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LETTER TO THE EDITOR

Does the absence of saturation preclude strong electron–phonon coupling?

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Abstract. Diffraction model calculations of electrical resistance for strong electron–phonon coupling in two- and three-dimensional alloys, incorporating Pippard–Ziman phonon ineffectiveness, are reported. It is shown that in an electron–phonon scattering based theory, although strong electron–phonon coupling is necessary, it is not a sufficient condition for the production of strong saturation in the normal-state resistivity. Thus, absence of saturation does not preclude strong electron–phonon coupling.

Recently Gurvitch and Fiory [1] argued against phonon-mediated superconductivity in $\text{La}_{1.825}\text{Sr}_{0.175}\text{CuO}_4$ (LSCO) and $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO). Their argument goes as follows: the previously known high- T_c alloys (e.g., the A15 alloys), which have strong electron–phonon coupling, all display strong negative deviations from linearity, in the normal state resistivity $r(T)$, referred to as saturation [2, 3]. The normal-state resistivities of LSCO and YBCO are not saturated. Thus, one does not have strong electron–phonon coupling in LSCO and YBCO.

Gurvitch and Fiory [1] further suggest that their arguments do not depend on specific models for resistivity saturation. Essentially, [1] contends that absence of saturation in the normal-state resistivity precludes strong electron–phonon coupling. This is a very interesting hypothesis, which deserves close scrutiny. Does the hypothesis hold in the three-dimensional case? Does the layered, essentially two-dimensional nature of the new superconductors vitiate the force of arguments based upon experience in three dimensional high- T_c alloys?

In order to provide some answers to these questions, the results of calculations of normal-state resistivity in two and three dimensions for a simple model, which contains the essential physics of the problem are presented.

To obtain the simplest form of the diffraction model and to simplify the numerical procedure, we assume (i) spherical or circular Fermi surface, (ii) single-branch Debye phonon spectrum, (iii) constant scattering t -matrices, and (iv) a solid having a single ion type.

These assumptions are incorporated into the diffraction model as described by Ziman [4], Faber [5] and Baym [6], generalised by incorporation of the Pippard–Ziman phonon ineffective principle [7] as articulated in [4].

The strength of the electron–phonon interaction is chosen to yield agreement with

the strong saturated normal-state resistivity of the A15 alloy, Nb_3Sn^3 , for reasonable choices of other parameters.

For purely normal scattering in the large electron mean free path l limit (i.e., no phonon ineffectiveness) in three dimensions, these assumptions yield standard Bloch-Grüneisen theory.

The diffraction model concepts employed have been developed and applied in a series of articles by Cote and Meisel [8–10]. The implications of phonon ineffectiveness for degradation of T_c in disordered superconductors [11, 12] and for the Eliashberg function [13] have been discussed. Diffraction model calculations incorporating Pip-pard–Ziman phonon ineffectiveness have yielded good agreement with details of the temperature dependence of the electrical resistivity in amorphous metals [14–20]. Pertinent reviews of many of the ideas employed in this work may be found in [21, 22].

Following these procedures one obtains for the isochoric resistivity in the two dimensional case with e the electron charge and v_F the Fermi velocity, the expression

$$r(t) = [4/(ev_F)^2] \int_0^1 dy y^2 (1 - y^2)^{-1/2} |t(2k_F y)|^2 S^r(2k_F y, l) \quad (1a)$$

$$r(t) = [4/(ev_F)^3] \langle |t|^2 \rangle \int_0^1 dy y^2 (1 - y^2)^{-1/2} S^r(2k_F y, l). \quad (1b)$$

We refer to $S^r(K, l)$ as the resistivity static structure factor for electron mean free path l . The resistivity static structure factor $S^r(K, l)$ with scalar argument K is equal to $S^r(\mathbf{K}, l)$ averaged over orientations of the scattering vector \mathbf{K} , involves a sum (integral) over the phonon spectrum, and incorporates saturation effects. (The $\langle \rangle$ notation implies an average value of 0 and, since we assume constant t -matrices, is redundant here.)

The corresponding isochoric results in three dimensions are

$$r(t) = [3/(ev_F)^2] \int_0^1 dy y^3 |t(2k_F y)|^2 S^r(2k_F y, l) \quad (2a)$$

$$r(t) = [3/(3v_F)^2] \langle |t|^2 \rangle \int_0^1 dy y^3 S^r(2k_F y, l). \quad (2b)$$

The resistivity static structure factor in perfectly crystalline alloys is expressed in terms of the phonon part of the Van Hove dynamical structure factor $S'(\mathbf{K}, \Omega)$ as

$$S^r(\mathbf{K}, l) = \int_{-\infty}^{\infty} d\Omega \quad xn(x) S'(\mathbf{K}, \Omega) P(\Omega, l) \quad (3a)$$

where for k_B Boltzmann's constant and \hbar Planck's constant, $x = \hbar\Omega/k_B T$, $n(x) = 1/(\exp(x) - 1)$ is the phonon occupation number, and $P(\Omega, l)$ is a factor included to describe saturation. Replacing $P(\Omega, l)$ by unity yields the standard expression for $S^r(\mathbf{K})$. (N.B., $S'(\mathbf{K}, \Omega)$ appears because Bloch waves are not *elastically* scattered in perfect crystals.) The appropriate form for $S^4(K, l)$ in three dimensions is

$$S^r(K, l) = \int \frac{d\mathbf{K}}{4\pi} S^r(\mathbf{K}, l). \quad (3b)$$

In the two-dimensional case, the integral is over ordinary angles and the denominator is 2π .

The phonon part of the dynamical structure factor in Sham–Ziman approximation

[24] is

$$S'(\mathbf{K}, \Omega) = \sum_{q,j} \frac{(\hbar \mathbf{K} \cdot \mathbf{e}(q, j))^2}{2NM\hbar\Omega(q, j)} [a(\mathbf{K} - \mathbf{q}) \delta(\Omega - \Omega(q, j)) (n(q, j) + 1) + a(\mathbf{K} + \mathbf{q}) \delta(\Omega + \Omega(q, j)) n(q, j)] \quad (4)$$

where the sum runs over phonon branches j and phonon wavevectors \mathbf{q} , $\mathbf{e}(q, j)$ is the j -branch polarisation vector at \mathbf{q} , $\Omega(q, j)$ the j -branch phonon dispersion, and $n(q, j) = n(x)$, defined above, for $x = \hbar\Omega(q, j)/k_B T$; N the ion number density, M the ion mass, and $a(\mathbf{k})$ the geometric structure factor. For three-dimensional crystalline materials

$$a(\mathbf{k}) = [(2\pi)^3/V_0] \sum_{\mathbf{G}} \delta(\mathbf{k} - \mathbf{G}) \quad (5)$$

where the sum runs over reciprocal-lattice vectors \mathbf{G} and V_0 is the unit cell volume. In two dimensions one has $(2\pi)^2$ and a two-dimensional δ -function.

The function $P(\Omega, l)$ describes saturation of the electron–phonon interaction. The form selected is based on the Pippard–Ziman phonon ineffectiveness principle [4, 7]: ‘Phonons whose wavelengths $2\pi/q$ exceed the electron mean free path l are ineffective electron scatterers.’

Good agreement with measured $r(T)/r(\theta)$ in amorphous metals, and the degradation of the superconducting critical temperature T_c in disordered A15 superconductors has been obtained with *sharp cut-off phonon ineffectiveness*:

$$P(\Omega, l) = H(|\Omega| - \Omega_c(l)) \quad (6)$$

where $H(x)$ is the Heaviside function and for a Debye phonon spectrum

$$\Omega_c(l) = \Omega_D a/l = (6\pi^3)^{1/3} \Omega_D/(q_D l) \quad (7)$$

where a is a representative lattice spacing, q_D is the Debye wavenumber, and Ω_D is the Debye frequency. The form for the cut-off value Ω_c is chosen to completely cut off the electron–phonon interaction when the electron mean free path is equal to the lattice spacing a .

Incorporating the approximations enumerated above, the resistivity static structure factor for electron mean free path l in three dimensions assumes the form

$$S^r(K, l) = \beta(K) \frac{\theta}{l} \sum_{\mathbf{G}} \int \frac{d\mathbf{K}}{4\pi} (n(z) + 1) n(z) P(\Omega|\mathbf{K} - \mathbf{G}|, l) H(q_D - |\mathbf{K} - \mathbf{G}|) \quad (8)$$

(and similarly in two dimensions) where q_D is the Debye wavenumber

$$z = \hbar\Omega(|\mathbf{K} - \mathbf{G}|)/k_B T = (\theta/T) |\mathbf{K} - \mathbf{G}|/q_D$$

$$\beta(K) = (\hbar K)^2/(Mk_B\theta)$$

and $H(x)$ is the Heaviside function again. The Heaviside function appears because for a Debye spectrum, the phonon wavenumber q does not exceed q_D .

We assume that there are six (equal in magnitude) smallest reciprocal-lattice vectors \mathbf{G} ($G = 2\pi/a$) contributing Umklapp terms to the resistivity (and mass enhancement factor) in three dimensions, etc, and use the same constant t -matrix for normal and Umklapp scattering.

Although not an essential element of the argument, we allow for residual resistivity

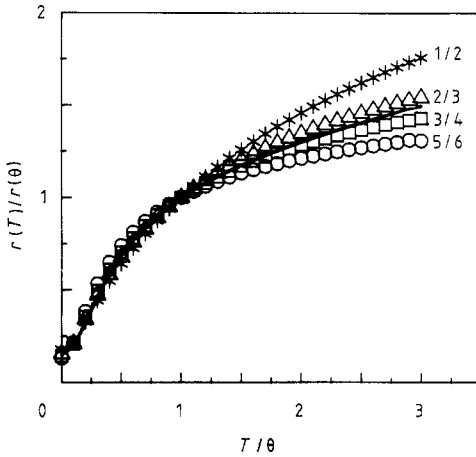


Figure 1. Normalised isochoric resistivity versus T/θ for $2k_F = 1.6q_D$ in the three-dimensional case. (N.B., shortest $G = 1.612q_D$ for all figures.) Values of $a/l(3\theta)$ are indicated. The full curve is for Nb_3Sn from Woodard and Cody [3] for $\theta = 200$ K.

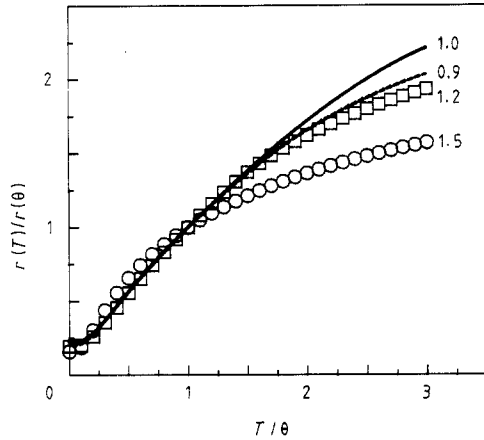


Figure 2. Normalised isochoric resistivity versus T/θ for $l(3\theta) = 1.5a$ in the two-dimensional case. Values of $2k_F/q_D$ are indicated. The straight line is a guide for the eye.

as observed in LSCO, YBCO and Nb_3Sn . The residual resistance is assumed to be due to a random distribution of defects, which produces constant terms in the geometrical structure factor. A k -independent term in $a(k)$ engenders a weakly T -dependent term in the electrical resistivity, which is approximated as a T -independent part of $r(T)$ here.

As is customary, computed isochoric $r(T)/r(\theta)$ are compared with isobaric experimental measurements. As discussed, for example, by Mott and Jones [23], for $T > \theta$

$$(r(T)/r(\theta))|_p \approx (r(T)/r(\theta))|_v(1 + 2\alpha\gamma T)$$

where α is the thermal expansion coefficient and γ Grüneisen's constant. For typical metals $2\alpha\gamma \approx 10^{-4} \text{ C}^{-1}$. Although the correction is negligible in the A15 superconducting alloys, it can yield observable effects.

The calculation of $r(T)$ proceeds as follows.

(i) values are selected for $2k_F/G$, the relative residual resistivity $r(0)/r(3\theta)$, and for $a/l(3\theta)$.

(ii) The integral in equation (2b) or (3b) is calculated at $T = 3\theta$.

(iii) The proportionality constant relating $a/l(T)$ to the respective integrals when combined with the residual resistivity part is computed.

(iv) Then $a/l(T)$ is computed self consistently for a set of T values.

Figure 1 shows isochoric results computed in three dimensions. Parameters were chosen to approximate those for Nb_3Sn : $2k_F/G = 0.99$, $r(0)/r(3\theta) = 0.1$. A variety of values were assumed for $a/l(3\theta)$. Representative results and, assuming $\theta = 200$ K, the experimental resistivity curve for Nb_3Sn of Woodard and Cody [3] are shown. The data fall about midway between the computed values obtained for $a/l(3\theta) = \frac{2}{3}$ and $\frac{3}{4}$. The data could be fit with either of these values of $a/l(3\theta)$ if one changed θ by about 10%; the data are also consistent with computed results for $\theta = 200$ K, $2k_F/G = 0.93$, and $a/l(3\theta) = \frac{3}{4}$. The values of a/l in figure 1 are in the range suggested in [1] for A15 alloys.

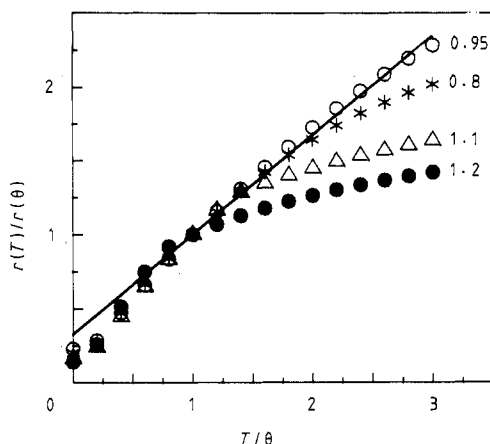


Figure 3. Normalised isochoric resistivity versus T/θ for $l(3\theta) = 1.5a$ in the three-dimensional case. The smooth curves pass through the same point set as the symbols and are used for clarity. Values of $2k_F/q_D$ are indicated.

Figures 2 and 3 show results of calculations for $a/l(3\theta) = \frac{2}{3}$, $r(0)/r(3\theta) = 0.1$, and a selection of $2k_F/G$ values in two and three dimensions, respectively. The shape of the computed $r(T)/r(\theta)$ versus T curves is strongly dependent on $2k_F/G$. The least curvature is obtained in both figures at $2k_F/G \approx 0.6$. Although a/l values along all the curves in figures 2 and 3 are large, of the order appropriate for the A15 alloys, one would not describe the curves for $2k_F/G = 0.6$ as saturated. Even smaller negative curvature is obtained for $2k_F/G$ near 0.6 and smaller (although, still representative of strong electron-phonon coupling) values of a/l .

The following conclusions can be drawn from this study.

(i) The simplest form of the diffraction model, incorporating Pippard–Ziman phonon ineffectiveness and reasonable parameters yields agreement with the strongly saturated $r(T)/r(\theta)$ in A15 alloys.

(ii) Similar results, including saturated $r(T)/r(\theta)$, are obtained in two and three dimensions. Thus, saturated resistivity curves do not require three-dimensional structure and lack of saturation in the ceramic superconductors cannot be attributed to their layered structure.

(iii) The extreme linearity in the normal-state resistivity reported for the ceramic superconductors, especially for $T < \theta$, cannot be explained by this model. However, the negative curvature exhibited in the resistivity versus temperature data of Johnson *et al* [25] for example, is consistent with results presented here for reasonable parameter choices.

(iv) Significant Umklapp contributions to the resistivity can occur for relatively large phonon wavevectors (which are relatively immune to phonon ineffectiveness) for values of $2k_F/G$ near 0.6. Therefore, relatively small negative deviations from linearity may result for strong electron–phonon coupling if $2k_F/G$ is near 0.6. Thus, absence of saturation in the electrical resistivity does not preclude strong electron–phonon coupling.

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