Kohn Anomaly in Conventional Superconductors: A Surprise

M.P. Das[a] and R. Chaudhury[b]

[a]*Research School of Physics and Engineering, The Australian National University Canberra 0200, Australia.*
[1]Email: mukunda.das@anu.edu.au
[b]*S. N. Bose National Centre for Basic Sciences, Sector-3, Block-JD,Salt Lake Kolkata 700098, India*

Kohn anomaly occurs in normal metals as a kink in the phonon spectrum around $2k_F$, arising out of screened Coulomb interaction. Recently as a major surprise, neutron spin-echo experiments on elemental (conventional) superconductors Pb and Nb reveal a very important and striking relation that Kohn (anomaly) energy, w_{KA} equals twice the superconducting gap energy, $\Delta(0)$. From the theoretical perspective the Kohn anomaly and the BCS pairing theory do not seem to belong to a common platform. In this paper we explore the microscopic origin of this novel phenomenon and discuss its implication to the standard model BCS theory.

1. Introduction

Occurrence of Kohn anomaly in a metallic system, normal or superconducting, depends on the nature of screening of the electric field of the ionic lattices. The latter determines the energy and lifetimes of phonons. In the normal metals, which are so successfully described by the Fermi liquid theory, the Kohn singularity arises as a consequence of sharp discontinuity of the electron distribution function f_k in the momentum space. The k-space gradient of the longitudinal static dielectric function exhibits a logarithmic divergence at $2k_F$, where k_F is the Fermi momentum.

In 1959 Walter Kohn [1] examined the longitudinal static (ω=0) dielectric function. This function screens the effective ionic pair potentials in the q-space. Kohn showed that for $q < 2k_F$ (q is the phonon momentum) virtual excitations are created with conservation of energy, while for $q > 2k_F$ such excitations are no longer possible. Therefore, the KA arises from the discontinuity of the Fermi function. Kohn predicted that the logarithmic singularity of the dielectric function produces a kink in the phonon spectrum and one sees the image of the FS at $2k_F$. Within a couple of years Kohn anomaly was experimentally observed by Brockhouse , Rao and collaborators [2,3] in the normal phase of Pb. Following this result a number of authors also observed Kohn anomaly in many metallic systems, particularly more in lower dimensions [4].

2. Phonons in Superconductivity

Phonons have a pivotal role in various properties of condensed matters. The Bardeen-Cooper-Schrieffer (BCS) pairing theory for superconductivity has been quite successful for the interpretation of most of the experimental data obtained from the conventional low-temperature superconductors. In this theory the attractive pairing interaction arises from the mediation of phonons to the pair of electrons near the Fermi surface. Nevertheless, the theoretical formulation of the BCS suffers from several limitations. In the simple BCS calculational framework the pairing interaction $V_{k,k'}$ is simplified by a square well model. This incorporates the static electronic screening effects in the long wave-length limit of the random phase approximation (RPA) as appropriate to a metal; however it neglects the detailed phonon spectrum of the material. In the strong coupling version of the pairing, what is known as Eliashberg theory for the conventional superconductors, the role of phonons are explicit and are worked out in detail (see for example, J. Carbotte [5]). However, its implication to Kohn anomaly seems to have scanty discussion/analysis in the literature. In this context Scalapino [6] notes -"Although the effective pairing interaction involves phonons, it is difficult to see any direct connection between the Kohn anomaly energy and the energy gap."

The recent neutron spin-echo experiments by Aynajian et al. [7] on elemental conventional superconductors Pb and Nb in the superconducting phase, question this conventional wisdom. It clearly brings out the severe limitation of the conventional treatment of the superconducting phase and the pairing mediated by the phononic modes, for not including all the characteristics of the dielectric response function of the system. More elaborately, this highlights the utmost importance of the restructuring and refinement of the conventional BCS/Eliashberg scheme with incorporation of the salient features of the electronic (quasi-particle) spectrum in the superconducting phase. Besides, these new experiments also motivate one to theoretically calculate the phonon lifetime or linewidth in the superconducting phase.

3. Results

Mathematically, the phenomena of Kohn anomaly can be briefly described in the following way: The static (ω=0) electronic polarizability function P(q) for the normal electrons in a 3-dimensional metal is given in RPA as

$$P(q) = (N(0)/4x)\,[2x + (1-x^2)\ln|(1+x)/(1-x)|],$$

where x is given as $x= [q/ 2k_F]$; k_F being the Fermi wavevector and N(0) is the electronic density of states at the Fermi surface. The corresponding longitudinal dielectric function is given as

$$\varepsilon(q) = 1+ [4\pi e^2/q^2]P(q)$$

The above electronic dielectric function possesses the property that its derivative with respect to q diverges at $q = 2k_F$. This result is the well-known Kohn singularity.

When one studies a coupled electron-phonon system in a normal metal within the RPA and the resulting phonon modes are calculated with the above dielectric function, the phonon dispersion function $\omega(q)$ is found to display a singularity at $q=2k_F$. More precisely, the q-space derivative of the real part of the dynamic dielectric function corresponding to the electronic component, diverges at q near $2k_F$. This causes the screened phonon dispersion function itself to exhibit non-analyticity from the following relation.

$$\partial\,[\mathrm{Real}\ \{\varepsilon(q,\omega_{\mathbf{q}})\}] / \partial q = \text{infinity for } q = 2k_F\,,$$

This happens at that value of ω_q, which we call energy of Kohn anomaly. It is naturally expected to be much smaller than the frequency corresponding to the Fermi energy E_F.

A much more challenging task in condensed matter physics is the theoretical exploration starting from a microscopic model to answer the question whether the Kohn anomaly can also occur in the superconductors. The recent experimental observations (Aynajian et al. [7]) with clear signature of the Kohn anomaly in the superconducting phases of Pb and Nb have provided fresh impetus to initiate theoretical investigations. Here we establish the microscopic origin of these effects by presenting our results based on some simple (at the level of RPA) preliminary calculations and arguments.

First of all, we calculate the electronic polarizability corresponding to a BCS superconductor under the mean field treatment. This can be done in a straightforward way by making use of Bogoliubov transformation to diagonalise the mean field BCS Hamiltonian in terms of the non-interacting fermionic quasi-particles. One can then apply the standard linear response theory to calculate the electronic response functions.

The detailed and elaborate calculations involving the above approach lead to the result that indeed the static electronic (quasi-particle-quasi-hole) polarizability in a BCS superconductor exhibits singularity at $q = 2k_F$ under certain conditions.

$$\{ 2k_F [\partial P_s(q)/ \partial q] /[P_s(q = 2k_F)] \} \approx 2 \ln [2/ (k_F\xi)],$$

where, P_s is the electronic polarizability in the superconducting phase, ξ is the superconducting coherence length given by $\xi = k_F/\pi\Delta$ and the numerator (the derivative) is evaluated at $q = 2k_F$.
The above expression shows that the polarizability diverges logarithmically at the wave-vector $2k_F$, when the superconducting coherence length becomes very large or extremely small with respect to the lattice spacing. This is a very genuine manifestation of "Kohn-like singularity"! Thus, the true Kohn anomaly behaviour is expected to occur both in the conventional weak coupling superconductors as well as in the novel superconductors characterized by the "real space pairing", independent of the mechanism for the pairing interaction. It is also worthwhile to remark that we do recover the usual Kohn singularity appropriate to the normal metal from our expression, in the limiting case of the superconducting gap becoming vanishingly small.

The next important issue is the theoretical investigation of the consequences for the phonon spectrum in the presence of the above Kohn-like singularity. The aim obviously is to examine if there exists a Kohn anomaly in the superconducting phase. The microscopic input required for this study appears in the form of an additional term describing the coupling between the Bogoliubov quasi-particles and the phonons, in the Hamiltonian. The objectives are two-fold. First of all, it is important to investigate whether the Kohn-like singularity leads to a non-analyticity in the phonon-dispersion function. Secondly, it also enables us to calculate the line-widths of the phonon modes under this condition to examine whether the theoretical line-widths exhibit the same behaviour as shown by the experimental ones. It is quite remarkable that the experimental line-widths are found to acquire a maximum at the phonon energy equal to 2Δ. This implies a very strong coupling between the phonon modes and the quasi-particles in the superconducting phase.

The coupling between the Bogoliubov quasi-particles and the phonons is derived from the usual electron-phonon interaction by taking into account the Bogoliubov transformation matrix elements. It may be recalled that these transformation matrix elements connect the quasi particle operators (of the superconducting phase) to the normal electron operators. Thus, the effective Hamiltonian for studying the Kohn anomaly in the superconducting phase becomes very similar to that used in the normal metallic phase, except for the presence of the appropriate BCS coherence factors (Schrieffer [8]). The detailed nature of the Kohn anomaly in the superconducting phase is therefore also decided by the wave-vector dependence of these coherence factors. The dressed phonon frequency spectrum $\omega_q \sim q$ produced by the dielectric response of the quasi-particles (ε_s) in the superconducting phase is determined under the RPA. The minimum quasi-particle-quasi-hole pair creation energy 2Δ is hidden here through the expressions for the dynamic electronic polarizability and is the prime source for the location (position) of the occurrence of Kohn anomaly in the superconducting phase. The dressed phonon spectrum exhibits all the principal features of Kohn anomaly seen experimentally in the phonon dispersion function ($\omega_q^{\{exp\}}$ vs. q) (Aynajian et al. [7]).

4. Conclusion

In summary, we discuss here the important microscopic processes responsible for the Kohn anomaly observed experimentally in the superconducting phases of some of the conventional superconductors. The confirmed appearance of this anomaly in the superconducting phases of real materials has tremendous consequences for the microscopic theories as well. It brings out the genuine need for a modification and an improvement over the conventional approach followed within the BCS pairing theory.

For the superconductors based on the phonon mediated pairing, the BCS theory assumes the phonon spectrum to remain essentially unchanged when the metal becomes superconductor. The occurrence of Kohn anomaly at the phonon energy of 2 times the superconducting gap Δ in the experiment of Aynajian et al, is a kind of challenge to this assumption. The incorporation of Kohn anomaly in the modelling of the BCS pairing interaction would be of immense importance towards achieving the goal of correct understanding of real superconducting materials.

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