the case in the present model. In the present model, the Coulomb quasigap is caused by a repulsive momentum dependent interaction, with a small cutoff ξ_1. We propose a model theory possessing these features

elsewhere [40].

There is also some experimental indication that an increase of the velocity near the Fermi Surface is associated with a high T_c. Measurements of Uemura et al. [41] show that T_c is approximately proportional to Λ_L^{-2} (Λ_L is the London penetration depth), which in turn is proportional to the velocity.

Band-structure calculations employ the LDA, in which the interaction is assumed to be local in r-space, and consequently (essentially) k-independent. Therefore the k-dependent features that we consider by using momentum dependent interactions are not considered. We suggest that close to the Fermi surface, we must use a theory that goes beyond LDA and takes into account the momentum dependence of the exchange and correlation potentials.

The quasiparticle DOS in the superconducting state is sensitive to the structure of the superconducting gap parameter and can be a useful quantity to guide the understanding of the mechanism leading to the high temperature superconductivity. This quantity can be measured in tunneling conductivity experiments. Experimentally, in high temperature superconductors, such as YBCO, BSCCO, NCCO, BKBO, [42] a sharp maximum is observed in the tunneling conductivity and the energy of this maximum is conventionally called the "gap". However the tunneling conductivity does not vanish below that maximum, but extends smoothly down to a very low energy $\delta^{(0)}$, which is commonly called the "Zero Bias Anomaly" (ZBA). A similar situation is observed very clearly in the organic superconductor ET [43]. $\delta^{(0)}$ in YBCO is about 4 meV, and in ET it is about 0.35 meV, i.e. 5 to 10 times less than the "gap". There is not yet a consensus about the origin of states in the "gap", or the ZBA. Recent experiments by Renner et al. [44], definitely established an appreciable tunneling conductivity inside of the "gap" in BSCCO. This finite tunneling conductivity is sometimes attributed to a gap varying with angle [15], as in d-wave superconductivity. However a similar effect can be otained by a gap function with s symmetry that varies in the energy direction as described in this paper. For instance the (symmetric and antisymmetric) solutions $\Delta(\xi)$ of the gap equation for a repulsive potential that oscillate as a function of ξ as shown in Fig. 5 give strongly varying excitation energy $E(\xi) = \sqrt{\xi^2 + \Delta^2(\xi)}$ (Fig. 5) and finite DOS in the "gap" (Fig. 7).

6   Discussion

Eliashberg treated the ω-dependent interaction (due to the electron-phonon coupling) for strong coupling. It is important to note, however, that the concepts of a "frequency dependent interaction" and "strong coupling" are distinct and independent: a momentum dependent interaction may be treated for the case of strong coupling, as we do here, and an ω-dependent Eliashberg formalism may be used in the weak coupling limit. Also, it is important to point out that the reduction of T_c is *not* an essential consequence of strong coupling and renormalization alone, but of retardation as well.

Usually, the momentum renormalization X is considered as a normal-state effect that
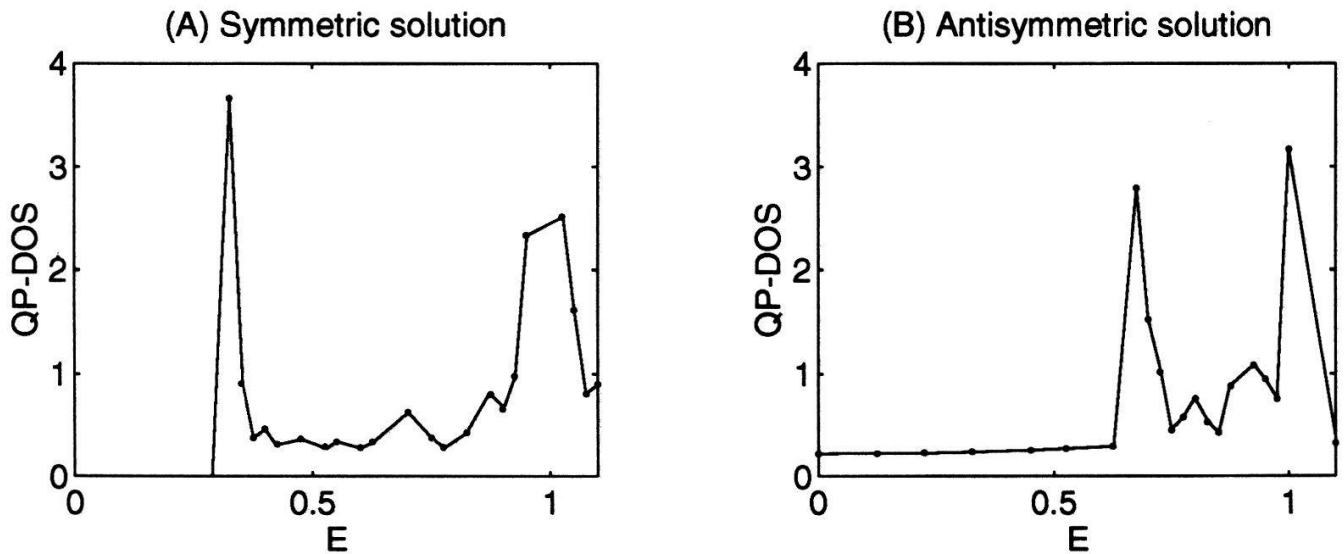
Figure 7: Superconducting quasiparticle DOS for a symmetric solution (A) and an antisymmetric one (B) (given in Fig. 5) as function of the excitation energy E.

can be absorbed in a renormalized band. We found however, that for some interactions depending on momentum the superconducting state can have a strong influence on X, and thus, we have to solve coupled nonlinear integral equations for X and for the superconducting order parameter ϕ, generalizing the Hartree-Fock scheme. These equations are very similar to the standard Eliashberg equations along the ω imaginary axis.

However, the differences between an interaction that depends on momentum and one that depends on frequency are subtle, and at the same time very profound. For an ω-dependent interaction the kernels of the integral equations are analytic in ω away from the real axis. For a k-dependent interaction, the kernels of the integral equations are not necessarily analytic in the complex-ξ plane. Analyticity is a very severe restriction, that drastically limits the allowed solutions. Thus, the manifold of allowed solutions for a k-dependent interaction is so much richer (table 1).

A major physical difference is, that a momentum dependent interaction causes the velocity to *increase* for a repulsive interaction, and to *decrease* for an attractive one. An ω-dependent interaction *always decreases* the velocity. In the normal state ($T > T_c$), the single particle states for an attractive k-dependent potential are unstable, when λ is greater than a certain threshold.

The physical reason why the electron-phonon interaction in metals gives rise to a weakly momentum dependent interaction is that the coupling is almost local in space [45, 46], as the interaction is screened with a screening length that is considerably shorter than the interatomic distance. This physical reason may no longer apply in layered materials like the high temperature superconductors, where non locality is important [47].

Coupling originating from electron-electron interactions in layered and composite materials was considered in the theories of "excitonic" superconductivity by Little [8], Allender,

Bray and Bardeen (ABB) [10] and Ginzburg [9]. In the description of this mechanism, the results from the electron-phonon mechanism were taken over, with the frequency rescaled to the higher exciton frequency, but without consideration of the possibility that the momentum dependence may play an essential role. In the Little mechanism the electron-exciton interaction may be regarded as local (in the relevant direction), therefore $X \approx 1$. In the Ginzburg and ABB mechanisms this is not the case, since the excitons are extended, therefore the Nambu-Gor'kov [2] theory of superconductivity in these models should be reevaluated, taking notice of the momentum dependence of the interaction from the very start.

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