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Pair-breaking effects on charge imbalance in superconductors

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Using quasi-classical Green function, a general formalism for calculating charge imbalance and its relaxation in non-equilibrium superconductors is presented. The formalism is applicable at arbitrary temperatures, under conditions when the width of quasi-particle state is appreciable due to pair breaking processes and when strong-coupling effects are significant. In the limit of small pair-breaking and for a weak coupling superconductor the collision term in the formalism reduces to the one in the quasi-particle Boltzmann equation.

1 Introduction

During last few decades, the dynamics of non-equilibrium superconductors have received considerable attention. One of the important aspects of non-equilibrium superconductivity has been centered around the concept of charge imbalance. The interesting observation is the quasi-particle tunnelling current at zero bias voltage in a superconductor–insulator–normal metal junction in which superconductor is driven out of equilibrium by tunnel injection[1]. The magnitude of the charge imbalance is determined by the competition between generation mechanism and pair-breaking processes, which relax the charge imbalance. This and several other non-equilibrium effects have been couched in two different theoretical frameworks. One method of treating such phenomenon is using the Boltzmann equation for quasi-particle distribution using Bogoliubov quasi-particle of BSC theory in which superfluid correlations enter through changes in the quasi-particle and coherence factors that occur in transition probabilities. Such a description was first used by Tinkham[2] and Pethick & Smith[3]. This approach, though, is physically appealing, but is limited since it is applicable only when width of quasi-particle state is small and pair-breaking effects are treated as a perturbation. The other method is based on using quasi-static Green function developed by Eliashberg[4], Eilenberger[5] and Sehmid & Schon[6]. The kinetic equations for the Green function may be conveniently derived using the Keldysh[7] techniques for non-equilibrium problems.

In this paper, kinetic equation for charge imbalance for the case of electron-phonon scattering in a form which is directly applicable to strong-coupling superconductors is derived. Such an equation was first obtained by Schmid & Schon[8]. Its derivation has been discussed in detail by Hu[9]. The author's formalism is a general one, as it is applicable at arbitrary temperatures and when strong coupling effects are significant. For a weak coupling superconductor, the kinetic equation for charge imbalance derived by Schmid & Schon[6] is recovered. In the limit of small pair-breaking and for a weak coupling, the collision term in the formalism is shown to be reduced to that in quasi-particle Boltzmann equation.

2 Kinetic Equation

In the Green function method, the kinetic equation is derived from the matrix equation obtained by subtracting the Dyson equation for the ζ - integrated Green function from its conjugate:

$$[\hat{g}_0^{-1} - \hat{\Sigma}, \hat{g}] = 0 \qquad \ldots(1)$$

where

$$\hat{\Sigma} = \begin{pmatrix} \Sigma^R & \Sigma^K \\ 0 & \Sigma^A \end{pmatrix} \qquad \ldots(2)$$

and

$$\hat{g} = \begin{pmatrix} g^R & g^K \\ 0 & g^A \end{pmatrix} \qquad \ldots(3)$$

are the self-energy and ζ-integrated Green function in Keldysh space, consisting of advanced (A), retarded (R) and Keldysh (K) component, all of which are matrices in Nambu space. In the stationary case and in the absence of a vector potential the matrix g_o^{-1} is:

$$\hat{g}_0^{-1} = \tau_3 E + i\frac{\overline{P}}{m}.\frac{\partial}{\partial \bar{r}} - e\Phi \quad \ldots(4)$$

where E is the energy variable , $\overline{P} = P_F\hat{P}$ is the momentum, $\bar{r}$ the position coordinate and Φ is the electrostatic potential. The Pauli matrices in Nambu space are denoted by τ_i (i = 1, 2, 3).

Introducing a distribution matrix h by the definition:

$$g^K = g^R h - h g^A \quad \ldots(5)$$

and using the equations of motion corresponding to the diagonal components of matrix Eq. (1), one arrives at the following 2×2 matrix equation in Nambu space:

$$g^R y - y g^A = 0 \quad \ldots(6)$$

where

$$Y = \Sigma^K + h\Sigma^A - \Sigma^R h + [g_0^{-1}, h] \quad \ldots(7)$$

Following Ref. 7, one may take h to be diagonal and introducing the scalar distribution functions f_L and f_T by the definition:

$$h = (1 - 2 f_L) - 2 f_T \tau_3 \quad \ldots(8)$$

under isotropic conditions f_T and f_L depend only on energy E; furthermore f_T is even and $(1-2f_L)$ odd under reversal of the sign of E.

In the case of electron-phonon scattering, the retarded and advanced self-energies are written in the customary form:

$$\Sigma^R = \tau_3 (1 - z)E - i\,\tau_1 \Phi \quad \ldots(9)$$

$$\Sigma^A = \tau_3 (1 - z^*)E - i\,\tau_1 \Phi^* \quad \ldots(10)$$

The re-normalization function z and the gap function Φ are given below in Eqs (18–19). In this case, g^R and g^A may be written in the simplest form:

$$g^R = \alpha\,\tau_3 + \beta\,\tau_1 \quad \ldots(11a)$$

and

$$g^A = -\alpha^*\,\tau_3 + \beta^*\,\tau_1 \quad \ldots(11b)$$

where

$$\alpha = N_1 + iR_1 \quad \ldots(12a)$$

and

$$\beta = N_2 + iR_2 \quad \ldots(12b)$$

The diagonal part of Eq. (1) then becomes:

$$ZE\,\beta - i\,\Phi\,\alpha = 0 \quad \ldots(13)$$

which together with the normalization condition[5,10]:

$$\alpha^2 + \beta^2 = 1 \quad \ldots(14)$$

determines α and β. The kinetic equation corresponding to the off-diagonal part of Eq. (7) contains terms proportional to f_T, which may be combined into single collision integral I (f_T). The resulting kinetic equation has the form:

$$X = I(f_T) \quad \ldots(15)$$

where, the driving term, denoted by X, may be due to tunnel injection, due to temperature gradient in the presence of super-flow or due to other phenomena, which generate charge-imbalance.

When the phonons are assumed to be in equilibrium the self-energies Σ^K, Σ^R and Σ^A involve g^R, g^A and g^K, as well as the effective phonon density of states $\alpha^2\ F(E)$. The explicit expression may be found in Ref. 8. The collision integral resulting from Eq. (7) then becomes:

$$I(f_T) = -2\,(N_1 \text{ Im } ZE + N_2 \text{ Re }(\Phi)\, f_T(E)$$

$$+ \int_{-\infty}^{\infty} dE^1\, \beta(E, E^1)\,\{N_1(E)\, N_1(\acute{E})$$

$$+ N_2(E)\, N_2(E^1)\}\, f_T(E^1) \quad \ldots(16)$$

where

$$\beta(E, E^1)$$

$$= \pi\,\alpha^2 F(\,|E-E^1|\,)\,\frac{\cos\ hE^1/2T}{\sin\ h(|E^1 - E|/2T)\cos\ hE/2T} \quad \ldots(17)$$

The collision integral (16–17) applies to strong-coupling superconductors and is valid for both clean and dirty superconductors in the absence of anisotropy. In the presence of anisotropy such as associated with super-current, the collision integral remains valid in the dirty limit.

In order to find f_T from the kinetic Eq. (15), one must, in general, first solve the Eliashberg[4] equations for Z and Φ, which in the present notation have the form:

$$(1-Z)\,E = \frac{-1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\,E^{1}\, N_1\,(E^{1})$$

$$\int_{-\infty}^{\infty} \mathrm{d}\,E^{11}\, \frac{\beta(E^{1}, E^{1}-E^{11})}{E^{1}-E^{11}-E-i\delta} \qquad \ldots(18)$$

and

$$\Phi = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\,E^{1}\, R_2\,(E^{1})$$

$$\int_{-\infty}^{\infty} \mathrm{d}\,E^{11}\, \frac{\beta(E^{1}, E^{1}-E^{11})}{E^{1}-E^{11}-E-i\delta} \qquad \ldots(19)$$

These Eqs (16–19) must, in general, be solved self-consistently. In weak coupling case, one may, however, replace in Eqs (18–19) the functions $N_1(E)$ and $R_2(E)$ by their values in BCS theory, given in Eqs (25–28) below.

The collision integral in Eq. (16) differs in form from obtained by Schmid & Schon[6] and Hu[9] by term multiplying $f_T\,(E)$ involving integrals of the form $\int dE^{1}\, N_2(E)\; N_2(E^{1})$, such terms appear in the gap equation for Re Φ, and should be considered as strong-coupling corrections to the BCS energy gap. In a weak-coupling calculations, where Re $\Phi = \Delta$ Re Z (o), these terms should be neglected for consistency.

In the case of electron-phonon scattering action alone, it may be convenient for calculation purposes and ready comparison with the Boltzmann equation, to write $I\,(f_T)$ in the equivalent form:

$$I\,(f_T) = -2\,(N_1\,\mathrm{Im}\,ZE - R_2\,\mathrm{Im}\,\Phi\,)\frac{N_1^2}{(N_1^2-R_2^2)^2}\; f_T\,(E)$$

$$+\int_{-\infty}^{\infty} dE^{1}\beta(E,E^{1})\{N_1(E)N_1(E^{1})+N_2(E)N_2(E^{1})\}f_T(E^{1}) \qquad \ldots(20)$$

The term multiplying $f_T\,(E)$ in Eq. (20) is identical with the corresponding 'scattering out' term obtained by Ambegaokar & Tewardt[10] for the case of thermal conductivity in the presence of electron-phonon scattering, since the following identities hold for electron-phonon scattering only:

$$N_1\,\mathrm{Im}\,ZE - R_2\,\mathrm{Im}\,\Phi = \mathrm{Im}\,\{\sqrt{(ZE)^2-\Phi}\}\;(N_1^{\,2}-R_2^{\,2}) \qquad \ldots(21)$$

and furthermore:

$$N_1^{\,2}-R_2^{\,2} = \frac{1}{2}\left\{1+\frac{E^2-|\Phi/z|^2}{|E^2-(\Phi/z)^2|}\right\} \qquad \ldots(22)$$

Introducing the important parameters τ_{in}, characterizing the strength of inelastic electron-phonon interaction, defined as the normal state inelastic relaxation time at T_c and at Fermi energy:

$$\frac{1}{\tau_{in}} = \frac{2\;\mathrm{Im}\;ZE}{\mathrm{Re}\;Z}\bigg|_{\substack{T=T_c\\E=0}}$$

$$= \frac{4\pi}{\mathrm{Re}\;Z(0)}\int_0^{\infty}\mathrm{d}E\,\frac{\alpha^2F(E)}{\sin\;h(E/T_c)} \qquad \ldots(23)$$

While solving the kinetic Eqs (15–17), one shall always use a Debye model, where, $\alpha^2 F = bE^2$. Here, b is of order the inverse Debye temperature $\odot_D$ squared.

For this model, one gets:

$$\frac{1}{\tau_{in}} = \frac{14\pi\zeta(3)T_c^3 b}{\mathrm{Re}\;Z(0)} \qquad \ldots(24)$$

If, furthermore, $\alpha^2 F = 0$ for $E > \odot_D$ one has Re $Z(0) = 1+\lambda$ where $\lambda = b\,\odot^2_D$

To simplify the equations, the author suppresses in the remainder of this paper, all strong-coupling effects, including the trivial effects of re-normalization Re $\Phi \cong \Delta\,(1+\lambda)$ and Re $Z \cong 1+\lambda$

Now, considering the expressions for N_1 and R_i ($i = 1, 2$) in the number of cases.

(i) *Quasi-particle limit*

If pair-breaking is neglected, one finds:

$$N_1\,(E) = \frac{|E|}{\sqrt{E^2-\Delta^2}}\,\odot(\,|E|-\Delta) \qquad \ldots(25)$$

$$R_1\,(E) = \frac{E}{\sqrt{\Delta^2-E^2}}\,\odot(\Delta-|E|\,) \qquad \ldots(26)$$

and

$$N_2\,(E) = \frac{|\Delta|}{\sqrt{\Delta^2-E^2}}\,\odot(\Delta-|E|) \qquad \ldots(27)$$

$$R_2(E) = \frac{|\Delta|}{\sqrt{E^2-\Delta^2}} \text{Sgn E } \Theta(|E|-\Delta) \quad ...(28)$$

Thus, N_1 is the usual BCS density of states.

Pair-breaking mechanism leads to a smearing of densities of states (25–28). The characters of the smearing depend on the particular mechanism under consideration, while an arbitrary small rate of electron-phonon scattering always makes a superconductor gap-less, it takes finite spin-flip scattering rate to render it gapless[11].

(ii) *Scattering by magnetic impurities*

In the presence of magnetic impurities scattering, in addition to electron-phonon scattering, the equation of motion in Eq. (13) becomes:

$$ZE\,\beta - i\,\Phi\,\alpha + i\,\Gamma_s\,\alpha\,\beta = 0 \quad ...(29)$$

where Γ_s is the spin-flip scattering rate:

Neglect electron-phonon scattering in Eq. (29) entirely, setting $Z = 1$ and $\Phi = \Delta$, the normalization condition in Eq. (14) is then used to eliminate β, which results in a quartic equation for α.

$$\Gamma_s^2\,\alpha^4 - 2\,iE\Gamma_s\alpha^3 + (\Delta^2 - E^2 - \Gamma_s^2)\,\alpha^2 + 2\,i\,E\,\Gamma_s\,\alpha + E^2 = 0 \quad ...(30)$$

For a weak pair-breaking ($\Gamma_s << \Delta$) and for energies close to Δ one may neglect the quartic term in Eq. (30) and one then finds $N_1(E) = 0$ for:

$$|E| < \Delta - \frac{3}{2}(\Gamma_s{}^2\,\Delta)^{1/3} \quad ...(31)$$

Eq. (30) can be solved numerically for number of cases so as to account for different experimental observations.

(iii) *Scattering by phonons*

Calculating Im ZE and Im Φ from Eqs (18–19) together with Eqs (25) and (28) it is found that, ImΦ changes sign from negative to positive at energies of the order of $4k_BT$. From Im ZE and ImΦ one can calculate value of N_2 which also changes sign at high energies[5]. One can ascertain the contribution of phonon scattering alone, by solving Eq. (29) with $\Gamma_s = 0$. When both scattering by magnetic impurities and phonons are present, one must solve the full Eqs (14) and (29) numerically.

3 Quasi-Particle Limit of the Collision Term

In case of weak pair-breaking, the collision term I in the form given in Eq. (16) is essentially the usual collision term in the quasi-particle approach. Previously, this has been demonstrated by Entin-Wholman & Orbach[12], for the limiting case $\Delta << T$, for which the imaginary part of the gap, ImΦ, may be neglected. To show this equivalence at arbitrary temperatures, the author expanded the collision term in Eq. (16) to first-order in pair-breaking rates associated with electron-phonon and spin-flip scattering. One finds upon expanding the solutions of Eqs (13–14) that:

$$\text{Re } ZN_2 = \frac{\Delta E}{(E^2-\Delta^2)^{3/2}}(\text{Im } ZE - \frac{E}{\Delta}\text{Im}\Phi) + \frac{\Delta E^2}{(E^2+\Delta^2)^2}\Gamma_s \quad ...(32)$$

It is convenient to introduce the single particle decay rate for a scattering by phonons, $2\,\Gamma_p$ by the definition:

$$\Gamma_p = \text{Im } ZE - \frac{\Delta}{E}\text{ Im }\Phi$$

$$= \frac{1}{2}\int dE^1\,N_1(E^1)\,B(E^1,E)\left(1-\frac{\Delta^2}{EE^1}\right) \quad ...(33)$$

It follows from Eqs (32–33):

$$2\text{Re}\Phi N_2 = \frac{2|E|}{(E^2-\Delta^2)^{1/2}}\left(\frac{E^2\Gamma_p}{E^2-\Delta^2} - \text{Im } ZE\right) + 2\frac{\Delta^2E^2}{(E^2-\Delta^2)^2}\Gamma_s \quad ...(34)$$

Inserting this result into Eq. (16), one finds that, Im ZE term in Eq. (34) precisely cancels the N_1ImZE term in Eq. (16). The $N_1\,N_1{}^1$ term in the integral may be neglected when pair-breaking is weak and introducing the variable:

$$\zeta = \sqrt{E^2-\Delta^2}\ \text{Sign } E \quad ...(35)$$

The kinetic equation takes the form:

$$X = I(f_T) = -\left[2\left(\frac{E}{\zeta}\right)^3\Gamma_p + 2\frac{\Delta^2}{E^2}\left(\frac{E}{\zeta}\right)^4\Gamma_s\right]f_T(E)$$

$$+\frac{E}{\zeta}\int_{-\infty}^{\infty} + d\zeta^1\,B(E,E^1)\,f_T(E^1) \quad ...(36)$$

Introducing

$$q = \frac{\zeta}{E} \quad \ldots(37)$$

as the effective charge of a quasi-particle, Eq. (36) takes the form:

$$q^2 X = q^2 I(f_T) = -2\left[\Gamma_p + \frac{\Delta^2}{E^2}\frac{E}{\zeta}\Gamma_s\right]\frac{f_T}{q}$$

$$+ q \int_{-\infty}^{\infty} d\zeta^1 q(\zeta^1) B(E, E^1) \frac{f_T(\zeta^1)}{q(\zeta^1)} \quad \ldots(38)$$

Defining $f_T(\zeta)/q(\zeta)$ as the quasi-particle distribution where the quasi-particle energies are negative, below the Fermi-surface, the operator on the right hand side of Eq. (38) is precisely the usual Boltzmann equation collision term and therefore to complete the identification one needs merely to compare driving terms. For the specific use of tunnel injection Schmid & Schnon[6] found:

$$X = \frac{\pi}{\hbar} N_n(0) \mid T_{NS} \mid^2 N_1(E) [f^{\circ}(E - ev) - f^{\circ}(E + ev1)] \quad \ldots(39)$$

where T_{NS} is the tunnelling matrix element, $N_n(0)$ is the density of states in the normal metal used to inject electrons into the superconductor and V is the injection voltage. The driving term in the Boltzmann equation is just:

$$X_{Boltz} = \frac{\pi}{h} N_n(0) \mid T_{NS} \mid^2 q(E)[f^{\circ}(E - ev) - f^{\circ}(E + ev1)] \quad \ldots(40)$$

and therefore in the quasi-particle limit $qN_1 = 1$, one finds:

$$X_{Boltz} = q^2 X \quad \ldots(41)$$

4 Conclusion

In this paper, a formalism, based on quasi-classic Green function, for calculating charge imbalance at arbitrary temperature and for arbitrary amount of pair-breaking is presented. It is also shown, explicitly, how in the weak-coupling case one recovers the usual quasi-particle Boltzmann equation when pair-breaking is small. An interesting feature of these calculations is that the collision term in the Boltzmann equation corresponds to the terms in the Green function approach having different origin. The basic formalism described can be applied to a variety of other non-equilibrium phenomenon.

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