Chapter 4

Theory of detection of x-rays by superconductors

Two new processes occur in a superconducting film when it is used as a detector of x-rays. One of these processes is the scattering of the x-ray by a single electron which gives rise to the broadening of the x-ray line. Another process describes the breaking of a Cooper pair by the x-ray which also contributes to the width of the x-ray. The line width arising from the single electron process depends on $T^4$ whereas that arising from the pair breaking process varies almost as $T^6$ at low temperatures. Lines occur at $\hbar \omega \pm 2\Delta$, and at $\hbar \omega_q$ where $\hbar \omega_q$ is the energy of the x-ray and $2\Delta$ is the gap of the superconductor.
Recently, the superconducting tunnel junctions have been used to measure the nonequilibrium quasiparticle population caused by the x-rays absorbed into the superconducting thin films. This energy breaks the Cooper pairs and the resulting quasiparticles tunnel across the barrier until they recombine to form Cooper pairs. A measurement of this current gives a measure of the x-ray energy. It is possible to achieve energy resolution better than 10 eV for 6 KeV x-rays [1]. Niobium based x-ray detector being developed [2] for the European Space Agency requires a highly theoretical approach combined with advanced device process development. The latest work demonstrates an exceptional energy resolution of 53 eV when cooled to 1.5 K. The superconducting films of NbN/BN have been shown to exhibit photoresponse to visible light [3]. It has been pointed out by Jochum et al [4] that new detectors have initiated important discoveries. Kraus et al[5] have pointed out that the rate of relaxation of particles down to the gap edge is,
\[ \gamma \propto E^3/\tau_o \]
where \( E \) is the energy of excitations and \( \tau_o \) is a time constant characteristic of the material. Several properties of the detectors of x-rays using superconducting junctions have been reported [6-9] but the quantum theory of widths and shifts has not yet been solved. The phonon scattering has been considered to be important [10-14] for the processes to take place but Burstein et al [15] have considered the use of superconductors as detectors of microwaves in which the photons play an important role. In the B.C.S. theory [16], the phonon operators of the Hamiltonian are eliminated to derive the attractive interaction between the electrons so that the phonon effects are found in the coupling constant. Thus the pair formation and breaking by phonons is stronger than by photons but the frequency of the x-ray is very large so that the two, phonon and photon resonances are far apart and hence do not interfere. Therefore it is of interest to determine the spectrum of the scattered
x and 7-rays. The solar x-rays can be detected using the superconductors. However, a monochromatic source of x-rays and a detector, both with an energy resolution of the order of the superconducting gap is not yet available. When ever such a technology is developed it will be necessary to have a calculation of shifts and widths, particularly because the widths determine the resolution of the instrument. Hence our calculation is of interest in the area of astrophysics and astronomy also. Further, the prospects of developing superconducting tunnel junctions as efficient detectors of x-rays[24] makes the study of detection of x-rays using superconductors more interesting.

In this work, we construct the Hamiltonian for the interaction of x-rays with Cooper pairs in a superconductor. As the x-ray hits the Cooper pair, it breaks the pair into two electrons and the x-ray is scattered. The spectrum of the scattered x-ray consists of several frequencies. One of the frequencies is the same as that of the incident x-ray, $\hbar \omega_q$, as in the Rayleigh scattering and there are sidebands at $\hbar \omega_q \pm 2\Delta$. We have performed the Bogoliubov transformation on the pair breaking interaction which we have used to calculate the self energy of the x-ray. This self energy corresponds to a broadening of the x-ray. We find that in a three dimensional superconductor, this broadening depends on temperature as $T^4$ for the electron scattering process and as $T^6$ for the pair breaking process at low temperatures.

We consider the x-rays interacting with the conduction electrons so that the unperturbed Hamiltonian of the system is described as,

$$H_o = \sum_q \hbar \omega_q \beta_q^\dagger \beta_q + \sum_{k,\sigma} \epsilon_{k,\sigma} (c_{k,\sigma}^\dagger c_{k,\sigma} + c_{-k,-\sigma}^\dagger c_{-k,-\sigma})$$  \hspace{1cm} (1)$$

where $\hbar \omega_q$ is the single particle energy of one x-ray. The $\beta_q^\dagger$ and $\beta_q$ are the boson creation and annihilation operators for the x-ray. The single particle energy of the electrons of wave
vector $k$ and spin $\sigma$ in the conduction band is $\epsilon_{k\sigma}$. The wave vector of the x-ray is $q = \omega/c$ where $c$ is the velocity of light. The attractive interaction between the electrons is given by

$$H_a = -V \sum_{k,k'} c_{k',\sigma}^\dagger c_{-k,-\sigma}^\dagger c_{-k,-\sigma} c_{k,\sigma}$$

This interaction is useful for the formation of spin singlet zero momentum pairs as in the B.C.S. theory [16,17] and is diagonalized by the

$$c_k = u_k d_k + v_k d_k^\dagger$$

where $k$ is associated with spin $\sigma$ and $-k$ with $-\sigma$. The coefficients $u_k$ and $v_k$ are real, where $u_k$ is an even function of $k$ and $v_k$ is an odd function of $k$, $u_k = u_{-k}$, $v_{-k} = -v_k$ with $u_k^2 + v_k^2 = 1$. The gap is written in terms of pair operators,

$$\Delta_k = V \sum_{k'} c_{-k,-\sigma}^\dagger c_{k,\sigma}$$

$$\Delta_k^* = V \sum_{k'} c_{k,\sigma}^\dagger c_{-k,-\sigma}$$

The interaction of the x-ray photon with the conduction electrons is described by

$$H'_{pe} = i \sum_{k,k',q} G_{k,k',q} c_{k',q}^\dagger c_{k,\sigma} \beta_q^\dagger \delta(k - k' - q)$$

$$+ i \sum_{k,k'',q} G_{k,k'',q} c_{k'',q}^\dagger c_{-k,\sigma} \beta_q \delta(k'' - q + k) + h.c.$$

where $G = gV^{-1/2}$ with

$$g = \frac{e\hbar}{mc} \left( \frac{\hbar \omega_q}{\kappa} \right)^{1/2}$$

where $\kappa$ is the dielectric constant of the medium and $m$ is the mass of the electron. One of the terms in the second-order energy operator of the above interaction is given by

$$H'_2 = - \sum_{k,k',k'',q,q'} (\epsilon_{k'} - \epsilon_k + \hbar \omega_q)^{-1} G_{k,k',q} G_{k,k'',q} c_{k'',q}^\dagger c_{-k,k'} \beta_q^\dagger \beta_q \delta(q - k' - k'' - q') + h.c.$$
Using anti commutators for the electron operators, the product of the electronic operators in the above can be written as

\[
\hat{c}^+_{k\mu} e_{-k\nu} \hat{c}^+_{k\nu} e_{k\mu} = \delta_{k,k''} \hat{c}^+_{k\mu} e_{k\mu} - e_{-k\nu} \hat{c}^+_{k\nu} e_{k\nu} - \delta_{k,k'} \hat{c}^+_{k\mu} e_{k\mu} + e_{-k\nu} \hat{c}^+_{k\nu} e_{k\nu}
\] (8)

from which leaving out the first three terms which describe single particle electron scattering by photons, we write the interaction corresponding to pair formation and breaking as

\[
H'_2 = \sum_{k,k',k'',q,q'} (\epsilon_{k'} - \epsilon_k + \hbar \omega_{q'})^{-1} G_{k,k',q} G_{k,k'',q} e_{k} \hat{c}^+_{k\mu} \hat{c}^+_{k\nu} e_{-k\nu} \hat{c}^+_{k\nu} e_{k\mu} \delta(q - q' - k' - k'')
\] (9)

Including the sum over intermediate states, one more contribution to the above interaction occurs which we calculate and include in the above so that

\[
H''_2 = \sum_{k,k',k'',q,q'} \left[ (\epsilon_{k'} - \epsilon_k + \hbar \omega_{q'})^{-1} + (\epsilon_{k''} - \epsilon_{-k} + \hbar \omega_{q''})^{-1} \right] G_{k,k',q} G_{k,k'',q} \times e_{k} \hat{c}^+_{-k\mu} \hat{c}^+_{k\nu} \beta^\dagger_q \beta^\dagger_{q'} \delta(q - q' - k' - k'') + h.c.
\] (10)

This means that the x-ray photons can break pairs of electrons into single electrons and pairs can be made by shining x-rays on electrons but the electromagnetic energy, \(H^2/8\pi\), is small compared with \(k_B T_c\). Hence this mechanism is too small to predict the transition temperatures but it can be effective for detecting x-rays, due to different frequency regime. Since the wave vector dependence in the coupling constant is small, we write the above interaction as,

\[
H' = \sum_{\sigma} \sum_{k,k',k'',q,q'} D_{k,k',k'',q,q'} \beta_{q'} \beta^\dagger_q e_{k,\sigma} \hat{c}^+_{-k,\sigma} \hat{c}^+_{k',\sigma} \hat{c}^+_{k'',\sigma} \delta(q - q' - k' - k'') + h.c.
\] (11)

where \(h.c.\) stands for the hermitian conjugate of the previous terms. Using the commutators for bosons and anticommutators for fermions, the above interaction can be written as,

\[
H = H'_a + H'_s + H'_p
\] (12)
where the first term in (13a) is a constant. The second term describes a small negative shift in the x-ray energy. The third term gives the reduction in the single particle energy of electrons in the conduction band. The term given by (13b) is a positive pairing interaction and hence its effect is to reduce the strength of attractive interaction given by (2). The expression (13c) shows that the x-rays are scattered by single electrons and (13d) shows that pairs are broken by the x-rays. Upon rearranging the various terms, the Hamiltonian of the system becomes,

\[ H = H_0 + H'_a + H'_s + H'_p \]  
(14)

where

\[ H_0 = \sum_{\sigma} \sum_{k,q} D_{k,q} \rightarrow \sum_{\sigma} \sum_{k,q} D_{k,q} \beta_{q}^{\dagger} \beta_{q} - \sum_{\sigma} \sum_{k,q} D_{k,q} (c_{k,\sigma}^{\dagger} c_{k,\sigma} + c_{-k,-\sigma}^{\dagger} c_{-k,-\sigma}) \]  
(15)

\[ H'_a = -V \sum_{k'_q} c_{k'_q,\sigma}^{\dagger} c_{-k'_q,-\sigma} c_{-k,-\sigma} c_{k,\sigma} \]  
(16)

with
\( \hbar \omega'_q = \hbar \omega_q - \sum \epsilon_{k,q} D_{k,q} \) \tag{17a}

\( \epsilon'_{k,\sigma} = \epsilon_{k,\sigma} - \sum q D_{k,q} \) \tag{17b}

and

\( V' = V - \sum q D_{k,k',q} \) \tag{17c}

in which the first term is a constant and the single particle energy of the x-ray has been slightly reduced. Similarly, the single particle energy of the electrons is also reduced by a small amount. The transformation (3) substituted in (16) gives the ground state energy with single particle energies shifted by the pair breaking energy \[17\]. The transformed form of the scattering interaction of (13c) is found to become,

\[
H'_s = \sum \sum D_{k,q,q'} v_{k} v_{k'} \beta_{q'}^{\dagger} \beta_{q} + \sum \sum D_{k,k'',q,q'} (u_{k} u_{k''} \beta_{q'}^{\dagger} \beta_{q} d_{k''}^{\dagger} d_{-k})
+ v_{k} v_{k''} \beta_{q'}^{\dagger} \beta_{q} d_{k}^{\dagger} d_{-k''} \delta(q - q' - k - k'') + h.c. \] \tag{18}

There are terms with \( k \) replaced by \(- k\) and also charge non-conserving terms containing factors of the type \( d_{-k''} d_{-k} \) or \( d_{k}^{\dagger} d_{k''}^{\dagger} \) but all such terms cancel each other so that there is no charge non-conserving interaction. The pair breaking Hamiltonian may be expressed as

\[
H'_p = H'_p(0) + H'_p(1) + H'_p(2) + H'_p(3) + H'_p(4) \tag{19}
\]

where

\[
H'_p(0) = \sum \sum D_{k,k',q} u_{k} u_{k'} v_{k} v_{k'} (d_{k}^{\dagger} d_{k} - d_{-k}^{\dagger} d_{-k}) \beta_{q'}^{\dagger} \beta_{q}
+ 2 \sum \sum D_{k,k',q,q'} v_{k} v_{k''} d_{k'}^{\dagger} d_{-k''} \beta_{q'}^{\dagger} \beta_{q} \delta(q - q' - k' - k'') + h.c. \tag{20}
\]

Upon decoupling, it is seen that this interaction gives a shift in the single particle frequency of the x-ray which depends on the number density of electrons. The second term in (20)
gives the electron scattering within a band. Next we write the terms which contain a pairing operator of the form $d_k d_{-k}$ which annihilates a fermion pair as,

$$H'_p(1) = \sum_{\sigma} \sum_{k,k'',q} D_{k,k'',q} u_k^2 u_{k''} v_{-k''} d_k d_{-k} \beta'_q \beta_q$$

$$+ \sum_{\sigma} \sum_{k,k'',q,q'} D_{k,k'',q,q'} u_k v_{k'} v_{k''} d_{-k'} d_{-k''} \beta'_{q'} \beta_{q'} \delta(q - q' - k' - k'')$$

$$- \sum_{\sigma} \sum_{k,k',q} D_{k,k',q} u_k v_{k'} v_{-k'} d_{-k} \beta'_q \beta_q$$

$$- \sum_{\sigma} \sum_{k,k',k'',q,q'} u_k u_{k'} v_{k'} v_{k''} d_{-k} d_{-k'} \beta'_{q'} \beta_{q'} \delta(q - q' - k' - k'') + h.c.$$  

(21)

We now write the interaction terms in which pairs are broken into two particles by the x-ray as,

$$H'_p(2) = \sum_{\sigma} \sum_{k,k'',q,q'} D_{k,k'',q,q'} u_k^2 u_{k''} d_{k'} d_{k''} d_k d_{-k} \beta'_q \beta_q \delta(q - q' - k' - k'')$$

$$- \sum_{\sigma} \sum_{k,k',k'',q,q'} D_{k,k',k'',q,q'} v_k v_{k''} d_{-k} d_{-k'} \beta'_q \beta_{q'} \delta(q - q' - k' - k'') + h.c.$$  

(22)

The terms which do not conserve the quasiparticle number unless pairs are formed are given below,

$$H'_p(3) = \sum_{\sigma} \sum_{k,k',k'',q,q'} D_{k,k',k'',q,q'} [u_k v_{k'} v_{k''} d_{-k} d_{-k'} d_{-k''} \beta'_q \beta_q$$

$$+ u_k v_{k'} v_{k''} d_{-k} d_{-k'} d_{-k''} \beta'_{q'} \beta_{q'} + u_k u_{k'} v_{k''} d_{-k} d_{-k'} d_{-k''} \beta'_q \beta_{q'}$$

$$+ u_k u_{k'} v_{k''} d_{-k} d_{-k'} d_{-k''} \beta'_{q'} \beta_{q'}] \delta(q - q' - k' - k'') + h.c.$$  

(23)

Now we write those terms which are quadratic in pair breaking upon interaction with the
This completes the definition of our Hamiltonian. Considering the single particle energies and the attractive interaction as given by (16), we find that the coherence factors are given by,

$$u^2_k = \frac{1}{2} \left[ 1 + \frac{\epsilon'_k}{(\epsilon'^2_k + \Delta^2)^{1/2}} \right]$$

and

$$v^2_k = \frac{1}{2} \left[ 1 - \frac{\epsilon'_k}{(\epsilon'^2_k + \Delta^2)^{1/2}} \right]$$

where the single particle energy is given by (17) which is slightly shifted from that in the conduction band due to shining with x-rays.

The width of the x-ray as measured by the superconducting detector is given by $\hbar/\tau$ where $\tau$ is the life time of the x-ray due to the interaction with the superconductor as calculated from the imaginary part of the self energy,

$$\frac{1}{\tau_q} = \frac{2}{\hbar} \text{Im} \Sigma_q$$

using Dirac's identity

$$\lim_{\epsilon \to 0} \frac{1}{x \pm i\epsilon} = \frac{P}{x} \mp i\pi \delta(x)$$

where the first term on the right hand side indicates that the Cauchy’s principal value has to be evaluated for determining the real part. The width of the x-ray is caused by two important processes. One of these is the electron scattering process given by (18) and the other is the pair breaking process given by (22). The total width is given by $\hbar \omega_q \sim \hbar (1/\tau_s + 1/\tau_p)$. 

\[ \text{Chap 4 : Theory of detection of x-rays. ...} \]
Chap 4 : Theory of detection of x-rays. ..

The method of calculation of the two mechanisms occurring here is similar to that used for the radiation damping from the magnon-photon interaction [18] and recombination in electron-hole droplets in semiconductors [19].

The first term of (18) gives rise to a shift of the energy of the x-ray as \( \sum \sum D_{k,q}u_k^2n_q \) to which we add also the term \( \sum \sum D_{k,q}u_k^2n_q \) where \( n_q = [\exp(\hbar \omega_q/k_BT) - 1]^{-1} \) is the number density of the x-ray. This term does not contribute to the life time of the x-ray. Therefore, we calcualte the self energy of the x-ray due to the second term of (18) as

\[
\Sigma^x_q(1) = \sum_{k,k'',q'} \frac{2G_1^2\zeta_1 \delta(q - q' - k - k'')}{E - \hbar \omega_{q'} - \epsilon_{k''} + \epsilon_k}
\]  

(28)

where

\[ G_1 = D_q u_k u_{k''}, \]

(29a)

and

\[ \zeta_1 = (1 + n_{q'})(1 - f_{k''})f_{-k} + n_{q'} f_{k''}(1 - f_{-k}) \]

(29b)

and \( f_k \) is a Fermi distribution

\[ f_k = [\exp(\epsilon_k - \epsilon_F)/k_BT + 1]^{-1}. \]

A factor of 2 arises due to two spin configurations. Using the Dirac's identity (27), the imaginary part of the above is found to be,

\[
Im \Sigma^x_q(1) = 2\pi \sum_{k,k'',q'} G_1^2 \zeta_1 \delta(q - q' - k - k'') \delta(\hbar \omega_q - \hbar \omega_{q'} - \epsilon_{k''} + \epsilon_{-k})
\]

(30)

where we took \( \hbar \omega_q \) for \( E \). We eliminate \( k'' \) using the first \( \delta \) function and then near small \( k \), \( \hbar \omega_q \approx \hbar \omega_{q'} \), so that the second \( \delta \) function gives \( \frac{1}{\hbar c} \delta(q - q') \). Then using (26) we find the life time of the x-ray as,

\[
\frac{1}{\tau_1} \approx \frac{2V\omega^2}{\pi \hbar^2 c^3} \sum_k G''_1 \zeta_1 \]

(31)

where

\[ G''_{1} = D_q u_k^2, \]

(32)
\[ \zeta''_1 = f_{-k}(1 - f_{-k})(2n_q + 1) \]  
(32b)

and \( V \) is the volume of the superconductor. In the case of a three dimensional superconductor the summation over \( k \) leads to \( T^3 \) dependence in the inverse life time. Another factor of \( T \) arise from \( n_q \) so that the rate given by (31) varies as \( T^4 \) at low temperatures. There is one more term in the interaction due to the symmetry in the Bogoliubov transformation given by the third term of (18). This term is of the form \( D_q v_k v_{q'-q''-k} \) in place of (29a) so that when we add this contribution to (31) we obtain

\[
\frac{1}{\tau_s} \approx \frac{2V\omega^2}{\pi^2 e^2} \sum D_q^2 \zeta''_1.
\]  
(33)

as the life time of the x-ray due to electron scattering from the processes of the form given by the second and third terms of (18). The first term of (20) does not contribute to the life time of the x-ray. The contribution of the second term is small compared with that calculated above. The contribution of all of the terms of (21) is real because of pair formation so that the imaginary part of the self energy is zero and only a shift occurs. This interaction becomes completely diagonalizable when pairs are introduced using the prescription given by (4). Sidebands are not produced by this interaction. Similarly (23) and (24) do not contribute to the width of the x-ray.

The broadening of the x-ray line due to pair breaking is given by the expression (22).

The self energy of the x-ray due to the first term of (22) is found to be,

\[
\Sigma_q^x(2) = \sum_{\sigma, k, k', k'', q'} \frac{F_1^2 \eta_1 \delta(q - q' - k' - k'')}{E + 2\epsilon_k - \epsilon_{k'} - \epsilon_{k''} - \hbar\omega_q'}
\]

where

\[
F_1 = D_{k, k', k'', q'} u_{k'}^2 u_{k'}^* u_{k''}^*
\]  
(35a)

\[
\eta_1 = (n_q' + 1)(1 - f_{k'}) (1 - f_{k''}) f_k f_{-k} + n_q' f_k f_{k''} (1 - f_k) (1 - f_{-k})
\]  
(35b)

in which \( 2\epsilon_k \) appears because we assumed \( \epsilon_k = \epsilon_{-k} \) in the denominator. We evaluate the sum over \( k'' \) by using the \( \delta \) function and then by using (26) and (27) we obtain the life time...
of the x-ray due to pair breaking from the first term of (12) as,
\[
\frac{1}{\tau_2} \sim \frac{2V(\omega + \frac{2\Delta}{\hbar})^2}{\pi \hbar^2 c^3} \sum_{k,k'} F''_1 \eta''_1^2
\]
where
\[
F''_1 = D_{k,k'} u_k^2 u_{k'} u_{(2\Delta/\hbar)c+k'}
\]
and
\[
\eta''_1 = [n(2\Delta + \hbar\omega) + 1](1 - f_{k'})(1 - f_{-k'-2\Delta/\hbar c})f_k f_{-k} + n(2\Delta + \hbar\omega)f_{k'} f_{-k'-2\Delta/\hbar c}(1 - f_k)(1 - f_{-k})
\]
Similarly, the second term of (22) gives,
\[
\frac{1}{\tau_3} \sim \frac{2V(\omega - \frac{2\Delta}{\hbar})^2}{\pi \hbar^2 c^3} \sum_{k,k'} F''_2 \eta''_2^2
\]
where
\[
F''_2 = D_{k,k'} u_k^2 u_{k'} u_{(2\Delta/\hbar c)+k'}
\]
\[
\eta''_2 = [n(\hbar\omega - 2\Delta) + 1](1 - f_k)(1 - f_{-k})f_{-k'} f_{-k'+2\Delta/\hbar c} + n(\hbar\omega - 2\Delta)f_k f_{-k}(1 - f_{k'})(1 - f_{-k'+2\Delta/\hbar c})
\]
The total life time of the x-ray due to pair breaking is
\[
\frac{1}{\tau_p} = \frac{1}{\tau_2} + \frac{1}{\tau_3}
\]
and the width of the x-ray is \(\hbar \delta \omega = \frac{\hbar}{2} \left( \frac{1}{\tau_2} + \frac{1}{\tau_3} \right) \) which is built up from the single quasiparticle scattering as well as pair breaking processes. The relaxation rates \(\tau_2\) and \(\tau_3\) suggest the occurrence of three lines one each at \(\omega\) and \(\omega \pm 2\Delta/\hbar\). The temperature dependence in the pair breaking process is a bit stronger than \(T^6\) at low temperatures. The calculations of \(\tau^{-1}\) involves \(\sum_{k,k'}\) which for a three dimensional solid is equivalent to \(\int \frac{1}{2}(m/\hbar^2)^3 \epsilon_k d\epsilon_k d\epsilon_{k'} \alpha \epsilon^3\) in agreement with the \(E^3\) dependence suggested by Kraus et al\(^5\). The resolution of the detector is limited by the line width determined from the life time of the x-ray (40).

The thermal and non-equilibrium response of superconductors as radiation detectors
has been studied by Zhang and Frenkel [20] and Epifani [21]. The x-ray operations of a thin film Nb superconducting strip particle detector is given by Parlato et al. [22] and by Gonsev et al. [23]. In the present work we have found the width of the x-ray as detected by a superconducting detector. Our calculation is thus of interest for the development of superconducting films as detectors. Since lines occur at $\omega, \omega \pm 2A$, we predict that there are side bands which affect the resolution of the detector. Since the gap is proportional to the transition temperature, the smaller the gap the better is the resolution of the detector. Hence the smaller the transition temperature, the better is the resolution. In the case of large $T_c$ the lines $\omega$ and $\omega \pm 2A$ will be well resolved.

We have found that the width of the x-ray line is determined by two processes. One of these is the process of electron scattering by x-rays and the other is the pair breaking. The width due to the former process depends on $T^4$ and that due to later is slightly stronger than $T^6$ at low temperatures. Both the mechanisms give zero line width at $T = 0$.

Since the x-ray frequency is much larger than the phonon frequency, creation of pairs by interaction of photons is possible at very low temperatures due to quantum mechanical effects.
Chap 4 : Theory of detection of x-rays.

References


