New form of pair interaction in superconductivity in pressure-sensitive systems

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An (electron) quasiparticle-phonon coupling proportional to the superconducting gap is considered. Eliashberg-type equations are derived and immediate consequences are discussed. These considerations apply to specific, yet interesting systems.

This paper addresses the following questions: which types of pair potential stabilizing or breaking up the Cooper pair can possibly be conceived, and where can we look for experimental evidence? A partial answer to these questions may yield insight into interesting and diverse systems such as the charge-density-wave (CDW) state of[1] $2H$-$NbSe_2$, or the heavy-fermion superconductor[2] (HFS) $CeCu_2Si_2$. Physically, the central observation will be a high-pressure dependence of the superconducting gap parameter Δ, indicating a great variation of Δ with lattice vibrations (phonons). This strong phonon-gap correlation can be parametrized by a new type of pair interaction between quasiparticles, in addition to the existing (and in most systems prevalent) Fröhlich-type and Coulomb interaction. While the stiffening of the lattice with increasing pressure tends to reduce the superconducting transition temperature T_c (it may however adversely *increase* T_c by increasing the quasiparticle density at the Fermi surface), for some materials there is a significant increase in T_c when pressure is applied (see Fig. 1). The same behavior can be expected from the pressure dependence of the gap function;[1] it may be estimated by

$$\delta T_c/\delta p \approx (\delta T_c/\delta\Delta)(\delta\Delta/\delta p) \approx (0.57/k_B)(\delta\Delta/\delta p) ,$$

where the BCS estimate $\Delta(T=0)/k_B T_c \approx 1.76$ has been used.

The phonon-quasiparticle interaction can be parametrized by a very general class of Yukawa potentials proportional to[3] $\Psi^\dagger(x)\Delta(x)\Psi(x)\varphi(x)$, where $\Psi=(\psi_s,\psi^\dagger_{-s})$ is the quasiparticle field in the two-component Nambu notation[4,5] and s is the spin index. φ stands for the phonon field, and Δ is a gap parameter yet to be calculated from self-consistent perturbation theory (Eliashberg theory). Its most general form is $\Delta(x)=\boldsymbol{\tau}\cdot\boldsymbol{\Delta}(x)$, where the τ_i's are the Dirac matrices.

The complete model in Lagrangian form reads[4,6] (arguments x have been dropped)

$$L = L_{\text{free}} + L_{\text{interaction}} + L_{\text{counterterm}} , \quad (1)$$

$$L_{\text{free}} = \Psi^\dagger[i(\partial/\partial t)1 - \epsilon_p\tau_3]\Psi + \tfrac{1}{2}(\partial_\mu\varphi)^2 + \tfrac{1}{2}(\nabla A_0)^2 , \quad (1a)$$

$$L_{\text{interaction}} = \Psi^\dagger(\mathbf{g}\cdot\boldsymbol{\tau}\varphi + e\tau_3 A_0)\Psi , \quad (1b)$$

$$L_{\text{counterterm}} = \Psi^\dagger(\phi_1\tau_1 + \phi_2\tau_2 + \phi_3\tau_3)\Psi . \quad (1c)$$

$A_0(\mathbf{x})$ is the Coulomb field (only the electrostatic part of the vector potential has been kept), e is the electric charge, and $\boldsymbol{\phi}=Z\boldsymbol{\Delta}$ are gap parameters times the quasiparticle field renormalization constant Z. Due to the specific form of L_{free}, a rotation in τ space along the τ_3 axis with angle $\theta=\tan^{-1}(\Delta_2/\Delta_1)$ can be performed such that Δ_2 and, therefore, g_2 vanishes; $\Delta_1 \to (\Delta_1^2+\Delta_2^2)^{1/2} \equiv \Delta$ and $g_1 \to (g_1^2+g_2^2)^{1/2} \equiv k$ (from now on, g_3 will be denoted by g). Hence, one is left with the standard Fröhlich and Coulomb interaction $(g\varphi+eA_0)\Psi^\dagger\tau_3\Psi$, and with a new type of coupling $k\varphi\Psi^\dagger\tau_1\Psi$. Since $k \propto \Delta$, this coupling vanishes for $\Delta=0$.

The Eliashberg theory of this model can be developed without conceptual difficulties. As long as the ratio between the square root of the compound and quasiparticle masses are small, Migdal's theorem can be applied even for strong-coupling materials.[5] From Dyson's equations one obtains[6] for the full quasiparticle propagator G and its

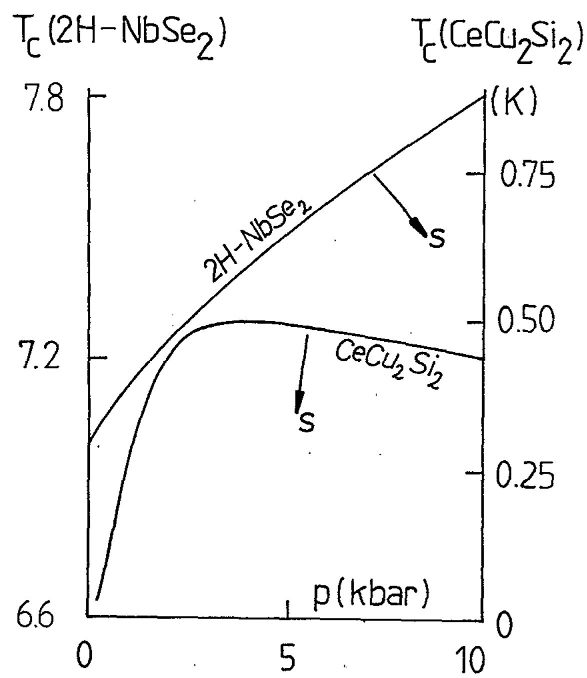

FIG. 1. Strong pressure dependence of the superconducting transition temperature T_c in the CDW state $2H$-$NbSe_2$ and the HFS $CeCu_2Si_2$, taken from references 1 and 2. For usual materials, with very few exceptions, $-0.05 < \delta T_c/\delta p < 0$ K/kbar.

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self-energy Σ in momentum representation (see Fig. 2).

$$G^{-1}(p)=G_0^{-1}(p)-\Sigma(p)=Z(p)\tilde{G}_0^{-1}(p)\ , \qquad (2a)$$

$$\Sigma(p)=i\int (k_{pp'q}\tau_1+g_{pp'q}\tau_3)G(p')\times(k_{pp'q}\tau_1+g_{pp'q}\tau_3)D(q)\frac{d^4p'}{(2\pi)^4}\ . \qquad (2b)$$

Here, D stands for the phonon propagator, the index zero denotes bare quantities, and $\tilde{G}_0$ (which includes the gap parameters) and Σ have been parametrized in the form

$$\tilde{G}_0^{-1}(p)=p_0 1-\left[\frac{\epsilon_p}{Z(p)}+\Delta_3(p)\right]\tau_3-\Delta(p)\tau_1+i\delta\ , \qquad (3a)$$

$$\Sigma(p)=[1-Z(p)]p_1 1+Z(p)[\Delta_3(p)\tau_3+\Delta(p)\tau_1]\ . \qquad (3b)$$

The evaluation of the system of Eqs. (2) is straightforward.[5] Assuming $|\mathbf{p}|\simeq|\mathbf{p}'|\simeq p_F$ (the Coulomb interaction has been omitted and enters in its standard form[5]), the results in the imaginary-frequency (Matsubara) representation are

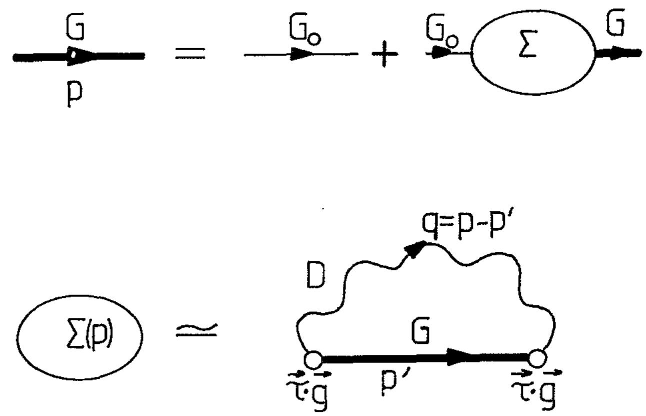

FIG. 2. The perturbative approximation scheme for calculation of the full quasiparticle propagator in the modified Eliashberg theory.

$$[1-Z(i\omega_n)]\omega_n=-\pi k_BT\sum_{m=-\infty}^{\infty}\frac{\omega_m}{[\omega_m^2+\Delta^2(i\omega_m)]^{1/2}}\int_0^\infty d\Omega\frac{2\Omega\alpha_+^2F(\Omega)}{(\omega_n-\omega_m)^2+\Omega^2}\ ; \qquad (4a)$$

$$Z(i\omega_n)\Delta(i\omega_n)=-\pi k_BT\sum_{m=-\infty}^{\infty}\frac{\Delta(i\omega_m)}{[\omega_m^2+\Delta^2(i\omega_m)]^{1/2}}\int_0^\infty d\Omega\frac{2\Omega\alpha_-^2F(\Omega)}{(\omega_n-\omega_m)^2+\Omega^2}\ . \qquad (4b)$$

After analytic continuation to real frequencies, (4) reads

$$[1-Z(p_0)]p_0=\int_{-\infty}^{\infty}dp_0'\int_0^\infty d\Omega\,\alpha_+^2F(\Omega)I(p_0+i\delta,\Omega,p_0')\mathrm{Re}\left\{\frac{p_0'}{[(p_0')^2-\Delta^2(p_0')]^{1/2}}\right\}\ , \qquad (5a)$$

$$Z(p_0)\Delta(p_0)=\int_{-\infty}^{\infty}dp_0'\int_0^\infty d\Omega\,\alpha_-^2F(\Omega)I(p_0+i\delta,\Omega,p_0')\mathrm{Re}\left\{\frac{\Delta(p_0')}{[(p_0')^2-\Delta^2(p_0')]^{1/2}}\right\}\ , \qquad (5b)$$

where

$$I(p_0+i\delta,\Omega,p_0')=\frac{N(\Omega)+1-f(p_0')}{p_0+i\delta-\Omega-p_0'}+\frac{N(\Omega)+f(p_0')}{p_0+i\delta+\Omega-p_0'}\ ,$$

and

$$N(\Omega)=(1-e^{\Omega/k_BT})^{-1}\ ,$$

$$f(p_0')=(1+e^{p_0'/k_BT})^{-1}\ .$$

Furthermore, when $B(q,\Omega)$ is the phonon spectral function and $\rho(0)$ is the quasiparticle density of states at the Fermi surface,

$$\alpha_\pm^2F(\Omega)\equiv\rho(0)\int_0^\infty\frac{qdq}{2p_F^2}(|k|^2\pm|g|^2)B(q,\Omega)\ .$$

The new type of pair interaction has been introduced previously[3] to explain a resonance structure in the Raman spectrum of CDW states. In this context, phonon polarization and charge screening have been discussed.[3] Some immediate consequences of the Eliashberg equations (5) shall be derived next.

An important observation concerns the sign of the coupling parameter $|k|^2$, as compared to $|g|^2$: One can introduce dimensionless quasiparticle-phonon coupling constants,[7] assuming $p_0,p_0'\ll\Omega$,

$$\lambda^\Delta\pm\lambda\equiv2\int_0^\infty\frac{d\Omega}{\Omega}\alpha_\pm^2F(\Omega)\ . \qquad (6)$$

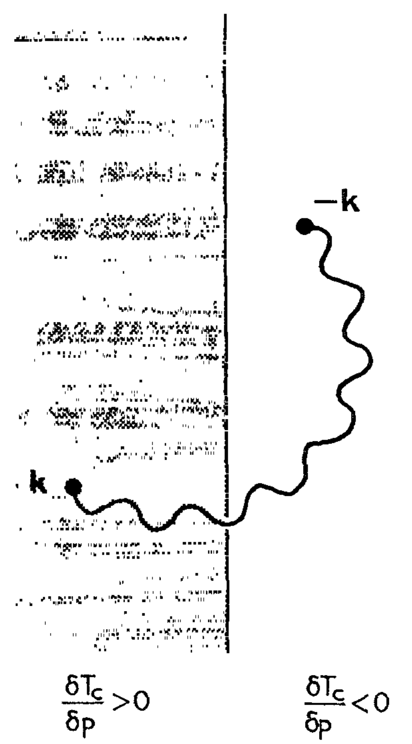

FIG. 3. Layers of negative and positive T_c-pressure gradients, yielding an attractive pair interaction.

λ is the usual quasiparticle-phonon coupling parameter of the BCS theory, and λ^{Δ} is defined analogously. Assuming a square-well form of the gap function $\Delta(p_0) \simeq \Delta\theta(\tilde{p}_0 - p_0)$, one obtains an equation for T_c in terms of the dimensionless coupling parameters:

$$T_c(\lambda,\lambda^{\Delta}) \simeq \frac{\tilde{p}_0}{k_B} \exp\left[-\frac{1+\lambda+\lambda^{\Delta}}{\lambda-\lambda^{\Delta}} \right] . \quad (7)$$

Since $\lambda^{\Delta} > 0$, the effect of the interaction is essentially to *reduce* the critical temperature, very similar to the Coulomb interaction. Hence, it can be inferred that the resulting pair interaction is *repulsive* and pair breaking. This can also be understood on more physical grounds, since the gap and the phonon amplitude are dynamically correlated: An increase of the gap function increases the potential energy of the lattice and therefore requires energy (very much as decreasing the distance between the constituents of the Cooper pair increases the potential energy of the Coulomb field).

The repulsiveness of the interaction in homogeneous three-dimensional systems would, however, be reversed for specific structures with (alternate) layers of positive and negative T_c-pressure gradients, as sketched in Fig. 3. When this gradient $|\delta T_c/\delta p|$ is of the same magnitude in both materials, the dimensionless coupling constant λ^{Δ} in Eq. (7) reverses its sign, yielding $T_c(\lambda, -\lambda^{\Delta})$. For such structures, the interaction becomes attractive and T_c increases.

In conclusion, it can be said that this pair interaction, parametrized by a direct gap-phonon coupling, can be applied to all types of materials with strong T_c-pressure correlation, such as the two systems $2H$-$NbSe_2$ and $CeCu_2Si_2$ mentioned above. It has the potential for important contributions to the dynamics of such systems.

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