

Koshino-Taylor coefficient in electrical resistivity

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At low temperatures the electrical resistivity of simple metals such as potassium has a T^2 term which is proportional to the concentration of impurities. This behavior was predicted by Koshino and Taylor. We provide an expression for the coefficient of the T^2 term. It is expressed as a function of the phase shifts of the scattering of the electron by the impurity.

At low temperature, the electrical resistivity of simple metals such as lithium and potassium varies with temperature according to¹⁻¹²

$$\rho(T) = AT^2 + \rho_0(1 + BT^2) + \delta\rho(T) . \tag{1}$$

The constant term ρ_0 is due to impurity scattering, and is proportional to their concentration. The first term AT^2 is intrinsic and comes from electron-electron umklapp scattering. The largest contribution to the coefficient A is from phonon-mediated interactions between the electrons.⁵ The term B is the subject of the present discussion. The extra term $\delta\rho$ is from a variety of effects: phonon drag,³ dislocations,^{6,7} size effects,^{13,14} and the effects of the impurities on the phonons.^{15,16}

The term B has two contributions: The Koshino-Taylor effect^{1,2} and dislocations.^{6,7} Here we wish to derive a new expression for the coefficient for the Koshino-Taylor effect.

The Koshino-Taylor effect is due to inelastic scattering of the electrons by impurities. Since the impurities are part of the lattice, the scattering by the electrons can excite phonons. The rate of scattering is also normalized by the Debye-Waller effect, which is given in terms of the thermal fluctuations of the impurity positions.

Accurate experimental data for B have become available for potassium and lithium.⁸⁻¹¹ It seems worthwhile to derive a more accurate expression for B , in order to provide a comparison between theory and experiment. Past derivations expressed B as an average over the scattering potential of the impurity. A better way to de-

scribe the potential scattering is in terms of the phase shifts of the electron scattering from the impurity. We adopt this approach and express B as a function of the phase shifts. The Friedel sum rule¹⁷ provides a constraint on the value of these phase shifts. Furthermore, the term ρ_0 provides another function of the phase shifts. These relations then allow B to be determined within bounds.

INELASTIC IMPURITY SCATTERING

Consider a distribution of impurities at sites R_j with a fluctuating displacement Q_j . This potential can be written as

$$\begin{aligned} V &= \sum_j V(\mathbf{r} - \mathbf{R}_j - \mathbf{Q}_j) \\ &= \sum_j \sum_q v_i(q) \exp[i\mathbf{q} \cdot (\mathbf{r} - \mathbf{R}_j - \mathbf{Q}_j)] . \end{aligned}$$

We expand it in powers of the displacement, and keep the first two terms:

$$\begin{aligned} V &= \sum_j \sum_q v_i(q) \exp[i\mathbf{q} \cdot (\mathbf{r} - \mathbf{R}_j)] \\ &\quad \times [1 - i\mathbf{q} \cdot \mathbf{Q}_j - (\mathbf{q} \cdot \mathbf{Q}_j)^2 / 2 + \dots] . \end{aligned}$$

This potential is used to evaluate the scattering in the second Born approximation. We retain terms of order $O(Q^2)$. The term $(\mathbf{q} \cdot \mathbf{Q})^2$ is part of the Debye-Waller factor. It is subtracted from the inelastic scattering of phonons. The net contribution to the self-energy of the electron is

$$\begin{aligned} \Sigma^<(p, \epsilon) &= n_i \int \frac{d^3q}{(2\pi)^3} [v_i(q)]^2 \int \frac{d^3q'}{(2\pi)^3} \frac{(q \cdot \xi')^2}{2\rho\omega'} \{ (N_{q'} + 1) [G^<(\mathbf{p} + \mathbf{q}, \epsilon + \omega_{q'}) - G^<(\mathbf{p} + \mathbf{q}, \epsilon)] \\ &\quad + N_{q'} [G^<(\mathbf{p} + \mathbf{q}, \epsilon - \omega_{q'}) - G^<(\mathbf{p} + \mathbf{q}, \epsilon)] \} . \end{aligned}$$

Primed q variables refer to the phonon, while unprimed q variables refer to the momentum transfer of the electron during the scattering. We use ρ here to mean the mass of the impurity divided by the volume of the unit cell. This self-energy vanishes if the energy of the phonon is set equal to zero. This formula is only valid if the impurity mass equals the mass of the host ions. Later we discuss the correction which is needed when the masses are different. We write

$$G^<(p, \epsilon) = i n_F(\epsilon) A(p, \epsilon) , \quad \Sigma^<(p, \epsilon) = i n_F(\epsilon) 2\Gamma_{KT}(p, \epsilon) ,$$

which defines the Koshino-Taylor energy uncertainty:

$$2\Gamma_{\text{KT}}(p, \varepsilon) = n_i \int \frac{d^3 q}{(2\pi)^3} [v_i(q)]^2 \int \frac{d^3 q'}{(2\pi)^3} \frac{(q \cdot \xi')^2}{2\rho\omega'} \{ [N_{q'} + n_F(\varepsilon + \omega_{q'})] A(\mathbf{p} + \mathbf{q}, \varepsilon + \omega_{q'}) \\ + [N_{q'} + 1 - n_F(\varepsilon - \omega_{q'})] A(\mathbf{p} + \mathbf{q}, \varepsilon - \omega_{q'}) - (2N_{q'} + 1) A(\mathbf{p} + \mathbf{q}, \varepsilon) \}. \quad (2)$$

We change the electron-impurity potential $v_i(q)$ to a T matrix¹⁷ between initial (p) and final (p') electron wave vectors. Furthermore we add a factor of $(1 - \cos\theta)$ to the integrand to account for the scattering back in the formula for the resistivity. The angle θ is between \mathbf{p} and \mathbf{p}' . The phonon part of the integrand is given by a function we define as $g(u)$:

$$(k_F^2/\rho) \sum_{\lambda} \int \frac{d^3 q'}{(2\pi)^3} \xi'_{\mu} \xi'_{\nu} \delta(u - \omega_{\lambda}(q')) = \delta_{\mu\nu} g(u), \quad (3)$$

where λ is the polarization of the phonon. The right-hand side is proportional to a delta function of the (x, y, z) components (μ, ν) which is required by cubic symmetry, which we are assuming. The function $g(u)$ is dimensionless. The delta function means that the factor $(q \cdot \xi')^2$ becomes

$$q^2 = (\mathbf{p} - \mathbf{p}')^2 = 2k_F^2(1 - \cos\theta).$$

The integral over p' decouples from the integral over phonon coordinates. It is useful to define the integral

$$I_{\text{KT}} = n_i \int \frac{d^3 p'}{(2\pi)^3} T_{pp'}^2 (1 - \cos\theta)^2 A(p', \varepsilon). \quad (4)$$

The same factors appear in the expression for the resistivity from impurity scattering. However, this factor, which we call I_i , has only one factor of $(1 - \cos\theta)$. It is a good approximation to evaluate both of these expressions as if the scattering were elastic. Then the T matrices can be expressed in terms of phase shifts,¹⁷ and the integral expressed in terms of them. We define S_j for $j = i$ or KT according to

$$I_j = \frac{4\pi n_i}{mk_F} S_j.$$

We find that

$$S_i = \sum_{l=1}^{\infty} l \sin^2(\delta_l - \delta_{l-1}), \quad (5) \\ S_{\text{KT}} = 2 \left[S_i - \sum_{l=1}^{\infty} \frac{l(l-1)}{2(2l-1)} \sin^2(\delta_l - \delta_{l-2}) \right].$$

Collecting all of these results gives the expression for the KT term in the resistivity

$$2\Gamma_{\text{KT}}(\varepsilon) = I_{\text{KT}} \int_0^{\omega_D} du \frac{1}{u} g(u) [n_F(\varepsilon + u) - n_F(\varepsilon - u)].$$

We write $n_F(\varepsilon - u) = 1 - n_F(u - \varepsilon)$ and the 1 term gives an uninteresting constant. At low temperature the T^2 term comes from the integral at small u . From Eq. (3) we find that $g = \gamma u^2$ at small u . Then the u integral is changed to $y = \beta u$ so that we find for Γ_{KT}

$$2\Gamma_{\text{KT}}(\varepsilon) = \gamma I_{\text{KT}} (k_B T)^2 z(\beta\varepsilon),$$

$$z(x) = \int_0^{\infty} dy y \left[\frac{1}{e^{x+y} + 1} + \frac{1}{e^{y-x} + 1} \right].$$

In calculating the conductivity, we have to average ε over its range of thermal values. This average is

$$\langle z \rangle = \int_{-\infty}^{\infty} d\varepsilon z(\beta\varepsilon) [-\partial n_F(\varepsilon)/\partial \varepsilon].$$

The above expression is a double integral in $x = \beta\varepsilon$ and y . It is easy to do the x integral first, and the result gives a y integrand of $2y \partial [y n_B(y)]/\partial y$. Then the y integral is also easy, so that $\langle z \rangle = \pi^2/3$. Our result is

$$2\Gamma_{\text{KT}} = \pi^2 \gamma I_{\text{KT}} (k_B T)^2 / 3.$$

The coefficient B is this expression divided by $\rho_0 T^2$. Thus we get that

$$B_{\text{KT}} = \pi^2 \gamma k_B^2 R / 3, \quad (6) \\ R = S_{\text{KT}} / S_i.$$

There remains just the task of evaluating the phonon contribution γ . From Eq. (3) it can be written as

$$\gamma = [k_F^2 / (2\pi^2 \rho)] \langle \xi_x^2 / c^3 \rangle,$$

where $\langle \rangle$ indicates an average over 4π of solid angle plus a summation over acoustic-phonon branches, and c is the phonon velocity which depends upon solid angle. For monovalent metals the density ρ can be written as the ion mass M times the particle density $k_F^3/3\pi^3$. Expressing k_F in terms of the electron density factor r_s by $k_F a_0 = 1.9192/r_s$, gives the expression

$$B_{\text{KT}} = (b R r_s / M) \langle \xi_x^2 / c^3 \rangle, \\ b = \pi^2 k_B^2 a_0 / (2 \times 1.9192),$$

which is our final expression. If we express M in atomic mass units and $\langle \rangle$ in terms of $10^{-15} \text{ s}^3/\text{cm}^3$, then $b = 1.48 \times 10^{-4} \text{ K}^{-2}$.

The only expression which may present difficulty is the ratio R in (6) between the phase-shift expression for the KT process divided by that for the impurity scattering. However, we find that this expression is simple to evaluate. First, we assume that the only nonzero phase shifts are s , p , and d . This approximation is accurate in simple metals, as shown by experiments on electron scattering from core holes.¹⁸ Second, the Friedel sum rule relates these three phase shifts to the impurity valence Z , which is the difference between the charge on the impurity and the host-metal ion.¹⁷

$$Z\pi/2 = \delta_0 + 3\delta_1 + 5\delta_2.$$

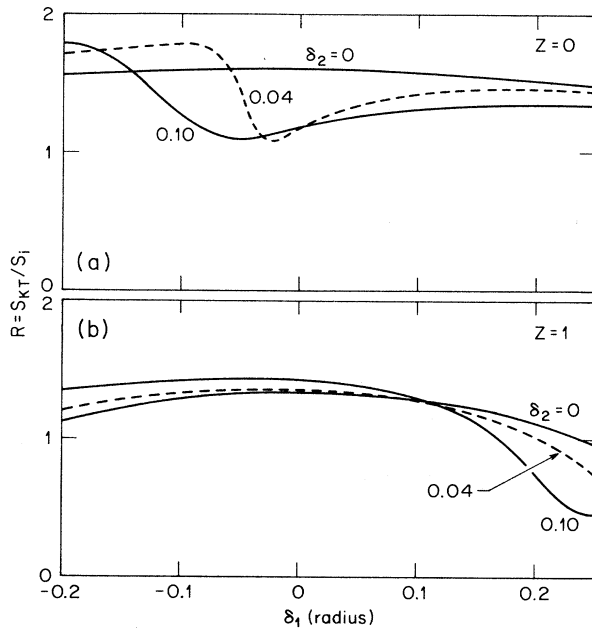


FIG. 1. The ratio R defined in Eqs. (5) and (6) is plotted as a function of phase shifts of an electron on the Fermi surface scattering from the impurity. The Friedel sum rule determines δ_0 once δ_1 and δ_2 are specified. Part (a) is for an impurity with the same core charge as the host ions ($Z=0$), and part (b) is for an impurity whose charge state differs by one ($Z=1$).

So if we vary δ_1 and δ_2 , then δ_0 is determined. Figure 1 shows a graph of R plotted for $Z=0$ and $Z=1$ for different values of the phase shifts. These values encompass the range of likely physical values. For $Z=0$, then, R has values between 1.06 and 1.80. For $Z=1$ the values are between 1.2 and 1.4. The parameter B has only a slight dependence upon the values of the phase shift for the impurity with $Z=1$, but a large dependence when $Z=0$.

The constant impurity resistance ρ_0 is also obtained by the fitting to the data. Using the standard formula¹⁹

$$\rho_0 = g(n_i/n_0)S_i,$$

$$g = 2h/e^2k_F = 1.42 \times 10^{-4} r_s \Omega \text{ cm}.$$

The experiments usually determine S_i . For $Z \neq 0$ this information puts another constraint upon the phase shifts. However, for $Z=0$, a knowledge of S_i does not help. Instead, it provides a scale factor for all of the phase shifts which factor out of the ratio when R is evaluated. For example, set $\delta_2 = \alpha S_i^{1/2}$. Since the phase shifts are all

small for $Z=0$ impurities, (5) can be approximated by setting $\sin^2 f = f^2$. Then the Friedel sum rule and the expression for S_i provide two equations for the unknowns δ_0 and δ_1 . Solving these two equations gives

$$\delta_0 = S_i^{1/2}(2\alpha \pm T),$$

$$\delta_1 = S_i^{1/2}(-\alpha \pm T/3),$$

$$T = (1 - 12\alpha^2)^{1/2}/\sqrt{2}.$$

The factor of S_i cancels out of the ratio $R = S_{KT}/S_i = F(\alpha)$. By varying α within its bounds of $\pm 1/12^{1/2}$, one finds the maximum value of R is 1.80 and the minimum value is 1.06. In Fig. 1(a) the curve for $\delta_2 = 0.04$ comes close to both of those bounds. Thus for $Z=0$ the knowledge of S_i does not provide any information towards determining R . Instead, it only provides a scale factor on the phase shifts.

All ions in the metal move together in long-wavelength acoustic motion. So there is no correction for the difference in the ion mass, or in the difference in bonding. This theory should apply to every impurity.

DISCUSSION

A new expression has been derived for the Koshino-Taylor coefficient for the low-temperature resistivity of simple metals. Here we wish to compare our result to the available experiment results.

For potassium we find for the average over sound-wave directions that $\langle \rangle = 0.466$. $Z=0$ for the rubidium impurity. Using $1.06 < R < 1.8$ gives in units of 10^{-5} K^{-2} the bounds on B of $0.93 < B < 1.58$. The experimental values^{11,12} of 1.20 and $1.23 \times 10^{-5} \text{ K}^{-2}$ are near the average of our extremal values. For this case we find that $S_i = 0.088$ and the phase shifts all have a magnitude of 0.1 rad.

For the cubic form of lithium we find that $\langle \rangle = 0.0452$. Using $R = 1.3$ for Mg impurities ($Z=1$) gives $B = 0.40 \times 10^{-5} \text{ K}^{-2}$. The experimental result¹¹ is $0.16 \times 10^{-5} \text{ K}^{-2}$. The comparison for lithium is inappropriate since it changes its structure at low temperature to the 9R phase,²⁰ which is hexagonal rather than cubic. The experiments are done at low temperature.

Experimental values are only available for lithium and potassium. Sodium and rubidium do not have a temperature regime where the T^2 is well defined. Thus the only comparison which is reasonable is for potassium.

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