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2008 J. Phys.: Condens. Matter 20 015215

(http://iopscience.iop.org/0953-8984/20/1/015215)

J. Phys.: Condens. Matter **20** (2008) 015215 (4pp) doi:10.1088/0953-8984/20/01/015215

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

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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 $Pb_{0.9}Bi_{0.1}$ 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 $Pb_{0.9}Bi_{0.1}$, 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 $\mathrm{d}I(V)/\mathrm{d}V$ of a superconductor–insulator–superconductor tunnel junction at the sum of the gaps. They found that the data on $Pb_{0.9}Bi_{0.1}$–insulator–$Pb_{0.9}Bi_{0.1}$ planar tunnel junction could be fitted quite well for voltages near twice the gap if the quasiparticle density of states

$$\rho(E) = \mathrm{Re}\,\frac{E}{\sqrt{E^2 - \Delta^2(E)}}, \tag{1}$$

in the expression for the tunneling current

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

is replaced by

$$\rho_D(E,\Gamma_\mathrm{D}) = \mathrm{Re}\,\frac{E - \mathrm{i}\Gamma_\mathrm{D}}{\sqrt{(E-\mathrm{i}\Gamma_\mathrm{D})^2 - \Delta_0^2}}, \tag{3}$$

with real and E-independent Γ_D and the measured gap edge Δ_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 Γ_D in (3) incorporates the quasiparticle lifetime effects. A good agreement between the measured $\Gamma_\mathrm{D}(T)$ 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 $Pb_{0.9}Bi_{0.1}$ was taken as a justification for the replacement of $\rho(E)$ with $\rho_D(E,\Gamma_\mathrm{D})$ and for the interpretation of parameter $2\Gamma_\mathrm{D}$ 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 ($T \ll T_\mathrm{c}$) 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 $LaRu_4P_{12}$ [9].

However, the *ansatz* (3) cannot be justified for a conventional strong coupling superconductor, such as $Pb_{0.9}Bi_{0.1}$ [1], from first principles. Indeed, $\rho(E)$ is given in terms of the diagonal electron Green's function in the superconducting state

$$G_{11}(\mathbf{k},E)=\frac{EZ(\mathbf{k},E)+\varepsilon_{\mathbf{k}}}{E^2Z^2(\mathbf{k},E)-\phi^2(\mathbf{k},E)-\varepsilon_{\mathbf{k}}^2},\qquad(4)$$

where Z is the complex renormalization function and ϕ is the complex pairing self-energy [10, 11], as

$$\rho(E)=-\frac{1}{\pi N(0)}\,\mathrm{Im}\sum_{\mathbf{k}}G_{11}(\mathbf{k},E),\qquad(5)$$

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

$$\rho(E)=\mathrm{Re}\,\frac{EZ(E)}{\sqrt{E^2Z^2(E)-\phi^2(E)}}\qquad(6)$$

$$=\mathrm{Re}\,\frac{E}{\sqrt{E^2-\Delta^2(E)}},\qquad(7)$$

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 $Z(E)=1-\mathrm{i}\Gamma_{\mathrm{D}}/E$ would give $\mathrm{Re}\,[(E-\mathrm{i}\Gamma_{\mathrm{D}})/\sqrt{(E-\mathrm{i}\Gamma_{\mathrm{D}})^2-\phi(E)}]$, where the pairing self-energy ϕ appears instead of the gap Δ, and the measured dI/dV gives Δ and not ϕ).

Instead of replacing $\rho(E)$ with $\rho_D(E,\Gamma_{\mathrm{D}})$ it is more reasonable to keep $\Delta(E)$ in (1) constant but complex for E not too far from the gap edge Δ_0, i.e. replace (1) with

$$\rho_\Delta(E,\Delta_2)=\mathrm{Re}\,\frac{E}{\sqrt{E^2-(\Delta_0-\mathrm{i}\Delta_2)^2}},\qquad(8)$$

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 $-2\,\mathrm{Im}\,\Delta(E=\Delta_0)$. Assuming that at $E=\Delta_0$ the imaginary parts Z_2 and ϕ_2 of Z and ϕ, respectively, are much smaller than the corresponding real parts one finds that

$$-\mathrm{Im}\,\Delta(E=\Delta_0)\approx\frac{\Delta_0Z_2(E=\Delta_0)-\phi_2(E=\Delta_0)}{Z_1(0)},\qquad(9)$$

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–phonon 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

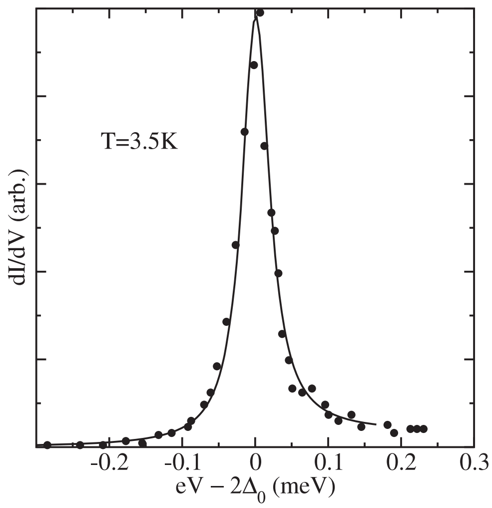

Figure 1. The calculated dI/dV (solid line) and the experimental data points (filled circles) from [1] at $T=3.5$ K. The data are plotted as a function of $eV-2\Delta_0$.

into three-dimensional granular aluminum [3] and quench-condensed two-dimensional films of Pb and Sn [4]. All that is required for

$$2\Gamma(\mathbf{k},E=\Delta_0)=-2\,\mathrm{Im}\,\Delta(\mathbf{k},E=\Delta_0),\qquad(10)$$

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

In the case of $Pb_{0.9}Bi_{0.1}$ we find that equation (8) produces fits to d$I(V)$/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 d$I(V)$/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 $Pb_{0.9}Bi_{0.1}$ [13]. Thus, the width of the peak in our calculated d$I(V)$/dV arises solely from the temperature dependent lifetime broadening and we could compare directly the value of the fit parameter Δ_2 in equation (8) with our solution $-\mathrm{Im}\,\Delta(E)$ 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])

$$\Gamma(E)=EZ_2(E)/Z_1(E)-\phi_1(E)\phi_2(E)/[Z_1^2(E)E]\qquad(11)$$

and compare its value at $E=\Delta_0$ with Δ_2 obtained from the fits with equation (8). We note, however, that there is a good agreement between the shapes of the calculated d$I(V)$/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

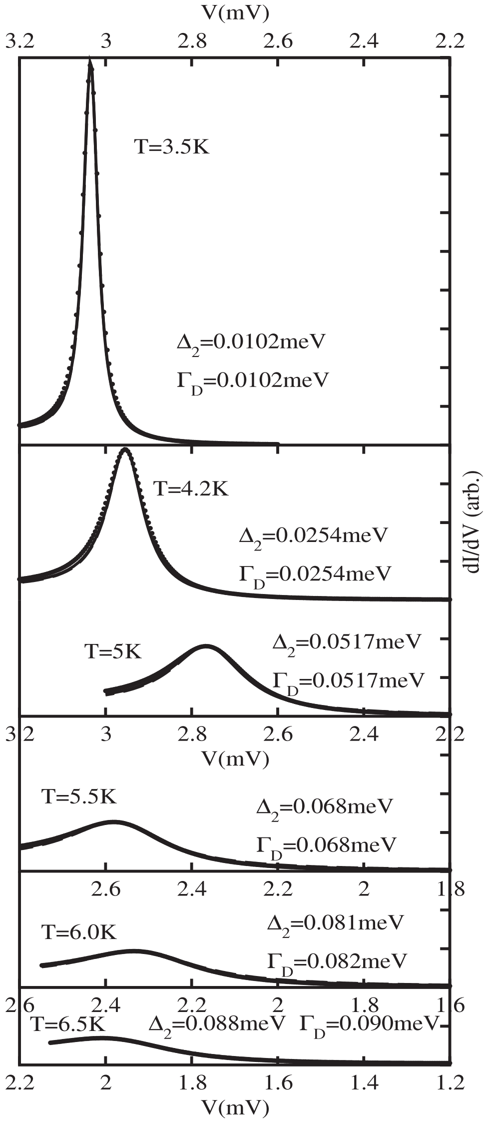

Figure 2. The calculated (filled circles) dI/dV at six different temperatures as a function of voltage and their fits with (8) (solid line) and with the Dynes formula (3) (dashed line) with Δ_2 and Γ_D as the only fit parameters, respectively.

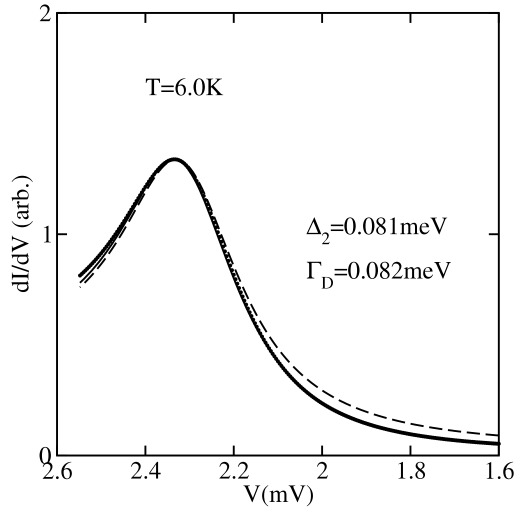

Figure 3. The calculated dI/dV (dots) at $T = 6$ K versus voltage and the fits with (8) (solid line) and (3) (dashed line), with Δ_2 and Γ_D as the only fit parameters, respectively.

pseudopotential $\mu^*(\omega_c) = 0.1034$, which was fitted to the experimental zero temperature gap edge $\Delta_0 = 1.54$ meV [13] for the cutoff $\omega_c = 100$ meV in the Eliashberg equations, we obtain somewhat higher values of Δ_0 than those found in [1]. As the Coulomb pseudopotential term in the Eliashberg equations is purely real it does not affect the imaginary parts of the solutions [10, 11].

In figure 2 we show the fits to the calculated dI/dV using the Dynes formula (3) and the formula with the complex gap (8). On the scale of figure 2, which was chosen to match the scale of figure 2 in [1], both equations (3) and (8) give equally good fits. Moreover, the values of the fit parameter Δ_2 turn out to be nearly the same as the values of the fit parameter Γ_D at all temperatures considered. One can understand why two different functional forms (3) and (8) give nearly identical fits to dI/dV with nearly identical fit parameters $\Gamma_D \approx \Delta_2$ from the fact that in the limit $\Gamma_D, \Delta_2 \ll \Delta_0$ the approximations (3) and (8) to $\rho(\Delta_0)$ give $\sqrt{\Delta_0/\Gamma_D}/2$ and $\sqrt{\Delta_0/\Delta_2}/2$, respectively and the height of the peak in dI/dV is most sensitive to the maximum in the quasiparticle density of states. However, it is clear that as the lifetime broadening grows compared to the gap edge, the difference between the fit parameters obtained with (3) and with (8) increases and the quality of fits with the Dynes formula deteriorates compared to the fits with (8) as illustrated in figure 3, in particular at lower voltages. The reason is that for $\Gamma_D, \Delta_2 \ll \Delta_0$ in the limit of small energy $\rho_D(E, \Gamma_D) = \Gamma_D/\Delta_0$, while $\rho_\Delta(E, \Delta_2) = (\Delta_2/\Delta_0^2)E$ to the first order in E, i.e. $\rho_D(E, \Gamma_D)$ does not vanish at $E = 0$. We note that the experimental *low-temperature* densities of states obtained for three-dimensional granular aluminum [3] do vanish at $E = 0$ (see figure 3 in [3]), while those obtained for two-dimensional quench-condensed tin films [4] do not (see figure 2 in [4]). The precise reason for such a difference between three-dimensional and two-dimensional disordered conventional superconductors is not known at the present time.

As one could have expected, the fitted values of Δ_2 turned out to be equal to the imaginary parts of our solutions $\Delta(E)$ of the Eliashberg equations at $E = \Delta_0$ to within a few percent at all temperatures considered. The values of Δ_2 extracted from the fits to the calculated dI/dV agree with the values of the fit parameter $\Gamma(\equiv\Gamma_D)$ reported in [1] before correction for the background to within a percent or two down to $T = 4.2$ K. At $T = 3.5$ K the difference is about 30% and yet the shapes of the calculated and measured dI/dV in figure 1 seem to agree quite well. A further reduction of the measured Γ by the background value of 0.01 meV would increase the difference between the lifetime broadening parameters to about 150%. At $T = 2.75$ K our fitted value (the fit is not shown here) is $\Delta_2 = 0.002\,26$ meV which is 80% lower than the measured Γ [1] or more than twice the measured value after the correction for the background. It is quite plausible that at low temperatures, when both the experimental and the theoretical data in the peak change very rapidly, it is difficult to determine

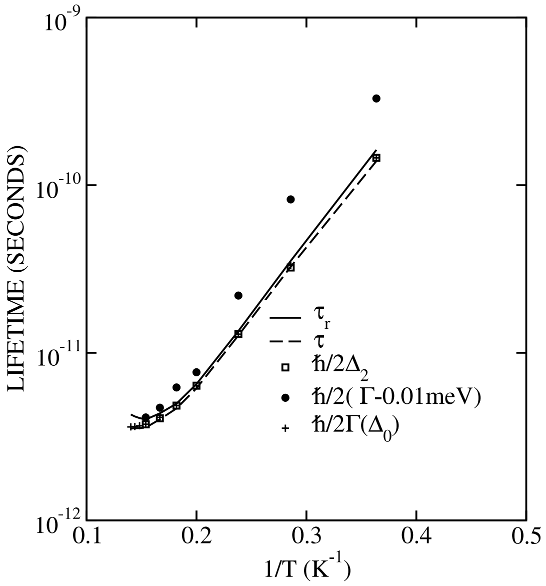

Figure 4. Quasiparticle lifetime at the gap edge determined in various ways (see the text) as a function of inverse temperature.

the actual maximum in dI/dV to which the fit parameters are most sensitive. It is likely that the maximum in dI/dV gets underestimated at low T having as a consequence too high values of the lifetime broadening parameter. We believe that is the reason for the discrepancies between our fitted values of Δ_2 and those found in [1] at low temperatures and that there is no need to invoke the intrinsic temperature-independent broadening parameter.

Finally, in figure 4 we show the temperature dependence of the quasiparticle lifetime τ at the gap edge obtained from $\hbar/\tau = 2\Delta_2$ (open squares) and $\hbar/\tau = 2(\Gamma - 0.01\text{ meV})$ (filled circles) with the values of Γ taken from figure 2 in [1]. In the same figure we show theoretical predictions for the recombination time τ_r (solid line) and the total lifetime τ (dashed line) at the gap edge based on approximate equations of Kaplan *et al* [2]

$$\frac{\hbar}{\tau_r} = C\int_{2\Delta_0}^{\infty} d\Omega\, \alpha^2(\Omega)F(\Omega)\frac{\Omega-\Delta_0}{\sqrt{(\Omega-\Delta_0)^2-\Delta_0^2}} \times \frac{\Omega}{\Omega-\Delta_0}[n(\Omega)+1]f(\Omega-\Delta_0), \quad (12)$$

$$\frac{\hbar}{\tau_s} = C\int_{0}^{\infty} d\Omega\, \alpha^2(\Omega)F(\Omega)\frac{\Omega+\Delta_0}{\sqrt{(\Omega+\Delta_0)^2-\Delta_0^2}} \times \frac{\Omega}{\Omega+\Delta_0}n(\Omega)[1-f(\Omega+\Delta_0)], \quad (13)$$

where $n(\Omega)$ is the Bose function, $C = 2\pi/\{Z_1(0)[1-f(\Delta_0)]\}$ and $\hbar/\tau = \hbar/\tau_r + \hbar/\tau_s$. A good agreement between the measured $\hbar/2(\Gamma - 0.01\text{ meV})$ and τ_r calculated according to (12) was taken as a justification of the Dynes formula (3) in [1]. We note that the integrand in (12) has a square root singularity at the lower limit of integration which has to be handled analytically if τ_r is not to be overestimated. Comparing figure 3 in [1] and figure 4 in this work it is clear that our calculated τ_r is considerably lower at the low temperatures than the one calculated in [1] as the filled circles in both figures represent $\hbar/2(\Gamma - 0.01\text{ meV})$. In addition, we show in figure 4 the lifetime calculated directly from our solutions of the Eliashberg equations in the quasiparticle approximation $\hbar/\tau = 2\Gamma(\Delta_0)$ (plus signs), where $\Gamma(\Delta_0)$ is computed using equation (11). The agreement between the values for the total quasiparticle lifetime τ 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 $2\Gamma/\Delta_0$, which seems to be the case in $LaRu_4P_{12}$ ($2\Gamma/\Delta_0 \approx 50\%$) [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).

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