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Kohn anomaly in phonon driven superconductors

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Abstract. Anomalies often occur in the physical world. Sometimes quite unexpectedly anomalies may give rise to new insight to an unrecognized phenomenon. In this paper we shall discuss about Kohn anomaly in a conventional phonon-driven superconductor by using a microscopic approach. Recently Aynajian et al.'s experiment showed a striking feature; the energy of phonon at a particular wave-vector is almost exactly equal to twice the energy of the superconducting gap. Although the phonon mechanism of superconductivity is well known for many conventional superconductors, as has been noted by Scalapino, the new experimental results reveal a genuine puzzle. In our recent work we have presented a detailed theoretical analysis with the help of microscopic calculations to unravel this mystery. We probe this aspect of phonon behaviour from the properties of electronic polarizability function in the super-conducting phase of a Fermi liquid metal, leading to the appearance of a Kohn singularity. We show the crossover to the standard Kohn anomaly of the normal phase for temperatures above the transition temperature. Our analysis provides a nearly complete explanation of this new experimentally discovered phenomenon. This report is a shorter version of our recent work in JPCM.

Occurrence of Kohn anomaly in normal conventional metals predicted by W. Kohn [1] and soon after observed in experiments [2,3], is well understood over the past five decades [4]. This anomalous feature originates from the discontinuity of electron occupation number at the Fermi surface and the dielectric screening of the bare phonon modes by the electrons of the Fermi sea. In contrast, the apparent signature of the occurrence of the similar phenomenon even in elemental conventional superconductors, as observed experimentally in recent times, still look rather mysterious [5]. Based on an extension of our recent works [6,7], we present in this paper some quantitative aspect of our theoretical and microscopic analysis on the background of recent observations. The experiments involve resonant spin-echo spectroscopy with neutrons in real superconducting materials. Moreover, we also discuss the possible implications of these studies towards a full understanding of results from another important experimental technique viz. ultrasonic attenuation even for conventional superconductors, considering the various electron-phonon processes [8-10].

We begin with the results of our investigation mostly on the phonon dispersion due to the emergence of the superconducting gap in conventional superconductors. Recently Johnston et al. studied theoretically and computationally the consequences for the phonon line-widths under this situation [11]. They performed a standard BCS calculation of the phonon line-width and showed the ratio of twice the energy gap at T=0 to the Kohn energy ($2\Delta(0)/\hbar\omega_{qKA}$) is close to unity in comparison with the experiments of Aynajian et al. [5].

We calculate the frequency and wave-vector dependent total electronic polarizability function ($P_s(q, \omega)$) in the superconducting phase. All the details can be found in ref. [7]. Making use of the retarded and advanced fermionic Green functions corresponding to Bogoliubov quasi-particles and quasi-holes respectively, we obtain the polarization bubble in the random phase approximation (RPA).

In the static limit ($\omega \rightarrow 0$) the q-space derivative of the polarization function is

$$dP_s(q)/dq = (2\pi N(0)m / \hbar^2 k_F)\,[(-1/q^2)\ln(A/B) + (1/q)\,\{(1/A)(dA/dq) - (1/B)(dB/dq)\}], \qquad (1)$$

where $A = 2[(\{\hbar^2 q/(2m)(q-2k_F)\}^2 + \Delta^2]^{1/2} + (\hbar^2 q/m)(q-2k_F)$ and B is same as A excepting that in the expression $(q-2k_F)$ is replaced by $(q+2k_F)$. The quantities N(0), m, k_F, and Δ occurring in the above equation represent electronic density of states at the Fermi level for one kind of spin (in the normal phase), conduction electron mass, Fermi wave-vector and the superconducting gap respectively.

The q-space derivative of the electronic polarizability function as shown above, in the superconducting phase at T=0, evaluated at $q = 2k_F$ possesses the following property. When it is scaled down by the quantity $P_s(q=2k_F)/2k_F$, it exhibits a logarithmic divergence in the limiting situation of the superconducting coherence length ξ becoming either (i) extremely large or (ii) vanishingly small, in comparison to the lattice spacing or more correctly the average inter-electron distance. This spectacular feature in fact, is an analogue of Kohn singularity in the BCS superconducting phase and the very large coherence length limit is expected to be reached in the conventional phonon- driven superconductors implying that Kohn singularity can occur quite naturally in these systems [7].

By taking the limits $\Delta \rightarrow 0$ and $q \rightarrow 2k_F$ it can be seen easily from the previous expressions (see eqn. (1)) that in this limit $dP_s(q)/dq$ reducing to $dP_N(q)/dq$ diverges. Thus, we recover the usual Kohn singularity for normal metals, as expected from microscopic considerations.

Next we focus on the nature of the q-space derivative of the static electronic polarizability function for any general wave-vector and explore its relation with the renormalized phonon dispersion function as well. This is for a microscopic investigation into the possible existence of Kohn anomaly in real BCS superconductors with phonon based pairing mechanism.

For a superconductor at very low temperature, where the electron-phonon interaction is crucial for BCS superconductivity, the phonons get renormalized because of creation and destruction of quasi-particles and quasi-hole pairs in the electron-phonon scattering processes. Furthermore, in the case of elemental conventional superconductors, neglecting the vertex corrections in the spirit of Migdal's approximation the Dyson Equation for the phonon self-energy in the superconducting phase leads to the following approximate equation in the region $\omega << \omega_D$ [12, 7].

$$\omega^2(q) = \omega_0^2(q)\,[1 + |g(q)|^2 P_s(q)], \qquad (2)$$

where $\omega(q)$ and $\omega_0(q)$ are the renormalized and bare phonon dispersions respectively and $\omega_0(q)$ is taken according to the Debye model (relevant for an acoustic phonon). The quantity P_s is the polarizability function in the superconducting phase. Therefore, any anomaly in the dressed phonon spectrum has its origin in the functional property of this polarizability function. This nearly static approximation ($\omega \rightarrow 0$) would not lead to any signature of damping of the phonon modes. In fact, to study the complete effect on the line-width of the phonon modes, one has to go beyond the RPA for the polarizability function adopted here and to consider the vertex corrections in the finite frequency regime.

The above eqn. (2) leads to the following important relation between the derivative of the dispersion function and that of the polarizability function :

$$2\omega(q)\, d\omega(q)/dq = \omega_0^2(q)\, |g(q)|^2\, dP_s(q)/dq, \qquad (3)$$

assuming g(q) to be a rather slowly varying function of q or nearly a constant and hence we neglect its derivative with respect to q.

Now considering the experimental observation of Aynajian et al to be a genuine manifestation of Kohn anomaly in the superconducting phase [5], represented by the occurrence of the point of inflexion (not discontinuity or divergence) in the observed i.e. the renormalized phonon dispersion function at a wave-vector near $q = 2k_F$, we must have (making use of equation (3)),

$$[dP_s(q) / dq]_{q\sim 2kF} = 0. \quad (4)$$

Thorough examination and inspection involving the combination of the equations (1) and (4), lead to the conclusion that the equation (4) can indeed have solution quite close to $q = 2k_F$. In fact, the solution occurs at $q = 2k_F \pm \delta$, where $\delta << 2k_F$ and is +ve. Furthermore it turns out that δ is of the order of $\sim \Delta/\hbar v_F$, for $\Delta << E_F$ (which holds easily for weak coupling phonon mediated superconducting pairing) and v_F being the Fermi velocity.

Quite interestingly it is also found that the parameter δ is material dependent and is essentially of the order of the inverse of the superconducting coherence length. Therefore, the measurement of the latter would give an estimate for δ. Again it can be shown that in the limit $\Delta \rightarrow 0$, we have $\delta \rightarrow 0$ leading to the Kohn anomaly exactly at $q = 2k_F$. Thus, we recover the normal state scenario exactly.

Next we consider the pairing in the superconducting phase to be mediated by the phonons, as is the case with the elemental s-wave superconductors Pb and Nb, the likely candidates for exhibiting Kohn anomaly in the superconducting phase. This enables us to further rewrite the BCS equation for the superconducting gap at zero temperature by considering the mediator phonons to be predominantly the dressed phonons which themselves exhibit the Kohn anomaly at the onset of the superconducting transition from the normal state. Purely isotropic weak coupling BCS gap function (Δ_0) at T=0K would then satisfy the following approximate equation under such condition [assuming a jellium model and keeping in mind that at Kohn anomaly $\hbar\omega(q) = 2\Delta_0$] [7],

$$\Delta_0 \sim 3.5\, \Delta_0 \exp[-\hbar^2 (3\pi^2)^{(2/3)}/3n^{(1/3)}m|g_{eff}|^2], \quad (5)$$

where $|g_{eff}|^2$ is the Fermi surface averaged effective electron-electron (more correctly the Landau quasiparticle-quasiparticle residual) attractive interaction in the normal phase at the onset of superconducting transition, mediated primarily by the phonons undergoing Kohn anomaly at the same time and 'n' is the conduction electron density.

For simplicity, making use of the jellium model in calculating the usual BCS attractive coupling constant 'g' and incorporating the standard values for the parameters corresponding to the above elemental superconducting materials, we find that indeed the above equation (5) can be obeyed quite realistically. Therefore, our proposal that the observations of Aynajian et al indicate a true occurrence of Kohn anomaly in the phonon driven BCS superconducting phase of a 3d Fermi Liquid metal has a very strong microscopic support.

Our work presented here has an interesting and a very natural connection with the acoustic attenuation problem studied both theoretically and experimentally earlier for some of the conventional BCS superconductors [8-10, 12]. In particular, the notable feature of ultrasonic waves exhibiting a discontinuity in attenuation at energy of the phonon equal to twice the superconducting gap, even at finite temperature as observed in various experimental phonon mechanism based 3-dimensional superconducting systems like Nb and Nb_3Sn, are directly related to our investigation reported here [8]. In fact abrupt changes in phonon life times have also been detected near T_C in Nb_3Sn. These results are very much consistent with the observed peak in the phonon line-width occurring at the above mentioned value of phonon energy seen in the very high resolution measurements involving resonant spin echo spectroscopy with neutrons [5]. The magnitude of the jump or discontinuity in the ratio of attenuation in the superconducting state to that in the normal state was predicted to be the highest (about 1.57) for energy of the ultrasonic phonon equal to twice the superconducting gap [9]. This feature is unlike that seen for the usual phonon attenuation in the pure acoustic regime ($\hbar\omega/2\Pi << 2\Delta$) both experimentally and theoretically [14]. Moreover, there is a substantial phonon softening (about 3%) observed below T_C in Nb_3Sn [8, 10].

The detailed quantitative calculation of the line-width or attenuation for these ultrasonic phonons around Kohn anomaly point can be carried out by retaining the frequency dependence in the self-energy diagrams corresponding to our calculations involving quasi-particle-quasi-hole excitations and preferably with inclusion of vertex correction as well. Johnston et al. have done such a calculation (neglecting vertex corrections) taking into account also the electronic structure for Pb and Nb [11]. However, the very important change in the phonon dispersion function from the bare linear one near q_{KA} is completely neglected in their calculation. Alternatively, it is easier to understand the substantial enhancement of attenuation at Kohn anomaly point in terms of simple 'Fermi's golden rule' type of calculations by considering the increase in the number of possible scattering channels in this region.

The possibilities of occurrences of Kohn singularity and Kohn anomaly with non-conventional pairing schemes in exotic systems are rather hypothetical ones , since no materials belonging to this class have been found to exhibit these effects clearly either in the normal or in the superconducting phases. Some of these questions have been discussed by Flatte [13].

In summary**, i**n this short report we have tried to present a more realistic analysis of the occurrences of both Kohn singularity and Kohn anomaly in the superconducting phase, keeping in mind the real condensed matter systems. Our calculations strongly indicate that the acoustic dispersion can indeed display anomaly at the phonon energy equal to 2Δ in the real phonon driven BCS superconductors. We also highlight that our microscopic approach is very different from that proposed in [5, 14-16] for an explanation of Kohn anomaly in superconductors. Besides, our analysis and calculational results establish a genuine and strong microscopic justification for the observations of Aynajian et al. regarding the simultaneous occurrences of both singularity in phonon dispersion function and a sharp peak in phonon line-width, to be unified and identified with a Kohn anomaly in the BCS superconducting phase based on phonon mechanism for pairing. This is in sharp contrast to the proposal of Johnston et al. [11] that these two phenomena are different and the strong similarity between them is just a coincidence.

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