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BRIEF REPORTS

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Effects of screening on the thermal resistivity of metals due to electron-electron scattering

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The thermal resistivity of metals due to electron-electron scattering is calculated by using the static-screening potential with the screening length determined by the compressibility which is derived from the Monte-Carlo values for the correlation energy. The result is compared with other theories and experiment. It is found that the resistivity depends quite sensitively on the screening length, with the theory based on the approximate correlation energy differing significantly from the present result. Compared with other more sophisticated theories, the present simple model is found to agree with experiment reasonably and competitively well, and much better than the result with the Fermi-Thomas screened-Coulomb potential. The inclusion of core polarization and band mass changes the thermal resistivity by up to 35% for sodium, potassium, rubidium, and cesium and by an order of magnitude for lithium. [S0163-1829(99)01915-3]

I. INTRODUCTION

Electron-electron correlations play an important role in the transport processes in metals.[1] Experimentally, one measures the transport coefficients and singles out the information about the electron-electron correlations among other effects. As for thermal resistivity, for example, both the electrons and phonons contribute as carriers of heat. Their heat transport may be impeded by electron-phonon, electron-impurity, and electron-electron scattering as well as phonon-phonon scattering. In this case, one measures the temperature dependence of the thermal resistivity and extracts the contribution from electron-electron scattering.[2–7] Such an analysis for different metals gives rise to valuable information about the interelectron potential, where many-body effects modify the bare Coulomb interaction significantly. Theoretically, many schemes have been proposed to take into account the many-body effects in calculating the thermal resistivity.[8–11] In the present paper we adopt the following model to study the effects of electron-electron scattering on the thermal resistivity of metals. We use the screened Coulomb interaction with the effective potential composed of the bare Coulomb potential divided by the dielectric function, where we use the static long-wavelength limit of the dielectric function. Then, the effective potential is characterized by the screening length, which is the only density-dependent parameter in the theory. It is sufficient to require that the static long-wavelength limit of the dielectric function satisfy the compressibility sum rule[12] in order to determine this screening length uniquely. The compressibility sum rule expresses the self-consistency condition that the static response of the system to the long-wavelength perturbation (the static long-wavelength limit of the dielectric function) be equal to the compressibility. Here, one may utilize the accurate density-dependent ground-state energy obtained via the Monte Carlo method[13,14] to calculate the compressibility via thermodynamic relations. The basic assumption in the present theoretical scheme is that the screening of the bare electron-electron interaction is appropriately described with the use of the static long-wavelength limit of the dielectric function. The advantage of the present one-parameter theory is its simplicity. This is also a natural extension of the previous theories with the screened Coulomb interaction, such as the Thomas-Fermi, Bohm-Pines,[15] and Hubbard[16] approximations. The construction of the effective potential to be consistent with the compressibility sum rule has been carried out previously by Kukkonen and Wilkins.[9] However, accurate data as an input for the compressibility were not available at that time: only the ground-state energy, calculated by use of certain approximations, was available. We shall see that the thermal resistivity depends on the compressibility (through the screening length) quite sensitively. Our model agrees reasonably well with experimental data for alkali metals. The inclusion of core polarization and band mass changes the result to some degree.

In Sec. II, we describe our model. In Sec. III, we present our results and compare them with the results of other theories and experiment.

II. THE MODEL

We assume the electron-electron interaction potential to be of the screened-Coulomb form[8]

$$V(r)=e^2(e^{-q_s r}/r). \tag{1}$$

Here, e is the electronic charge. In order to determine the screening wave number q_s, we regard Eq. (1) as a bare Coulomb potential which is screened by a static dielectric function in Fourier space,

$$V(q)=4\pi e^2/\epsilon(q,0)q^2 \tag{2}$$

with $\epsilon(q,0)=1+q_s^2/q^2$. We further assume that the static dielectric function is approximated by its long-wavelength limit. Then, the screening wave number q_s may be uniquely determined by the compressibility sum rule[12]

$$\lim_{q\to 0}\epsilon(q,0)=1+(q_{\mathrm{FT}}/q)^2(\kappa/\kappa_0), \tag{3}$$

where $q_{\mathrm{FT}}=(6\pi ne^2/E_F)^{1/2}$ is the Fermi-Thomas wave number, n the electron number density, and E_F the Fermi energy. The ratio κ/κ_0 is the compressibility normalized by its free Fermi gas value. The compressibility may be obtained from the density dependence of the ground-state energy through thermodynamic relations.

Kukkonen and Smith[8] used a screened Coulomb potential and calculated the scattering phase shifts numerically for $l=0$, 1, and 2 to obtain the scattering cross section. Then they used the exact solution of the Boltzmann equation[17,18] to derive the following interpolation formula for the thermal resistivity as a function of the dimensionless coupling constant r_s and the screening wave number:

$$W_{\mathrm{exact}}=1.10\times 10^{-8}(r_s^{5.04}/A^{3.06})T \ \ \mathrm{cm\ \ K/W} \tag{4}$$

with an estimated accuracy of 10% in the range $1.5<r_s<6$. Here r_s is defined by $r_s\equiv r_0/a_B$, where $r_0\equiv(3/4\pi n)^{1/3}$ is the mean particle distance, $a_B\equiv\hbar^2/me^2$ the Bohr radius, with n the electron number density, m the bare electron mass, and e the electronic charge. In addition, $A=q_s/r_s^{1/2}k_F$ with k_F the Fermi wave number. Since the present model adopts the same screened Coulomb potential, we shall use Eq. (4) in estimating the thermal resistivity.

Kukkonen and Wilkins[9] incorporated the compressibility sum rule into the interelectron potential in calculating the thermal resistivity. They obtained the compressibility from the ground-state energy which is calculated within various approximate theories.[16,19,20] Since thermal resistivity was found to be very sensitive to the screening length,[8,9] we instead use the accurate Monte Carlo data[13,14] for the ground-state energy in calculating the compressibility and the screening wave number. This has been done in Ref. 21. The screening wave number may be expressed in terms of the spin-parallel and spin-antiparallel screening wave numbers ($q_{\uparrow\uparrow}$ and $q_{\uparrow\downarrow}$) (Refs. 21 and 22) as

$$q_s=q_{\mathrm{FT}}/\{1+(1/2)[(q_{\mathrm{FT}}/q_{\uparrow\uparrow})^2+(q_{\mathrm{FT}}/q_{\uparrow\downarrow})^2]\}^{1/2}. \tag{5}$$

The simplest treatment of the lattice ions assumes that the electrons are immersed in a rigid, uniform, positively charged background. Such a system may be characterized by a dimensionless coupling constant r_s. In real solids, at least two effects modify the coupling constant r_s. First, the core electrons in the lattice ions form a polarizable medium. This will change the bare charge e^2 to the effective (or screened) charge e^2/ϵ_B, where ϵ_B is the dielectric constant of the background ions. Second, due to the interactions between the electrons and lattice ions (i.e., electron-phonon interaction) the electrons have an effective mass m_B rather than the bare mass m. Therefore, the electronic properties of real solids can be described in terms of an idealized electron system in an inert positive charge background with the mass and charge in the coupling constant replaced by m_B and e^2/ϵ_B so as to give an effective dimensionless coupling constant $r_s^*\equiv(m_B/m)r_s/\epsilon_B$.[9,10]

III. THE RESULTS AND DISCUSSION

The thermal resistivity calculated within the present model together with the results of other calculations and the experimental data are shown in Fig. 1. Note that the plot of our results in Fig. 1 (the fifth solid line from the top at cesium density) includes neither ionic polarizability nor band mass.

While the present model gives a thermal resistivity which is smaller than the experimental data for potassium, rubidium, and cesium, the agreement is satisfactory for copper, gold, and sodium. The Geldart-Taylor model[9,19] agrees with the experimental data for sodium and cesium, but give larger values for other metals. Two other models treated by Kukkonen and Wilkins[9]—the interpolation and the Hubbard approximation[16]—agree with the experimental data for sodium, but give larger values for other metals.

The inclusion of the effects of ionic core polarizability and band mass are found to modify the results to some degree. Such effects are shown in Table I. For sodium, these effects are small. For potassium, rubidium, and cesium, these effects change the thermal resistivity by about 35% in either direction. For lithium, on the other hand, these effects are marked, increasing the thermal resistivity by an order of magnitude, a tendency very similar to what MacDonald and Geldart[10] found. Namely, the thermal resistivity of lithium calculated within our scheme lies above those predicted by three other theories listed in Ref. 9.

The present model is a direct extension of the theory of Kukkonen and Smith,[8] where the electron-electron interaction was characterized by a single parameter, the screening length. The importance of satisfying the compressibility sum rule was stressed by Kukkonen and Wilkins.[9] They started with the relation between the electron-electron interaction and the proper vertex function. The latter is related to the ratio of the interacting and noninteracting proper polarizations in the long-wavelength limit, and this ratio was esti-

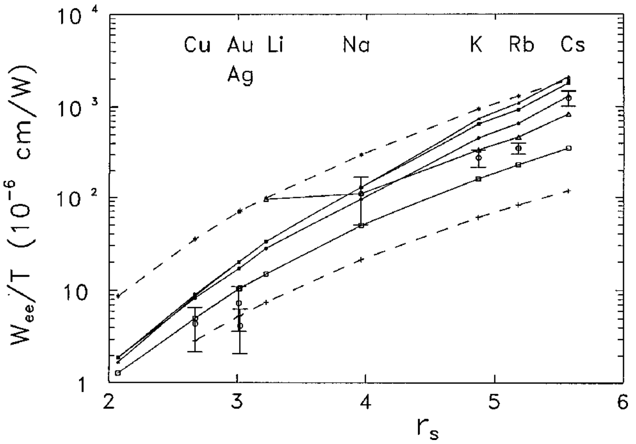

FIG. 1. Thermal resistivity due to electron-electron scattering as a function of density. The open circles with error bars are experimental values obtained by Laubitz for copper, gold, and silver (Ref. 2); by Cook *et al.* for sodium (Ref. 3); and by Cook for rubidium (Ref. 4), potassium (Ref. 5), and cesium (Ref. 6). The connected dashed or solid lines show theoretical values. The use of the Bohm-Pines (Ref. 15) and Thomas-Fermi screening lengths give the top and bottom dashed lines, respectively (Ref. 8). These dashed lines take into account neither the ionic polarizability (i.e., $\epsilon_B = 1$) nor the band mass (i.e., $m_B/m = 1$). The solid lines are, from top to bottom at the cesium density, the results of the interpolation by Kukkonen and Wilkins (Ref. 9), Hubbard approximation (Refs. 9 and 16), the theories of Geldart-Taylor (Refs. 9 and 19), and MacDonald-Geldart (Ref. 10), and the present calculation, respectively. The top three solid lines (at cesium density) due to Kukkonen and Wilkins (Ref. 9) include the ionic polarizability for Li, Na, K, Rb, and Cs, but do not include the band mass (i.e., $m_B/m = 1$). The MacDonald-Geldart results (Ref. 10) include the ionic polarizability (i.e., $\epsilon_B \neq 1$), the band mass (i.e., $m_B/m \neq 1$) as well as band correction, and the deviation from Matthiessen's rule. The calculated values at several metallic densities are connected by dashed or solid lines in order to guide the eye only. Individual metals have different core polarizabilities, so that the density dependence of the resistivity is not necessarily monotonic or smooth.

mated by the use of the compressibility sum rule. They obtained the compressibility from the ground-state energy which was calculated within various approximate theories.[16,19,20] In contrast, the present model incorporates the compressibility sum rule through the use of the accurate Monte Carlo data for the ground-state energy.[13,14]

Let us compare the present calculation with the model based on ''the interpolation formula'' [Eq. (29) in Ref. 9] by Kukkonen and Wilkins. By setting $m_B/m = 1$ for cesium, one obtains $r_s^* \rightarrow r_s/\epsilon_B = 4.46$, which is close to $r_s/\epsilon_B = 4.43$ in Ref. 9. At this density, one finds that their value for W_{ee}/T, 2100 in units of 10^{-6} cm/W, is much larger than ours, 95.6. (See the last entry in Table I.) The difference seems to reflect the sensitivity with which the thermal resistivity depends on the screening length.

MacDonald and Geldart[10] started with the transition probabilities expressed in terms of the four-point scattering function. The latter may be expressed in terms of the Landau Fermi-liquid parameters in the forward scattering limit. The Dy-Pethick approximation determines the ϕ dependence of the forward scattering function uniquely, where ϕ is the angle between the relative momentum of the initial state and that of the final state.[12] MacDonald and Geldart[10] compared their theory with that of Kukkonen and Wilkins.[9] As noted by MacDonald and Geldart,[10] this was by no means straightforward.

Most recently, Lundmark[11] used the Landau Fermi-liquid theory to examine the static and dynamic versions of five theories (i.e., ten theories total) and calculated W_{ee}/T for sodium and potassium. Among them, it is found that the static versions of the four theories (Hedin's *GW* approximation, RPA, SSTL, and Hubbard-corrected LDA) give values

TABLE I. The effects of ionic core polarization and band mass on the thermal resistivity. Here $\epsilon_B = 1 + 4\pi n_i \alpha_d$ is the dielectric constant of the background ions, where n_i and α_d are the number density and the polarizability of ions, respectively. The values for the ionic polarizability and band mass m_B are taken from Refs. 23 and 24, respectively, and $r_s^* = (m_b/m) r_s/\epsilon_B$. The quantities q_s^* (given in atomic units with a_B the Bohr radius), A^*, and W_{exact}^*/T are obtained with r_s replaced by r_s^* in Eqs. (4) and (5), etc. The last entry is for cesium with $m_B/m = 1$.

	r_s	α_d (10^{-24} cm^3)	ϵ_B	m_B/m	r_s^*	q_s^* (a_B^{-1})	A^*	W_{exact}^*/T (10^{-6} cm/W)
Li	3.22	0.02807	1.01634	1.54	4.88	0.512	0.589	163.6
Na	3.96	0.1401	1.04478	1.04	3.94	0.600	0.620	47.7
K	4.87	0.8086	1.1349	1.08	4.63	0.534	0.599	119.9
Rb	5.18	1.345	1.18125	1.10	4.82	0.517	0.591	152.7
Cs	5.57	2.343	1.24948	1.30	5.80	0.562	0.562	449.5
Cs	5.57	2.343	1.24948	1.00	4.46	0.550	0.605	95.6

in the range 65 (SSTL) – 73 (RPA) for sodium and 231 (Hedin) – 327 (Hubbard) for potassium all in units of 10^{-6} cm/W. Most of these theoretical values are within the error bars of the experimental data for each of these two alkali metals as listed in Fig. 1. On the other hand, it is also found that most of the dynamic versions of these theories as well as the static version of the LDA overestimate W_{ee}/T for potassium by a factor of 3 (SSTL) – 110 (LDA).

In comparison with these more sophisticated theories, the present model, in spite of its simplicity as a one-parameter theory, agrees competitively well with experiment.

In summary, let us emphasize the following points.

(i) The present theory is based on a simple model. The screening length is the only parameter in the theory.

(ii) The dielectric function, from which the screening length is derived, satisfies the compressibility sum rule *exactly*. The compressibility itself is determined from the density dependence of the ground-state energy, which is calculated by the Monte Carlo method with high precision.

Let us finally remark on the following issues which have not been considered in the present paper.

(i) Effects of the wave-number dependence of the static dielectric function: We have used the static dielectric function in the long-wavelength limit to derive the screening length. While this approximation simplifies the form of the effective potential greatly, the effects of the contribution from the finite wave-number region (finite momentum transfers) should be examined.

(ii) Dynamic effects: Similarly, the effects of the finite frequency may be examined. This corresponds to a finite energy transfer in scattering. Since two-particle scattering occurs in a degenerate fermion system, the typical energy transfer is of order k_BT due to the Pauli principle, where T is the temperature of the system. Therefore, $\hbar\omega \sim k_BT \ll E_F$, where E_F is the Fermi energy. Thus, the static approximation is justified.

(iii) Other ''solid state'' effects: Finally our model does not include effects arising from the fact that ions are mobile rather than an idealized rigid, uniform, positively charged background.

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