On the correct formula for the lifetime broadened superconducting density of states

Božidar Mitrović and Lee A Rozema

Department of Physics, Brock University, St Catharines, ON, L2S 3A1, Canada

E-mail: mitrovic@brocku.ca

Received 11 October 2007, in final form 14 October 2007
Published 7 December 2007
Online at stacks.iop.org/JPhysCM/20/015215

Abstract
We argue that the well known Dynes formula (Dynes et al 1978 Phys. Rev. Lett. 41 1509) for the superconducting quasiparticle density of states, which tries to incorporate the lifetime broadening in an approximate way, cannot be justified microscopically for conventional superconductors. Instead, we propose a new simple formula in which the energy gap has a finite imaginary part $-\Delta_2$ and the quasiparticle energy is real. We prove that in the quasiparticle approximation $2\Delta_2$ gives the quasiparticle decay rate at the gap edge for conventional superconductors. This conclusion does not depend on the nature of interactions that cause the quasiparticle decay. The new formula is tested on the case of a strong coupling superconductor Pb$_0$Bi$_0$ and an excellent agreement with theoretical predictions is obtained. While both the Dynes formula and the one proposed in this work give good fits and fit parameters for Pb$_0$Bi$_0$, only the latter formula can be justified microscopically.

Almost thirty years ago Dynes et al [1] proposed that the quasiparticle recombination time in a strong-coupled superconductor can be directly measured from the width of the peak in the tunneling conductance $dI(V)/dV$ of a superconductor–insulator–superconductor tunnel junction at the sum of the gaps. They found that the data on Pb$_0$Bi$_0$–insulator–Pb$_0$Bi$_0$ planar tunnel junction could be fitted quite well for voltages near twice the gap if the quasiparticle density of states

$$\rho(E) = \frac{E}{\sqrt{E^2 - \Delta(E)^2}} \quad (1)$$

in the expression for the tunneling current

$$I(V) \propto \int_{-\infty}^{+\infty} dE \rho(E) \rho(E + eV) [f(E) - f(E + eV)] \quad (2)$$

is replaced by

$$\rho_D(E, \Gamma_D) = \frac{E - i\Gamma_D}{\sqrt{(E - i\Gamma_D)^2 - \Delta_0^2}} \quad (3)$$

with real and $E$-independent $\Gamma_D$ and the measured gap edge $\Delta_0$. In (1) $\Delta(E)$ is the complex gap function and $f$ and $e$ in (2) are the Fermi function at temperature $T$ and the magnitude of electron charge, respectively. It was proposed [1] that the temperature dependent parameter $\Gamma_D$ in (3) incorporates the quasiparticle lifetime effects. A good agreement between the measured $\Gamma_D(T)$ and a microscopic calculation [1] based on the work by Kaplan et al [2] for a number of temperatures below the transition temperature $T_c$ of Pb$_0$Bi$_0$ was taken as a justification for the replacement of $\rho(E)$ with $\rho_D(E, \Gamma_D)$ and for the interpretation of parameter $2\Gamma_D$ as the inverse of the quasiparticle recombination lifetime. Formula (3) is now widely known as the Dynes formula and it has been applied to a variety of low temperature ($T \ll T_c$) tunneling experiments ranging from tunneling into the bulk [3] and thin film [4] inhomogeneous/ granular superconductors to the tunneling into a two-band superconductor MgB$_2$ [5] and tunneling into a novel superconductor CaC$_6$ [6, 7]. The Dynes formula was also recently used to describe the density of states obtained in photoemission studies of superconducting h-ZrRuP [8] and of filled skutterudite superconductor LaRu$_4$P$_{12}$ [9].

However, the ansatz (3) cannot be justified for a conventional strong coupling superconductor, such as Pb$_0$Bi$_0$ [1], from first principles. Indeed, $\rho(E)$ is given in terms of the diagonal electron Green’s function in the
superconducting state

\[ G_{11}(k, E) = \frac{E Z(k, E) + \varepsilon_k}{E^2 Z^2(k, E) - \phi^2(k, E) - \varepsilon_k^2}, \tag{4} \]

where \( Z \) is the complex renormalization function and \( \phi \) is the complex pairing self-energy \([10, 11]\), as

\[ \rho(E) = \frac{1}{\pi N(0)} \sum_k G_{11}(k, E), \tag{5} \]

where \( N(0) \) is the normal state density of states at the Fermi level. All interactions enter via the self-energy terms \( Z \) and \( \phi \) and assuming that they do not depend on momentum \( k \) one finds

\[ \rho(E) = \text{Re} \frac{E Z(E)}{\sqrt{E^2 - \Delta^2(E)}} \tag{6} \]

\[ \rho(E) = \text{Re} \frac{E}{\sqrt{E^2 - \Delta^2(E)}} \tag{7} \]

where in the last step \( Z(E) \) and \( \phi(E) \) have been eliminated in favor of the gap function \( \Delta(E) = \phi(E)/Z(E) \). Clearly, all the lifetime effects which enter via \( \phi(E) \) and \( Z(E) \) are ultimately incorporated in the complex gap function \( \Delta(E) \) and the tunneling current \( I(V) \) depends on the full complex gap function as is clear from equations (1) and (2). Note that (6) cannot be cast into the form (3) by a suitable choice of \( Z(E) \) (e.g., taking \( Z(E) = 1/\Gamma_0(E) \) would give \( \text{Re} \left[ (E - i\Gamma_0(E))/\sqrt{(E - \Gamma_0(E))^2 - \phi(E)} \right] \), where the pairing self-energy \( \phi \) appears instead of the gap \( \Delta \), and the measured \( dI/dV \) gives \( \Delta \) and not \( \phi \).

Instead of replacing \( \rho(E) \) with \( \rho_D(E, \Gamma_0) \) it is more reasonable to keep \( \Delta(E) \) in (1) constant but complex for \( E \) not too far from the gap edge \( \Delta_0 \), i.e. replace (1) with

\[ \rho_D(E, \Delta_2) = \text{Re} \frac{E}{\sqrt{E^2 - (\Delta_0 - i\Delta_2)^2}}, \tag{8} \]

where \( -\Delta_2 \) is the imaginary part of the gap at \( E = \Delta_0 \). It is well known that at a finite temperature the imaginary part of the gap at the gap edge is finite as a result of quasiparticle damping (see figure 45 in [11]). In fact, it is easy to prove that in the quasiparticle approximation [2] the quasiparticle decay rate at the gap edge is equal to \(-2 \text{Im} \Delta(E = \Delta_0)\). Assuming that at \( E = \Delta_0 \) the imaginary parts \( Z_2 \) and \( \phi_2 \) of \( Z \) and \( \phi \), respectively, are much smaller than the corresponding real parts one finds that

\[ -\text{Im} \Delta(E = \Delta_0) \approx \frac{\Delta_0 Z_2(E = \Delta_0) - \phi_2(E = \Delta_0)}{Z_1(0)}, \tag{9} \]

where \( Z_1(0) \) is the real part of \( Z(E = 0) \). Expression (9) is identical to the equation of Kaplan et al for the quasiparticle decay rate parameter \( \Gamma(E = \Delta_0) \) [2] (see equation (5) in [2]). This result is quite general and does not depend on the specific interactions leading to quasiparticle damping, i.e. whether it is the electron–photon interaction which was considered in [1, 2], or the dynamically screened Coulomb interaction in the presence of disorder which was assumed to be the cause of lifetime broadening in low temperature tunneling experiments into three-dimensional granular aluminum [3] and quench-condensed two-dimensional films of Pb and Sn [4]. All that is required for

\[ 2\Gamma(k, E = \Delta_0) = -2 \text{Im} \Delta(k, E = \Delta_0), \tag{10} \]

to be valid, where \( 2\Gamma(k, E = \Delta_0) \) is the inverse quasiparticle lifetime with \( k \) on the Fermi surface, is that the imaginary parts of \( \phi(k, E) \) and \( Z(k, E) \) are much smaller than their respective real parts near the gap-edge. Needless to say, (10) does not apply to unconventional superconductors characterized by \( \sum_{k \in FS} \Delta(k) = 0 \), where FS is the Fermi surface, for \( k \) near the gap nodes [12].

In the case of Pb_0.9Bi_0.1 we find that equation (8) produces fits to \( dI(V)/dV \) which are at least as good as those obtained with the Dynes formula (3). Instead of trying to fit the original data from [1], which in addition to the temperature dependent lifetime broadening were assumed to contain an intrinsic (background) width of 0.01 meV, we fitted \( dI(V)/dV \) calculated from the solutions \( \Delta(E) \) and \( Z(E) \) of the finite temperature Eliashberg equations [10, 11] on the real axis using the Eliashberg function \( \alpha^2(\Omega) F(\Omega) \) for Pb_0.9Bi_0.1 [13]. Thus, the width of the peak in our calculated \( dI(V)/dV \) arises solely from the temperature dependent lifetime broadening and we could compare directly the value of the fit parameter \( \Delta_2 \) in equation (8) with our solution – \( \text{Im} \Delta(E) \) for \( E \) at the gap edge. Moreover, we could calculate the decay rate parameter \( \Gamma(E) \) directly from our solutions of Eliashberg equations [2] (see equation (4) in [2])

\[ \Gamma(E) = \frac{E Z_1(E) / Z_1(0) - \phi_1(E) \phi_2(E) / [Z_1^2(E) E]}{[Z_1^2(E) E]} \tag{11} \]

and compare its value at \( E = \Delta_0 \) with \( \Delta_2 \) obtained from the fits with equation (8). We note, however, that there is a good agreement between the shapes of the calculated \( dI(V)/dV \) and the measured ones [1] down to \( T = 2.75 \) K as illustrated in figure 1 for \( T = 3.5 \) K. In figure 1 the results are plotted as functions of \( eV - 2\Delta_0 \) since with our choice of the Coulomb
Figure 2. The calculated (filled circles) $dI/dV$ at six different temperatures as a function of voltage and their fits with (8) (solid line) and with the Dynes formula (3) (dashed line) with $\Delta_2$ and $\Gamma_D$ as the only fit parameters, respectively.

The calculated $dI/dV$ (dots) at $T = 6$ K versus voltage and the fits with (8) (solid line) and (3) (dashed line), with $\Delta_2$ and $\Gamma_D$ as the only fit parameters, respectively.

...
measured quasiparticle lifetime \( \bar{\tau} \) is no need to invoke the intrinsic temperature-independent recombination time \( \tau \) and \( \bar{\tau} \) of Kaplan (dashed line) at the gap edge based on approximate equations (filled circles) with the values of \( \Gamma(\Delta_0) \) computed using equation (11). The agreement between the values for the total quasiparticle lifetime \( \tau \) at the gap edge obtained from the fits with formula (8) and both theoretical predictions is excellent.

In conclusion, we have shown that one can, indeed, obtain the total quasiparticle lifetime at the gap edge from the fits of the derivatives of the \( I-V \) characteristic of a superconductor–insulator–superconductor tunnel junctions using equation (8). The interpretation of the parameter \( 2\Delta_2 \) as the quasiparticle decay rate at the gap edge is microscopically justified. While the Dynes formula (3) gives correct values for the total quasiparticle lifetime, it cannot be justified for conventional superconductors. Hence the fact that it works, at least for the cases when the quasiparticle decay rate is less than about 20% of the gap edge, is a pure accident. It is likely that for larger values of \( \Gamma(\Delta_0) \), which seems to be the case in LaRu$_4$P$_{12}$ (\( 2\Gamma(\Delta_0) \approx 50\% \)) [9], equations (3) and (8) would give qualitatively and quantitatively different results.

**Acknowledgments**

This work was supported by the Natural Sciences and Engineering Research Council (NSERC) of Canada. The work of LAR was also supported in part through an NSERC Undergraduate Student Research Award (USRA).

**References**

[1] Dynes R C, Narayanamurti V and Garno J P 1978 Phys. Rev. Lett. 41 1509
[2] Kaplan S B, Chi C C, Langenberg D N, Chang J J, Jafarey S and Scalapino D J 1976 Phys. Rev. B 14 4854
[3] Dynes R C, Garno J P, Hertel G B and Orlando T P 1984 Phys. Rev. Lett. 53 2437
[4] White A E, Dynes R C and Garno J P 1986 Phys. Rev. B 33 3549
[5] Crabtree G, Kwok W and Canfield P C (ed) 2003 Physica C 385 1 Review issue on MgB$_2$
[6] Bergeal N, Dubost V, Noat Y, Sacks W, Roditchev D, Emery N, Hérold C, Maréché J-F, Lagrange P and Loupias G 2006 Phys. Rev. Lett. 97 077003
[7] Kurter C, Ozzyuzer L, Mazur D, Zasadzinski J F, Rosenmann D, Claus H, Hinks D G and Gray K E 2006 Preprint cond-mat/0612581
[8] Matsui H, Hashimoto D, Souma S, Sato T, Takahashi T and Shiratori I 2005 J. Phys. Soc. Japan 74 1401
[9] Tsuda S, Yokoya T, Kiss T, Shimojima T, Shin S, Togasi T, Watanabe S, Zhang C Q, Chen C T, Sugawara H, Sato H and Harima H 2006 J. Phys. Soc. Japan 75 0604711
[10] Schrieffer J R 1964 Theory of Superconductivity (New York: Benjamin)
[11] Scalapino D J 1969 Superconductivity ed R D Parks (New York: Dekker) pp 466–501
[12] Dahm T, Hirschfeld P J, Scalapino D J and Zhu L 2005 Phys. Rev. B 72 214512
[13] Dynes R C and Rowell J M 1975 Phys. Rev. B 11 1884