Kohn anomaly occurs in metals as a weak but discernible kink in the phonon spectrum around $2k_F$ arising out of screened Coulombic interaction. Over the years this has been observed in a number of normal metallic systems. As a major surprise however, the recent neutron spin-echo experiments on elemental (conventional) superconductors Pb and Nb reveal a very important and striking relation that Kohn (anomaly) energy equals twice the energy of the superconducting gap. In this paper we explore the microscopic origin of this novel phenomenon and discuss its implication to the standard model BCS Theory.

Keywords: Kohn anomaly; Kohn singularity; superconducting gap.

1. Introduction

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. Nevertheless, the theoretical formulation of the BCS suffers from several limitations. Most of the low-temperature superconductors are based on the phonon-mediated attractive pairing interaction. 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. More importantly, the effects of various special characteristics of the
electronic response functions either in the normal metallic phase or in the superconducting phase, particularly on the phonon energy and the linewidth are generally neglected. Although Brockhouse et al.\textsuperscript{1,2} made the first experimental observation of Kohn anomaly\textsuperscript{3} in normal metallic systems, such studies on superconductors were carried out only very recently, as late as in 2008. From the theoretical perspective too, the BCS model and the Kohn anomaly did not seem to belong to the same platform and were treated as rather two independent entities.

Occurrence of Kohn anomaly in a metallic system, normal or superconducting, depends on the nature of screening of the electric field of the ionic lattice. The latter determines the energy and lifetimes of phonons. It is worthwhile to mention that in the strong coupling version of the pairing (Eliashberg) theory for the conventional superconductors, the role of phonons are explicit and are worked out in detail (see for example, Marsiglio and Carbotte\textsuperscript{4}). However, its implication to Kohn anomaly seems to have scanty discussion/analysis in the literature. In this context Scalapino\textsuperscript{5} 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.\textsuperscript{6} on elemental conventional superconductors Pb and Nb in the superconducting phase, raises some interesting question on the conventional wisdom. It clearly brings out a 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, invoking the electron-phonon interaction under the Fermi golden rule scheme.

In a simple demonstration as done here, we would like to examine if the wave-vector at which the phonon linewidth exhibits the maximum, truly corresponds to the renormalized phonon energy of $2\Delta$ ($\Delta$ being the superconducting gap), as observed experimentally by Aynajian et al.\textsuperscript{6} Interestingly, the phonon dispersion function also shows an anomaly at around the same energy.\textsuperscript{6}

2. Kohn Anomaly In A Normal Metal

The Kohn singularity\textsuperscript{3} in the normal electron response function in a metal at low temperature, is a consequence of the sharp discontinuity of the electron distribution function in the momentum space at $k_F$, the Fermi wave-vector. This holds true for an ideal Fermi gas as well as for the Fermi liquid model (a model successfully describing real simple metals). Mathematically, it is manifested as the $k$-space gradient of the longitudinal static dielectric function exhibiting a logarithmic divergence at $2k_F$. This result can be readily derived from the RPA treatment of the weakly
interacting 3-dimensional electron gas, as was first shown by Kohn\(^3\) on the basis of the Lindhard response function\(^7,8\) for the electron-hole polarizability. Interestingly, when the combined system of interacting electrons and phonons are considered and treated under the RPA, the phonon spectrum gets renormalized. Moreover, the dispersion function of the renormalized phonons exhibits a non-analyticity viz. the k-space gradient of the dispersion function diverges at \(2k_F\). This property of the phonons in normal metals is the well-known “Kohn anomaly”. The origin of this anomaly is undoubtedly the Kohn singularity of the normal electron response function. The Kohn anomaly has been experimentally observed and confirmed in the normal phase of metals such as Pb\(^1\), where the electron-phonon coupling is rather strong.\(^7\)

Mathematically, the phenomena of Kohn singularity and Kohn anomaly can be briefly described in the following way:- The static electronic polarizability function \(\Pi(q)\) for the normal electrons in a 3d metal is given in RPA as

\[
\Pi(q) = \frac{N(0)}{4\pi} [2x + (1 - x^2)\ln |(1 + x)/(1 - x)|] 
\]

where \(x\) is the reduced wave vector and is given as \(x = \frac{q}{2k_F}\); \(k_F\) being the Fermi wavevector and \(N(0)\) is the electronic density of states at the Fermi surface for one kind of spin. The corresponding longitudinal dielectric function is given as

\[
\epsilon(q) = 1 + \frac{4\pi e^2}{q^2} \Pi(q) 
\]

The above electronic dielectric function can be shown to possess the property that its derivative with respect to \(q\), the wave vector, diverges at \(q = 2k_F\). This result is the well known Kohn singularity. Although, the above analysis is based upon a treatment corresponding to zero temperature, it is realistically valid for all temperatures \(T < < T_F\).

When one studies a coupled electron-phonon system in a 3d normal metal within the RPA and the resulting screening of the phonon modes is performed with the above dielectric function, the phonon dispersion function is found to display a singularity as well. 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. These may be described mathematically as,

\[
\frac{\partial [\text{Real}(\epsilon(q,\omega_q))]}{\partial q} = \infty 
\]

for \(q \approx 2k_F\), where \(\omega_q\) is the screened phonon frequency and is expected to be much smaller than the frequency corresponding to the Fermi energy \(E_F\).

The above electronic dielectric function when incorporated in the analysis of the coupled electron-phonon system within RPA, gives rise to the phenomenon of Kohn anomaly in the normal metal.
3. Kohn Anomaly In A Conventional Superconductor

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 of Aynajian et al. 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 for a superconductor, as modelled by BCS, 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.

Mathematically, it is manifested in the following expressions

$$\frac{2k_F \partial \Pi_s(q,0)}{\Pi_s(2k_F,0)} = 2 \ln \frac{2}{k_F \xi}$$

where, $\Pi_s$ is the electronic polarizability in the superconducting phase, $\xi$ is the superconducting coherence length and the numerator (the derivative) is also 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-like singularity 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 very 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 usual BCS Hamiltonian. The objectives are two-fold. First of all, it is very 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 linewidths of the phonon modes under this condition to examine whether the theoretical linewidths exhibit the same behaviour as shown by the experimental ones. It is quite remarkable that the experimental linewidths are found to acquire a maximum at the phonon energy equal to $2\Delta$. This probably 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 can be 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 (see also). These factors denoted by 'm' and 'n', are given by the following expressions:-

$$m(k, k') = u_{k'}v_k + u_kv_{k'}$$

and

$$n(k, k') = u_{k'}u_k - v_{k'}v_k$$

where $u$ and $v$ are the well known Bogoliubov coefficients; the quantity $q = k' - k$ denotes the wavevector of the phonon mediating the pairing interaction with $k$ and $k'$ being the electron wave-vectors. 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 screened phonon frequency spectrum $\tilde{\omega}_q$ produced by the dynamic (frequency dependent) dielectric response of the quasi-particles ($\epsilon_s$) in the superconducting phase, can also be easily determined under the RPA. Interestingly, the minimum quasi-particle-quasi-hole pair creation energy $2\Delta$ 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 renormalized phonon spectrum is expected to exhibit all the principal features of Kohn anomaly seen experimentally in the phonon dispersion function ($\omega_{QP} vs. q$).

The above formalism is also powerful enough to perform a calculation of the quasi-particle-phonon scattering rate in the superconducting phase, using the Fermi golden rule. The linewidth of the phonon modes ($\gamma_q$) is directly proportional to the scattering rate ($\frac{1}{\tau}$), which in turn can be calculated by making use of the quasi-particle-phonon interaction matrix elements and the average occupation numbers of these particles. Hence the contribution due to the above process can be estimated quantitatively at various temperatures in the entire $q$-space. This provides a very
direct route for the comparison of the theoretical predictions with the experimental results of Brockhouse et al.\textsuperscript{2} and Aynajian et al.\textsuperscript{6} and further strengthens the basis of our formalism.

4. Summary

In summary, we have tried to put forward and describe in this short note 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 two times the superconducting gap $\Delta$ in the experiment of Aynajian et al., challenges this assumption. These studies further imply that in the weak coupling BCS approach, the conventional static square well model for the phonon-induced effective attraction $V_{\text{eff}}(\omega = \zeta - \zeta')$ between the electrons ($\zeta$'s are the effective single electron energies measured from the chemical potential in the normal state) must be replaced by a more appropriate interaction kernel. This new realistic interaction function will have to include the contributions due to the presence of the expected non-analyticity in the phonon spectrum in the superconducting phase itself. Thus, the calculational scheme becomes much more self-consistent than in the usual treatment. This requires very sophisticated many-body approach to handle it.

Last but not the least, the incorporation of Kohn anomaly in the modelling of the BCS pairing interaction would be of immense importance towards achieving the goal of correct estimation of $T_c$ for real superconducting materials, driven by mechanism based on phonon mediated attractive interaction.

Further work involving detailed calculations is in progress.

References