Test of s-wave pairing in heavy-fermion systems due to Kondo volume collapse

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It is proposed to utilize resonant Raman scattering on heavy-fermion superconductors as a test for Cooper pairing via an effective phonon-mediated attraction due to the Kondo volume collapse. The suggested experiment might help to discriminate between singlet and triplet pairing.

Since the discovery[1] of heavy-fermion superconductivity (HFS) in concentrated Kondo systems, there has been an intensive search for the explanation of its remarkable properties.[2] As this report intends no review of the basic phenomenology (see, for instance, Ref. 2), we shall only be concerned with the discussion of a proposal put forward by Fulde and co-workers recently:[3] Their proposal suggests to explain standard Cooper-type pairing by means of a phonon-mediated attraction due to Kondo volume collapse (KVC), whether the constituents of the bound state originate from conduction-band electrons,[3] or from electrons of the impurity f band.[4]

KVC can be understood[5] heuristically as a rearrangement of the lattice below the Kondo temperature ($T < T_K$), when all impurity spins are strongly screened by conduction-band electrons. Since HFS occurs below T_K, the above mechanism has been put forward as a good candidate for an attractive pair interaction, which binds the strongly hybridized, immobilized electrons favorably into a relative s state.[3,4] In some sense, this effect is very similar to the appearance of low-lying phonon modes in a charge-density-wave structure, although there the phonon softening has completely different origins.

The goal of this report is a proposal to test this hypothesis. On physical grounds its basis is the observation that whenever the lattice supports vibrations (phonons) whose frequencies are of the order of twice the superconducting gap parameter Δ, then there is a strong enhancement in the Raman spectrum near 2Δ. This is due to the high concentration of quasiparticles at these phonon energies, such that an enhancement in the scattering amplitude is encountered and real-pair excitation sets in. This reasoning goes back to quite similar arguments[6–9] for the charged-density-wave system $2H$-$NbSe_2$.

The existence of low-lying phonon modes proves indeed to be essential for a strong enough signature. In the case of a derivation of pairing from KVC, the average phonon frequency was assumed[3] to be about ($k_B = h = 1$) 200 K, yielding a far-too-high-lying spectrum for resonant Raman scattering when the gap is of the order of about 1 K [here, the BCS relation $\Delta(T=0) \sim 1.76 T_c$ and $T_c(CeCu_2Si_2) \sim 0.5$ K was assumed]. However, as a result of a cutoff for this mechanism at T_K, where the compensating spins break up, phonons with frequency equivalents above T_K contribute little to Cooper pairing.[3] Hence, the characteristic phonon frequency is of the order of T_K or less: Were there no low-lying phonon modes, the mechanism due to the KVC would not be effective. This inevitably brings the effective phonon spectrum within one order of magnitude down to the desired energy scale of 2 K.

The model which I use to study Raman scattering is the standard Fröhlich-type interaction between phonons and quasiparticles in the superconducting s state:

$$H_{e\text{-ph}}^{\text{int}} = g(b + b^\dagger) \sum_k \Psi_k^\dagger \tau_3 \Psi_k, \tag{1}$$

where b stands for the phonon field operator, the quasiparticle field $\Psi_k^\dagger = (c_{k\uparrow}^\dagger, c_{-k\downarrow})$ is written in the Nambu notation,[10] and $\tau_3 = \text{diag}(1, -1)$. Low-order radiative corrections to the phonon dispersion relation

$$\nu^2 - \omega_0^2 - 2\omega_0 \Pi(\nu) = 0, \tag{2}$$

where ω_0 is the bare phonon frequency, can be calculated from polarization processes, with the lowest-order contribution to the phonon polarization Π drawn in Fig. 1: When $\beta = 1/T$,

$$\Pi^{(2)}(\nu_n) = -ig^2 T \sum_{\omega_m = 2\pi(2m+1)T} \int \frac{d^3k}{(2\pi)^3} \text{Tr}[\tau_3 G^T(k, \omega_m + \nu_n) \tau_3 G^T(k, \omega_m)]. \tag{3}$$

The evaluation of Eq. (3) is straightforward[6–9] if one assumes a constant gap Δ. For $T \neq 0$, the result for $\nu < 2\Delta$ is

$$\Pi^{(2)}(\nu) = -8g^2 N(\varepsilon_F) \Delta^2 \int_0^\infty dx \frac{\tanh[\frac{1}{2}\beta\Delta\cosh(x)]}{4\Delta^2[\cosh(x)]^2 - \nu^2} . \tag{4}$$

This reduces for $T = 0$ to

$$\Pi^{(2)}(\nu) = -8g^2 N(\varepsilon_F) \frac{\Delta}{\nu(4\Delta^2 - \nu^2)^{1/2}} \tan^{-1} \frac{\nu}{(4\Delta^2 - \nu^2)^{1/2}} . \tag{5}$$

As can be inferred from the functional form of Eq. (5), there is a characteristic signature of the phonon spectral weight due to increased (virtual) scattering of quasiparticle-hole pairs as the phonon frequency approaches twice the gap value from below: $\nu \to 2\Delta -$. The spectral weight $S(\nu) = -(1/\pi)\text{Im}D(\nu)$ [here, $D(\nu)$ stands for the phonon propagator] for

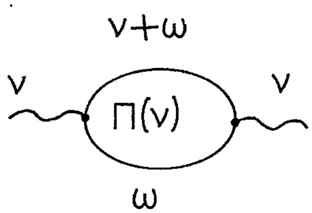

FIG. 1. Lowest-order contribution to the phonon polarization as evaluated in Eq. (3).

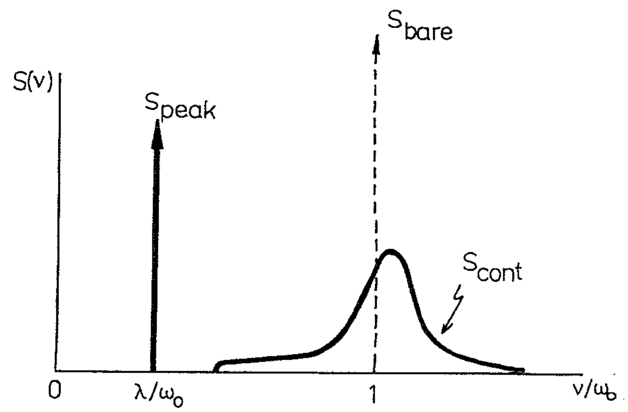

FIG. 2. The phonon spectral weight function due to polarization. Typical weight ratios between peak and continuum contributions are of the order of 10.

$\nu < 2\Delta$ is strongly peaked at $\lambda = [\omega_0^2 + 2\omega_0 \Pi(\lambda)]^{1/2}$ and for $\nu > 2\Delta$ broadened close to the bare phonon frequency (see Fig. 2). This effect should qualitatively pertain even for high-order contributions to the polarization Π in the case when Migdal's theorem is no longer valid. It gives rise to a strong enhancement of the Raman activity at a frequency below ω_0 (resonant Raman scattering). Since presently it is not possible to insert values for the parameters $\omega_0 \leq T_K (\sim 10$ K for $CeCu_2Si_2)$, $g^2 N(\varepsilon_F)$ ($\sim$ of the order of[3] 10^{-2}) and $\Delta \sim 1$ K from BCS estimates, only a qualitative picture of the phonon spectral weight has been drawn in Fig. 2. Nevertheless, the strong peak at λ should give a clear experimental signature.

A completely different behavior could be expected for gapless superconductivity[2] or for a magnitude of the gap which lies significantly lower than the BCS estimate. In this case, it would be very difficult to detect any signature, since the associated phonon frequency would be out of range of any conceivable experiment.

We now turn to the discussion of *s*- vs *p*-wave pairing discrimination for different scattering angles. Since the gap function in the relative $l = s = 1$ state (analogous to ^{3}He) is not isotropic and the superconducting order pertains up to macroscopic scales, deviations from isotropic *s* pairing ($l = s = 0$) could, at least in principle, be directly measured from resonant Raman scattering. In this case it is necessary to vary the angle of the incident beam relative to the sample. The situation is complicated by theoretical and technical obstacles, which I shall discuss below.

(i) Since the derivation of a resonant Raman scattering has been performed in the *s*-wave formalism, it can only be conjectured, that the same arguments hold true for triplet pairing as well. However, since the above arguments involved phase-space considerations, this can be expected.

(ii) Assuming a similar phase as for ^{3}He-*A*, with an angular dependence of the gap as $\Delta_{\mathbf{q}} = (\frac{3}{2})^{1/2} \Delta \sin(\mathbf{l}, \mathbf{q})$, where $\mathbf{q}$ stands for the phonon momentum and $\mathbf{l}$ is the angular momentum of the ($l = s = 1$) pair, this dependence on $\mathbf{q}$ could be readily smeared out by effectively averaging over great parts of the Fermi surface. For ^{3}He-*B*-type pairing, no anisotropy could be inferred from the very beginning, since there $\Delta_{\mathbf{q}} = \Delta$.

(iii) As has been shown[11] for H_{c2} measurements, the relative angular dependence of the (heavy) quasiparticle mass spoils the asymmetry argument.

(iv) Furthermore, all characteristic energy scales are very low. There have been Raman studies[12] on $CeAl_2$ down to 5 K and frequency shifts of 40 cm^{-1} (approximately 50 K). The scales of the suggested experiment are one order of magnitude lower, although not technically unfeasible.

In conclusion, it can be said, that under the assumption of a phonon mediated *s* pairing, resonant Raman scattering may be a decisive means to investigate the pair formation in heavy-fermion superconductors due to the Kondo volume collapse.

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