Journal of Nuclear Materials 385 (2009) 4–7

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

d-wave superconductive gap and related observables of $PuCoGa_5$

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ARTICLE INFO

PACS:
74.62.Dh
61.80.Jh
74.25.Qt
74.70.Dd

ABSTRACT

The real-axis formulation of the Eliashberg theory has been applied to $PuCoGa_5$, assuming d-wave symmetry and phonon-mediated pairing. Here, we present the calculated temperature dependence of the superconductive gap $\Delta(T)$ for a freshly prepared sample, and the variation of $\Delta(T = 2\text{ K})$ with increasing impurity scattering rate. We also present the calculated energy dependence of the quasiparticle density of state, together with the corresponding normalized tunnelling conductance at $T = 4$ K. These quantities could be compared with future tunnelling experiments that would also lead to a direct determination of the spectral density function. Finally, we show that the normal phase resistivity can be well reproduced up to room temperature assuming electron–phonon scattering within a two-band model.

1. Introduction

Despite several years of extensive investigation, the nature of the mediating bosons in the superconductive phase of $PuCoGa_5$ is still the object of debate. While the most commonly accepted viewpoint states that this fascinating material is an unconventional superconductor with spin fluctuations as pairing bosons [1], state-of-the-art Eliashberg calculations can qualitatively reproduce the whole available experimental evidence within a scenario of phonon-mediated superconductivity [2]; moreover, polarized neutron scattering experiments [3] have shown that the normal state of $PuCoGa_5$ is different from that anticipated for a Pu^{3+} ion, as the magnetic susceptibility in the normal state is small, temperature independent and dominated by orbital effects. On the other hand, neutron scattering experiments have recently demonstrated the presence of short-range magnetic fluctuations in the paramagnetic phase of the isostructural compound $NpCoGa_5$ [4]. An elucidation of the pairing-boson nature is crucial, especially since the search of ‘superconductivity without phonons’ has become a central issue in condensed-matter research [5].

In this work, we exploit the real-axis solution of the Eliashberg equations for $PuCoGa_5$, in order to calculate the temperature and impurity-scattering-rate dependence of the superconductive gap, the normalized quasiparticle density of states (NDOS), and the normalized tunnelling conductance. All these observables could be directly probed by Josephson junction experiments. In addition, we show that a two-band model can remove the discrepancy between the measured and the calculated resistivity curve $\rho(T)$ in the normal phase.

2. Theoretical model

In our previous work [2] we have experimentally and theoretically investigated the role of self-induced defects and disorder in modifying the superconductive properties of $PuCoGa_5$. Our experimental results were consistent with a dirty d-wave model for superconductivity with strong impurity scattering. The results of key experiments probing superconductive parameters (critical temperature, upper critical field, penetration depth) were well reproduced by assuming a phononic mechanism for superconductivity in the framework of the imaginary-frequency-axis formulation of the Eliashberg theory [6].

The present work is based on the real-frequency-axis formulation [7,8]. The two formulations are formally equivalent; the former, being based on a discrete set of imaginary frequencies, makes the calculation of T_C simpler, but the latter allows to estimate with precision several other physical quantities, by numerical solution of two coupled non-linear singular integral equations involving a frequency and temperature dependent complex gap $\Delta(\omega,T)$ and a renormalization function $Z(\omega,T)$. The input quantities entering the singular kernels of these equations are the spectral density function $\alpha^2F(\omega)$, describing the effective electron–electron interaction due to phonon exchange, the Coulomb pseudopotential μ^*, and the normal electronic density of states $N^N(\omega)$. Assuming a d-wave gap symmetry, $\alpha^2F(\omega)$ and μ^* can be expanded as

$$\alpha^2(\omega,\phi,\phi')F(\omega) = \alpha^2F_s(\omega) + 2\alpha^2F_d(\omega)\cos(2\phi)\cos(2\phi') \qquad (1)$$

and

$$\mu^*(\omega,\phi,\phi') = \mu^*_s + 2\mu^*_d(\omega)\cos(2\phi)\cos(2\phi'), \qquad (2)$$

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0022-3115/$ - see front matter © 2008 Published by Elsevier B.V.
doi:10.1016/j.jnucmat.2008.09.042

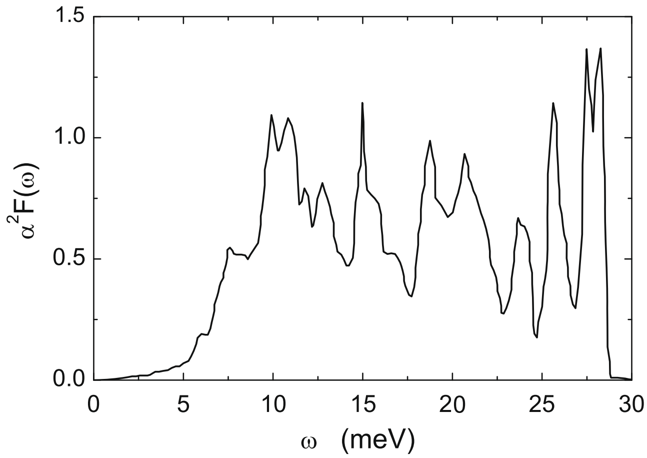

Fig. 1. Frequency dependence of the spectral density function $\alpha^2F(\omega)$ used in the calculations. This quantity describes the effective electron–electron interaction due to phonon exchange.

where ϕ and ϕ' are azimuthal angles defining the orientation of the electron wavevector in the *a*–*b* plane. The values of the relevant input quantities are given in our previous work [2]; $\alpha^2F(\omega)$, shown in Fig. 1, was obtained by rescaling the phonon density of states (PDOS) calculated ab initio by DFT methods [9], whereas $\mu_d^* = 0.247$ was fixed by the value of T_C. $N^N(\omega)$ was calculated using fully relativistic ab initio methods [10]. For the electron–phonon coupling constant, we use the phonon density of states calculated by Piekarz et al. [9], opportunely scaled in order to obtain $\lambda_s = \lambda_d = 2.1$. With these values, the effective electron–phonon coupling constant takes the value $\lambda_{s,eff} = 3.6$, which can be positively compared with the experimental value from specific heat measurements [11]. The impurity scattering rate Γ was also introduced into the equations as a free parameter in order to describe the effects of increasing lattice defects due to self-irradiation damage in aged samples.

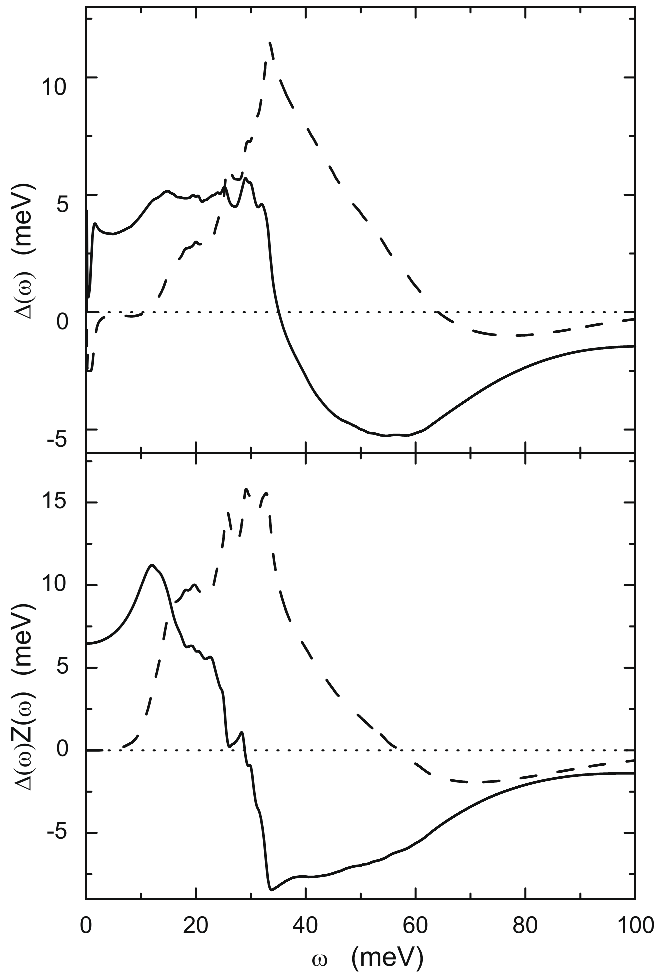

Fig. 2. Real (solid line) and imaginary (broken line) component of the complex gap function $\Delta(\omega)$ (upper panel) and of the renormalization function $Z(\omega)$ multiplied by $\Delta(\omega)$ (lower panel), calculated at $T = 4$ K for a $PuCoGa_5$ sample with $T_C = 18.5$ K.

3. Results and discussion

3.1. The superconducting phase

The real and imaginary parts of the complex gap function $\Delta(\omega)$ and of the renormalization function $Z(\omega)$ which result from our complete numerical solution of the Eliashberg equations at $T = 4$ K which would correspond to a fresh $PuCoGa_5$ sample ($T_C = 18.5$ K) are shown in Fig. 2. A visual inspection immediately shows that the real part of the gap function drops from positive to negative values in correspondence of the maximum of its imaginary part; this happens at the same energy where α^2F has a cutoff [9]. Once these functions are known, the superconductive energy gap $\Delta_0(T)$ at a given temperature T coincides with the value of ω which satisfies the relation

$$\mathrm{Re}[\Delta(\omega, T)] = \omega. \tag{3}$$

A calculation of $\Delta_0(T = 2\ \mathrm{K})$ as a function of Γ (and therefore of T_C for aged samples) is shown in Fig. 3. The predicted value (3.4 meV) obtained for a fresh sample could in principle be measured by several experimental probes, such as tunnelling measurements; despite the fact that the transuranic nature of this peculiar compound makes these experiments very difficult to be realized in practice, such a comparison could shed more light on the microscopic pairing mechanism. With this in mind, we also show the expected temperature dependence of the superconducting gap for a fresh sample in the inset of Fig. 3.

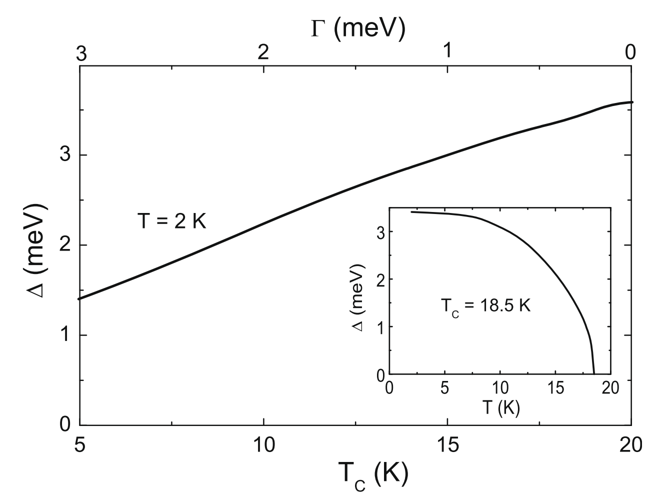

Fig. 3. Superconducting energy gap calculated at $T = 2$ K for $PuCoGa_5$ samples with different T_C resulting from different impurity content. The upper scale shows the corresponding value of the impurity scattering rate Γ. Inset: temperature variation of the energy gap for a freshly prepared sample ($T_C = 18.5$ K).

On the other hand, the spectral density α^2F can in principle be obtained directly by inversion of the current–voltage (I–V) characteristics of a metal–insulator–superconductor tunnelling junction. In this case, the I versus V curve is given by

$$I(V) \propto \int d\omega \frac{N(\omega)}{N(0)} [f(\omega) - f(\omega + V)], \quad (4)$$

where $f(\omega)$ is the Fermi function and the normalized quasiparticle density of states can be easily obtained from the calculated frequency-dependent gap function as

$$\frac{N(\omega)}{N(0)} = \int_0^{2\pi} \frac{d\phi}{2\pi} \mathrm{Re}\left[\frac{\omega N^N [Z(\omega)\sqrt{\omega^2 - 2\Delta^2 \cos^2 2\phi}]}{\sqrt{\omega^2 - 2\Delta^2 \cos^2 2\phi}}\right]. \quad (5)$$

The derivative of Eq. (4) with respect to V is the normalized tunnelling conductivity, which coincides with $N(\omega)/N(0)$ at zero temperature. Both $N(\omega)/N(0)$ and $dI/dV(T = 4\text{ K})$ corresponding to a freshly prepared sample have been calculated and are shown in Fig. 4 for comparison with future experiments.

3.2. The normal phase

One of the most important hints on the nature of the pairing bosons in the superconducting phase of $PuCoGa_5$ actually came from the resistivity measurements in the *normal* phase [2]. Indeed, in case of purely phonon-mediated pairing, the fit of $\rho(T)$ must contain the same electron–phonon-scattering matrix elements that appear in the Eliashberg equations for the superconducting state [12]. When this condition is imposed, the resistivity measured below 110 K for a freshly prepared sample can be fit (Fig. 5) with a reasonable plasma frequency $\Omega_p = 2.69$ eV, which compares well with the value of 1.78 eV obtained from the low-temperature experimental value of the penetration depth. However, above 110 K, the calculated linear increase of the resistivity does not fit at all the measured curve, as it fails to reproduce the saturation observed at high temperature. The temperature dependence of the electrical resistivity of $PuCoGa_5$ has been addressed in [13], considering both spin fluctuations and phonons as mediating boson. For the phonon case, these authors show that the shunting model proposed by Calandra and Gunnarsson [14] is partially successful in reproducing the S-shaped behavior of the resistivity.

Alternatively, the disagreement could be attributed to a failure of the one-band model used in the present calculation. A multiband approach can indeed be necessary to describe the superconductivity in $PuCoGa_5$, as a consequence of the bi-dimensionality of the Fermi sheets [10]. A second conduction band, as suggested for MgB_2 [15], could resolve the discrepancy. With this in mind, we have extended our calculations assuming a two-band model, one of which non-superconducting. Since this calculation involves a large number of free parameters (4 electron–phonon coupling constants, 2 plasma frequencies, and 3 different values of the impurity scattering rate), a unique solution should not be expected. However, we managed to show that this more rigorous treatment reproduces a behaviour similar to the shunting model [16]. In particular, imposing reasonable values to all parameters it is possible to obtain a calculated resistivity curve which is well in agreement with the experimental data in the range from T_C to room temperature (Fig. 5).

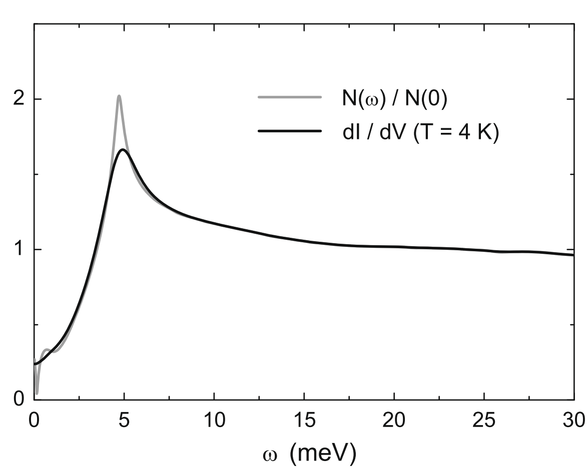

Fig. 4. Normalized quasiparticle density of states (grey line) and normalized tunnelling conductance at $T = 4$K (black line) calculated for a freshly prepared sample ($T_C = 18.5$ K).

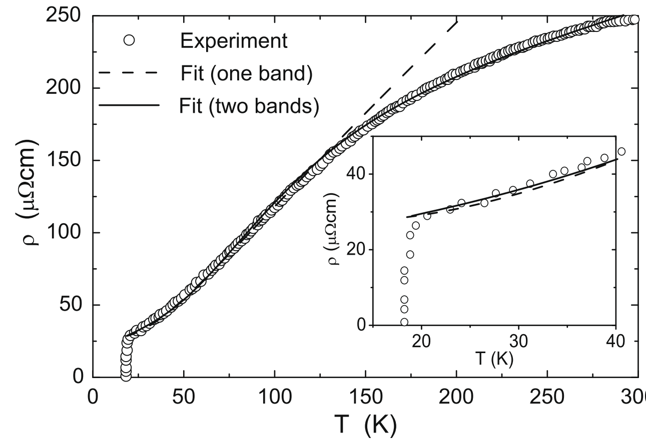

Fig. 5. Temperature dependence of the electrical resistivity calculated for a freshly prepared $PuCoGa_5$ sample ($T_C = 18.5$ K), within the one-band (dashed line) and the two-band model (solid line).

4. Conclusions

The nature of the pairing bosons of $PuCoGa_5$ has not yet been unambiguously identified. By focussing on a rigorous Eliashberg approach in the frame of a purely phonon-mediated *d*-wave superconductivity, we have calculated several physical observables (temperature and impurity-scattering-rate dependence of the superconductive gap, normalized quasiparticle density of states, and normalized tunnelling conductance). Future experimental determinations of these quantities could allow to set precise constraints on the parameters appearing in theoretical models, which would lead to more indications on the nature of the electron–boson coupling in the superconductive phase. This would be a considerable step forward towards the understanding of this fascinating compound.

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