

Electron–electron interactions and the electrical resistivity of lithium at low temperatures

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Abstract. The electron–electron interactions in lithium metal have been examined keeping in view the recent developments. The contribution of the electron–electron Umklapp scattering processes in the electrical resistivity of lithium at low temperatures has been evaluated using a simplified spherical Fermi surface model with isotropic transition probability. Our values of the electrical resistivity so obtained compare fairly well with the experimental results for lithium.

Keywords. Electrical resistivity; e–e interactions, temperature dependence.

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1. Introduction

Since 1968, a revolution has taken place in the field of low-temperature electrical resistivity of simple metals. Recent technological advances in measurements have yielded unexpected experimental results, which are totally at variance with earlier accepted theories. At liquid helium temperatures, the electrical resistivity of metals is governed mainly by electron–electron and electron–phonon interactions. Garland and Bowers [1] measured the electrical resistivity of aluminium, indium, sodium and potassium as a function of temperature from 1.2 K to 4.2 K. Their results clearly indicated the presence of a T^2 -term in the electrical resistivity of aluminium and indium. Sodium and potassium, however, did not show a T^2 -term.

More refined later measurements [2,3] for the electrical resistivity of sodium and potassium in the temperature region 0.5 K to 4.2 K have, however, indicated that these metals also have a T^2 -term.

The experimental results for lithium [4–6] clearly show a T^2 -term. Further, these experimental results for lithium show no sample dependence at all. The experimentally observed T^2 -term for lithium clearly suggests that the e–e scattering dominates the e–phonon scattering below 10 K [7].

The study of electron–electron interactions started with the pioneering work of Landau and Pomeranchuk [8,9] and Baber [10], who showed that e–e scattering, should contribute to $\rho(T)$ term of the form

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

with the coefficient A_{ee} being constant for a given metal.

Here A_{ee} contains both normal (A_{Nee}) and Umklapp (A_{Uee}) components. Although the actual scattering of electrons by other electrons is predominantly normal, such scattering is so ineffective in contributing to $\rho(T)$ in an alkali metal that A_{Uee} is predicted to dominate A_{Nee} .

A_{ee} has been estimated for simple metals like alkali metals etc. mostly by the three groups. The initial pioneering work was done by Lawrence and Wilkins [11] who assumed that the only interaction between the electrons was the repulsive Coulomb interaction. They obtained values of A_{ee} for K and Na.

A decade later, MacDonald *et al* [12] recalculated A_{ee} using a more sophisticated procedure, a more realistic Fermi surface, and most importantly, a higher-order phonon-mediated interaction between electrons. This phonon-mediated interaction increases A_{Uee} , but leaves A_{Nee} nearly unchanged. Given the difficulty of these calculations and their sensitivity to both the detailed shape of the Fermi surface and phonon-mediated scattering, even these values are probably uncertain by a factor of 2.

Similar values to those of MacDonald *et al* were obtained soon afterward by Awasthi [13] and Awasthi and Sathish [14] using a much less sophisticated procedure. These workers did not separate the resistivity into normal and Umklapp contributions, but rather took the lattice periodicity into account by means of an overlap integral involving the Bloch wave functions of electrons with their momenta separated by reciprocal lattice vectors. Their values compare fairly well with the experimental results. The three calculations just described all assumed that the electron distribution function is isotropic at low temperatures because $\rho(o)$ is dominated by impurity scattering. All these calculations thus yielded $A_{Uee} \gg A_{Nee}$.

In the light of the above background, we decided to examine the e–e interactions in lithium, an alkali metal, for which MacDonald *et al* estimated A_{ee} values, which are only about 7% of the experimental estimates.

Our work has the following characteristics:

1. We have taken into consideration, for our calculations, the phase change in lithium at low temperatures when it undergoes martensitic transformation. In the martensitic phase the structure of lithium becomes 9R instead of bcc.
2. This phase change is the root cause of lithium for its abnormal behavior as compared to other alkali metals.
3. Ours is the first quantitative treatment of low-temperature electrical resistivity of lithium with 9R structure. The work of Wiser [24] for lithium, as explained later in this paper, is only the qualitative estimate of low-temperature electrical resistivity in lithium using 9R structure.

2. Theoretical formulation

2.1 *Electron–electron scattering*

As is well-known, in the isotropic limit, the normal e–e scattering does not contribute to the electrical resistivity because in such collisions, the charge and the momentum are conserved. Umklapp processes, however, impart momentum to the lattice as a whole and they can thus contribute to the electrical resistivity. The magnitude of this contribution is, however, greatly reduced due to the operation of the Pauli’s exclusion principle.

2.2 *The scattering potential*

Although the free electrons of a metal have electrostatic Coulomb fields by which they repel one another, the field at large distances is screened out by collective motions of the electron gas, and there only remains a residual short-range interaction. The potential to be used in e–e scattering, as given by Bohm and Pines [15,16], is of the ‘screened Coulomb’ type with a screening distance of a few atomic dimensions. The form of the potential is as follows:

$$V(\mathbf{r}) = (1/r) \exp(-k_c r) \quad (\text{atomic unit}), \quad (2)$$

where k_c is the screening parameter.

According to Pines [17], the value of k_c can be determined from the relation

$$\beta = k_c/k_F = 0.353r_s^{1/2} \quad (3)$$

where r_s is the radius of the Wigner–Seitz sphere and k_F is the Fermi wave vector.

The self-consistency of the method adopted by Pines to evaluate k_c depends on β being quite small. If we believe relation (3), we find that the screening length in a degenerate electron gas is given by the relation

$$1/k_c = 1.47r_s^{1/2} \quad (4)$$

in Bohr units. This is about the same as the atomic radius in a typical metal. The effect of correlation is to decouple the electrostatic interactions between an atom and the others in the lattice, except for the few ions and electrons in their immediate neighborhood.

2.3 *Scattering probability*

In view of the presence of a screened Coulomb potential, electrons are deflected by each other and hence, a scattering occurs. Due to the change in the motion of electrons, there is a change in the wave vectors of the electrons and hence, change in energies. The scattering can be understood as a transition of electrons into

new energy levels. The probability of scattering is equal to the probability of the corresponding energy changes of electrons when they change to new energy levels.

Consider an electron in state \mathbf{k}_1 which is scattered into the state \mathbf{k}_3 by collisions with another electron in the state \mathbf{k}_2 which is itself being scattered into state \mathbf{k}_4 . According to Pauli's exclusion principle, this scattering process can take place if the initial electronic states \mathbf{k}_1 and \mathbf{k}_2 are filled and the final states \mathbf{k}_3 and \mathbf{k}_4 are empty.

In collisions, both momentum as well as energy should be conserved.

If $f_{\mathbf{k}_1}$, $f_{\mathbf{k}_2}$, $f_{\mathbf{k}_3}$ and $f_{\mathbf{k}_4}$ are the Fermi functions of the electrons, the transition probability is given by the golden rule as

$$T(\mathbf{k}_1, \mathbf{k}_2 \rightarrow \mathbf{k}_3, \mathbf{k}_4) = 2\pi/\hbar |\langle \mathbf{k}_3, \mathbf{k}_4 | V(\mathbf{r}) | \mathbf{k}_1, \mathbf{k}_2 \rangle|^2 f_{\mathbf{k}_1} \cdot f_{\mathbf{k}_2} (1 - f_{\mathbf{k}_3})(1 - f_{\mathbf{k}_4}) \times \delta(\varepsilon_{\mathbf{k}_3} + \varepsilon_{\mathbf{k}_4} - \varepsilon_{\mathbf{k}_1} - \varepsilon_{\mathbf{k}_2}). \quad (5)$$

The δ function in eq. (5) takes care of the energy conservation.

2.4 Normal and Umklapp scattering

In a normal scattering, the momentum is conserved in the following way:

$$\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4. \quad (6)$$

In these collisions, the electrons do not lose momentum at all and hence, they cannot give rise to any contribution to electrical resistivity.

Now, let us introduce the effect of the lattice on the electrons. We know that the wave function for the electrons in the lattice is not plane waves but they are the Bloch functions defined as

$$\psi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{r}) u_{\mathbf{k}}(\mathbf{r}), \quad (7)$$

with $u_{\mathbf{k}}(\mathbf{r} + \mathbf{l}) = u_{\mathbf{k}}(\mathbf{r})$ and \mathbf{l} is the lattice vector.

Using Born approximation, the matrix elements of $V(\mathbf{r})$ between initial and final states can be written as

$$\begin{aligned} & \langle \mathbf{k}_3, \mathbf{k}_4 | V(\mathbf{r}) | \mathbf{k}_1, \mathbf{k}_2 \rangle \\ &= \int \int \Psi_{\mathbf{k}_3}^*(\mathbf{r}_1) \Psi_{\mathbf{k}_4}^*(\mathbf{r}_2) V(\mathbf{r}) \Psi_{\mathbf{k}_1}(\mathbf{r}_1) \Psi_{\mathbf{k}_2}(\mathbf{r}_2) d^3\mathbf{r}_1 d^3\mathbf{r}_2. \end{aligned} \quad (8)$$

Here, $\psi_{\mathbf{k}}$'s are the Bloch functions for the electrons in the lattice.

On introducing (7) for the Bloch functions into eq. (8) and simplifying it, we find that the matrix elements of $V(\mathbf{r})$ contain the square of an overlap integral G given by

$$G = 1/\Omega \int_{\text{Cell}} u_{\mathbf{k}_1}^*(\mathbf{r}) u_{\mathbf{k}_3}(\mathbf{r}) \exp(i\mathbf{g} \cdot \mathbf{r}) d^3\mathbf{r}, \quad (9)$$

where $\mathbf{g} = \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4$, \mathbf{g} is the reciprocal lattice vector and Ω is the atomic volume.

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The integral (9) is to be evaluated over a Wigner–Seitz cell. Proceeding in a similar manner as discussed by Ziman [18] and by Rösler [19], we obtain the following expression for $\rho_{ee}(T)$ due to e–e Umklapp scattering processes:

$$\rho_{ee}(T) = (\pi^3 z / 16) (e^2 / v_F^* E_F^{*3}) k_B^2 (G^2 / \beta^{*2}) T^2 = A_{ee} T^2 \quad (10)$$

(for $g \cong 2k_F$), where z is the coordination number of the reciprocal lattice, v_F^* is the Fermi velocity ($= \hbar k_F / m^*$), E_F^* is the Fermi energy, k_F is the Fermi wave vector and k_B is the Boltzmann constant. Further, * (asterisk) on the symbols denotes that the value is evaluated with the effective mass of the electron in lithium.

In deriving the electrical resistivity $\rho_{ee}(T)$ from eq. (10), certain assumptions were made.

Most important of them are: (a) Umklapp scattering is isotropic, and (b) the Fermi surface is spherical.

To test theoretical predictions with these assumptions in mind, one has to choose none other than simple metals like alkali metals and aluminium where their Fermi surfaces are believed to be nearly spherical in nature.

In the expression for A_{ee} (eq. (10)), all the values are known except G .

We now proceed to evaluate this important factor, which plays a crucial role in the e–e Umklapp scattering processes.

3. Evaluation of the overlap integral

In order to evaluate G for lithium, we need to have the knowledge of the wave functions of the electron in lithium, which we have taken from [20]. The wave functions for the simple metals are generally obtained by using the Wigner–Seitz’s method [21,22]. This way, we find the wave functions of an electron in the lowest state of the metal, i.e., for $\mathbf{k} = 0$. Denoting the wave functions in the ground state by $\psi_0(\mathbf{r})$, a fair approximation to the wave function for higher states will be (within any one atomic sphere), $\psi_{\mathbf{k}}(\mathbf{r}) \cong \exp(i\mathbf{k} \cdot \mathbf{r})\psi_0(\mathbf{r})$, provided that \mathbf{k} lies within the first Brillouin zone, but not too near the boundaries.

To evaluate the overlap integral G , eq. (9) is simplified. On normalization, G can be written as

$$G = \frac{1}{g} \frac{\int_0^{r_s} |\psi_0(\mathbf{r})|^2 r \sin(\mathbf{g}\mathbf{r}) d\mathbf{r}}{\int_0^{r_s} |\psi_0(\mathbf{r})|^2 \mathbf{r}^2 d\mathbf{r}}, \quad (11)$$

(for $g \cong 2k_F$), where r_s is the radius of the Wigner–Seitz’s sphere for the metal concerned. The value of G for lithium has been evaluated numerically using Simpson’s rule. The range of \mathbf{g} has been taken from 0 to 2 in the units of k_F , the Fermi wave vector. By varying \mathbf{g} we are varying the angle between the incident and the scattered electrons. Figure 1 shows the variation of G^2 with \mathbf{g} , i.e. the angle between the incident and scattered electrons.

It is clear that for $\mathbf{g} = 0$, $G^2 = 1$ and then value of G^2 falls off very rapidly as \mathbf{g} increases. The important value for G^2 is for $\mathbf{g} \cong 2k_F$, which has been obtained by us very carefully. This is the value of G^2 which enters in our evaluation of $\rho_{ee}(T)$ for lithium as given by eq. (10).

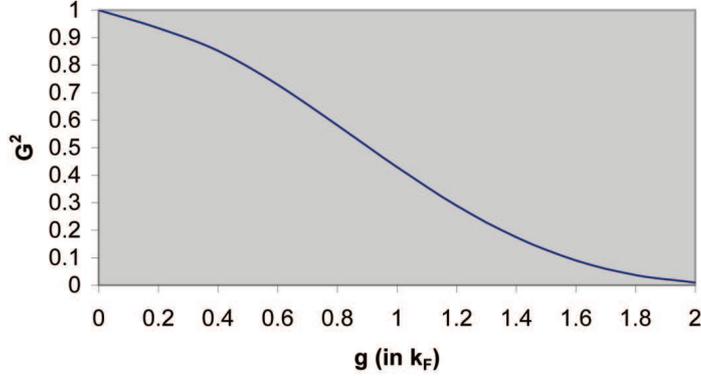


Figure 1. Variation of G^2 vs. g in lithium.

4. Results and discussion

Our value for A_{ee} for lithium calculated using the normal mass m of the electron is $0.04 \text{ p}\Omega \text{ cm K}^{-2}$. Obviously this value is almost 70 times less than the experimental value [23]. This clearly shows that lithium behaves very differently in its electrical properties at low temperature as compared to other alkali metals. This anomalous behavior in the electrical resistivity of lithium has been explained by Wisler [24] semi-quantitatively utilizing the findings of Overhauser [25] that at low-temperatures, lithium transforms into the 9R structure (which is also the structure for rare-earth metal Sm). This low-temperature structure of Li is very different from the bcc lattice that characterizes other alkali metals. Ashcroft [26] has shown that 9R structure resolves some longstanding anomalies in the optical properties of lithium. This structure can also explain the low-temperature electrical properties of Li.

The argument given to resolve quantitatively the enormous discrepancy in the values of A_{ee} between theory and experiment for Li in our work is based on the fact that the primitive rhombohedral unit cell of 9R structure contains three atoms. Therefore, monovalent Li has three electrons per unit cell (exactly as does aluminium, 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-wave function of a polyvalent metal. As a result, the pseudo-wave function of monovalent Li is similar to that of a non-transition polyvalent metal, rather than that of an alkali metal.

In order to insert the effect of the phase change of Li at low temperatures on the value of A_{ee} , we may do so by changing the values of the overlap integral G , E_F^* , v_F^* , β^* and z in eq. (10).

We find, through our calculations, using Bloch wave functions for lower \mathbf{k} values, that $G_{Li} \cong 0.10$, whereas $G_{Al} \cong 0.60$ [27]. Now using eq. (10) with G_{Al}^2 and other relevant values for the 9R structure of Li, we obtain $(A_{ee})_{Li} \simeq 3.20 \text{ p}\Omega \text{ cm K}^{-2}$, where we have used $m^*/m \cong 1.5$ for Li at low temperatures with 9R structure. For the sake of comparison the experimental values drawn from [4–6,23] are listed in

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Table 1. A_{ee} ($\text{p}\Omega \text{ cm K}^{-2}$) for lithium. Comparison between experiment and theory.

A_{ee}		
Experiment	Theory	
J Bass <i>et al</i> (1990)	MacDonald <i>et al</i> (1981)	Our proposed value [From eq. (10)]
2.8 ± 0.3	0.21	3.20

table 1. Theoretical estimates of A_{ee} for lithium as reported by MacDonald *et al* [12] have also been included in table 1 for comparison.

5. Conclusion

From table 1, it is obvious that our values of A_{ee} for lithium compare fairly well with the experimental data. The theoretical values reported by MacDonald *et al* [12] are only about 7% of the experimental data. It is concluded, therefore, that our approach renders fairly good results for $\rho_{ee}(T)$ in lithium, an alkali metal, at low temperatures.

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