

Electron-electron scattering resistivity of lithium

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1992 J. Phys.: Condens. Matter 4 L105

(<http://iopscience.iop.org/0953-8984/4/7/001>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.96

The article was downloaded on 11/05/2010 at 00:01

Please note that [terms and conditions apply](#).

LETTER TO THE EDITOR

Electron–electron scattering resistivity of lithium

N Wisert

Cavendish Laboratory, University of Cambridge, Cambridge, UK

Received 3 October 1991, in final form 13 December 1991

Abstract. The identification of the 9R rhombohedral structure as the low-temperature phase of lithium offers a resolution of the longstanding order-of-magnitude discrepancy between theory and experiment for the electron–electron scattering resistivity. In the 9R structure, the Fermi surface of monovalent lithium has many intersections with the Brillouin zone boundaries. This implies polyvalent-like behaviour for the electron pseudo-wavefunctions, which leads to an order-of-magnitude increase in the calculated electron–electron scattering resistivity.

Considerable progress has been made in recent years in our understanding of the electron–electron scattering contribution to the electrical and thermal resistivities of the non-transition metals (for reviews, see Kaveh and Wisert 1984, Wisert 1984, 1989). The low-temperature electrical resistivity of the non-transition metals is dominated by the electron–electron scattering term $\rho_{ee}(T)$, which varies quadratically with temperature, i.e.

$$\rho_{ee}(T) = A_{ee} T^2. \quad (1)$$

Measurements and calculations of A_{ee} have now been carried out for a number of non-transition metals, with generally good agreement between theory and experiment (for detailed references, see Kaveh and Wisert 1984).

The case of lithium, however, stands out as an anomaly. The experimental value of A_{ee} for Li, which has been confirmed in several laboratories (Krill 1971, Sinvani *et al* 1981, Yu *et al* 1983), is in complete contradiction to the best calculated value (MacDonald *et al* 1981):

$$\begin{aligned} A_{ee}(\text{Li}) &= 3.0 \text{ p}\Omega \text{ cm K}^{-2} && \text{(experiment)} \\ A_{ee}(\text{Li}) &= 0.21 \text{ p}\Omega \text{ cm K}^{-2} && \text{(theory)}. \end{aligned} \quad (2)$$

This striking discrepancy has not, of course, passed unnoticed, but previous attempts to explain it (Sinvani *et al* 1981) have not been satisfactory (Zhao *et al* 1986).

Here we propose a resolution of the discrepancy in equation (2) by utilizing the finding of Overhauser (1984) that at low temperatures, lithium transforms into the 9R structure (which is also that of the rare-earth metal Sm). This low-temperature structure of Li is very different from the BCC lattice that characterizes the other alkalis. Ashcroft (1989) has recently shown that the 9R structure resolves some longstanding anomalies

† Permanent address: Department of Physics, Bar-Ilan University, Ramat-Gan, Israel.

in the optical properties of Li. This structure can also explain the low-temperature electrical properties of Li.

The argument given here to resolve the enormous discrepancy in values of A_{cc} between theory and experiment for Li is based on the fact that the primitive rhombohedral unit cell of the 9R structure contains three atoms. Therefore, monovalent Li has three electrons per unit cell (exactly as does Al, with one trivalent atom per FCC unit cell). This implies that the Fermi surface intersects the Brillouin zone boundaries in many places, which is the characteristic feature of the pseudo-wavefunction of a *polyvalent* metal. As a result, the pseudo-wavefunction of monovalent Li is similar to that of a non-transition polyvalent metal, rather than that of an alkali metal. We shall see that this leads to an order-of-magnitude enhancement of the calculated coefficient, A_{cc} , in (1), thus bringing the calculated value into accord with the experimental value.

The pioneering 'modern-era' calculation of A_{cc} for the non-transition metals is surely that of Lawrence and Wilkins (1973), who wrote A_{cc} as a product

$$A_{cc} = A_0 \Delta \quad (3)$$

where the dimensionless quantity Δ is called the 'fractional Umklapp scattering'. The usefulness of (3) stems from the fact that A_0 depends primarily on the free-electron properties of the metal (i.e. on the basic electron-electron scattering rate), whereas Δ depends on the *deviations* from free-electron behaviour (i.e. on the fact that the electron pseudo-wavefunction may *not* be approximated by a single plane wave). Indeed, if the conduction electrons were truly free and describable by a single plane wave, then Δ and hence A_{cc} would vanish, even though $A_0 \neq 0$.

The determination of A_0 requires a comprehensive many-body analysis. MacDonald *et al* (1981) have carried out such a calculation for the alkali metals. For Li, they find

$$A_0 = 4 p \Omega \text{ cm K}^{-2}. \quad (4)$$

The heart of the present discussion of Li lies in the determination of Δ , the fractional Umklapp scattering. The value of Δ for the alkali metals differs markedly from its value for the polyvalent metals for the following reason. The (unnormalized) electron pseudo-wavefunction, $\psi_k(r)$, may be expanded into a sum of plane waves

$$\psi_k(r) = e^{ik \cdot r} + \sum_n C_n e^{i(k+G_n) \cdot r} \quad (5)$$

where the G_n are the non-zero reciprocal lattice vectors. Lawrence and Wilkins (1973) have shown that the fractional Umklapp scattering, Δ , depends on the magnitude of the coefficients $|C_n|^2$. If $\psi_k(r)$ were to be approximated by a single plane wave, with all the C_n set equal to zero, then $\Delta = 0$. Thus, it is precisely the *deviation* from single plane-wave behaviour for the electron pseudo-wavefunction that determines the magnitude of Δ .

For the alkalis—monovalent metals that crystallize in the BCC structure—the Fermi surface does not intersect the Brillouin zone boundaries. Therefore, a single plane wave is quite a good approximation to $\psi_k(r)$, with only very small corrections arising from the sum over the non-zero reciprocal lattice vectors indicated in (5). Since the coefficients C_n are *small*, so is Δ . The detailed calculations of MacDonald *et al* (1981) yield values for Δ for alkali metals in the range,

$$\Delta \sim 0.02\text{--}0.05 \quad (6)$$

where the alkalis have, of course, been assumed to have a BCC structure.

For the polyvalent metals, the situation is very different. The Fermi surface intersects the Brillouin zone boundaries in many places, so almost everywhere on the Fermi surface at least one of the C_n is of the order of unity. As a result, the value of Δ is much larger than for the alkalis. Lawrence and Wilkins (1973) calculated Δ for several non-transition polyvalent metals (Al, In, Mg, Zn, Cd) and found values in the range

$$\Delta \sim 0.4-0.6 \quad (7)$$

which is a full order of magnitude larger than the range of values for the alkali metals (6).

Although the calculation of Lawrence and Wilkins is not reliable in detail, there can be no doubt that there exists an order-of-magnitude difference between the value of Δ for the alkali metals and that for the polyvalent metals.

For lithium, the argument is now straightforward. At low temperatures, lithium transforms into the 9R crystal structure with three atoms and hence three electrons per unit cell. This implies that the electron pseudo-wavefunctions of Li resemble those of a polyvalent metal. Therefore, the value of Δ for Li will be given by (7), rather than (6). Taking $\Delta = 0.5$, according to (7), immediately leads to

$$A_{cc} = \Delta A_0 \approx 0.5 \times 4 \text{ p}\Omega \text{ cm K}^{-2} = 2 \text{ p}\Omega \text{ cm K}^{-2} \quad (8)$$

which is in quite reasonable agreement with the experimental value for Li of $A_{cc} = 3.0 \text{ p}\Omega \text{ cm K}^{-2}$.

References

- Ashcroft N W 1989 *Phys. Rev. B* **39** 10552
 Kaveh M and Wiser N 1984 *Adv. Phys.* **33** 257
 Krill G 1971 *Solid State Commun.* **9** 1065
 Lawrence W E and Wilkins J W 1973 *Phys. Rev. B* **7** 2317
 MacDonald A H, Taylor R and Geldart D J W 1981 *Phys. Rev. B* **23** 2718
 Overhauser A W 1984 *Phys. Rev. Lett.* **53** 64
 Sinvani M, Greenfield A J, Danino M, Kaveh M and Wiser N 1981 *J. Phys. F: Met. Phys.* **11** L73
 Wiser N 1984 *Contemp. Phys.* **25** 211
 ——— 1989 *High Temp.—High Pressures* **21** 25
 Yu Z Z, Haerle M, Zwart J W, Bass J, Pratt W P Jr and Schroeder P A 1983 *Phys. Lett. A* **97** 61
 Zhao J, Bass J, Pratt W P Jr and Schroeder P A 1986 *J. Phys. F: Met. Phys.* **16** L271