Comments and Addenda

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Spin-orbit coupling and electrical conduction in liquid metals

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The effect of spin-orbit coupling on the electrical resistivity ρ_R of liquid metals is studied and the appropriate extension of the Ziman formula for ρ_R is derived using the diagonality in spin index of some blocks of the square of the pseudopotential matrix. Application is made to liquid Cd.

In a recent paper,[1] which will be referred to as I, the use of nonlocal pseudopotentials in the calculation of the electrical resistivity ρ_R of liquid metals was studied and the nonlocal potential of Stark and Falicov[2] was used to compute ρ_R for liquid Cd. In I, it was assumed that the spin-orbit (SO) terms contained in the Stark-Falicov[2] pseudopotential could be ignored in calculating ρ_R. The validity of this assumption has now been examined in detail and a quantitative estimate of the effect of the SO interaction on ρ_R obtained.

The pseudopotential W (including the SO interaction) acting on an electron in the liquid metal can be written[2,3]

$$\begin{aligned}\langle \vec{k}s \,|\, W \,|\, \vec{k}'s' \rangle &= \frac{1}{N}\sum_{\nu} e^{i(\vec{k}-\vec{k}')\cdot\vec{R}_\nu}\{[\omega_L(|\vec{k}-\vec{k}'|) + \langle \vec{k}|\, \omega_{NL}\,|\vec{k}'\rangle]\delta_{ss'} \\ &\quad + i\omega_{SO}(\vec{k},\vec{k}')\vec{k}'\times\vec{k}\cdot\vec{\sigma}_{ss'}\} \\ &\equiv W_{\vec{k}s\vec{k}'s'}\,, \end{aligned} \tag{1}$$

where s, s' are components of the electron spin, $\vec{\sigma}$ are the Pauli matrices, $\vec{R}_\nu$ are the positions of the liquid-metal atoms, and, as in Ref. 2, I shall adopt for ω_{SO} the form

$$\omega_{SO} = \lambda_p + \lambda_d(\vec{k}\cdot\vec{k}')\,. \tag{2}$$

The remaining symbols of (1) are as defined in I.

In calculating the resistivity ρ_R, the SO term in (1) will be treated on the same footing as the other parts of the pseudopotential W.

The SO interaction causes transitions between two electronic bands (the spin-up and spin-down bands), whereas the method of Berger *et al.*[4] on which I is based was set up for a one-band system. The extension to the present two-band system is readily obtainable because of some special properties of W as shown below.

As in I, it is useful here to evaluate the Laplace transform $J^z(0^+)$ of the electric current j^z defined by

$$J^z(u) = \int_0^\infty dt\, e^{-ut} e^{iHt/\hbar} j^z e^{-iHt/\hbar}\,, \tag{3}$$

where H is now the pseudo-Hamiltonian

$$\langle \vec{k}s \,|\, H \,|\, \vec{k}'s' \rangle = \frac{\hbar^2 k^2}{2m}\delta_{\vec{k}\vec{k}'}\delta_{ss'} + W_{\vec{k}s\vec{k}'s'}\,. \tag{4}$$

If we set

$$\langle \vec{k}s \,|\, J^z(u) \,|\, \vec{k}'s' \rangle = J^z_{\vec{k}ss'}(u)\delta_{\vec{k}\vec{k}'} + J^z_{\vec{k}s\vec{k}'s'}(u)(1-\delta_{\vec{k}\vec{k}'})\,, \tag{5}$$

the equation of motion for $J^z(u)$ takes the form

$$uJ^z_{\vec{k}ss'}(u) = j^z_{\vec{k}s}\delta_{ss'} + \frac{i}{\hbar}\sum_{\vec{k}''s''}[W_{\vec{k}s\vec{k}''s''}J^z_{\vec{k}''s''\vec{k}s'}(u) - J^z_{\vec{k}s\vec{k}''s''}(u)W_{\vec{k}''s''\vec{k}s'}]\,, \tag{6}$$

$$\begin{aligned}(\hbar u - iE_{\vec{k}} + iE_{\vec{k}'})J^z_{\vec{k}s\vec{k}'s'}(u) &= (1-\delta_{\vec{k}\vec{k}'})i\Big(\sum_{s''}[W_{\vec{k}s\vec{k}'s''}J^z_{\vec{k}'s''s'}(u) - J^z_{\vec{k}'ss''}(u)W_{\vec{k}s''\vec{k}'s'}] \\ &\quad + \sum_{s''\vec{k}''}[W_{\vec{k}s\vec{k}''s''}J^z_{\vec{k}''s''\vec{k}'s'}(u) - J^z_{\vec{k}s\vec{k}''s''}(u)W_{\vec{k}''s''\vec{k}'s'}]\Big)\,, \end{aligned} \tag{7}$$

where

$$E_{\vec{k}} = \frac{h^2k^2}{2m} + \langle \vec{k}s \,|\, W \,|\, \vec{k}s \rangle \tag{8a}$$

as in I and

$$j^z_{\vec{k}s} = \langle \vec{k}s \,|\, j^z \,|\, \vec{k}s \rangle . \tag{8b}$$

Equations (6) and (7) are the two-band analogs of (2.12) and (2.13) of Ref. 4. Following Berger *et al.*,[4] (7) can be solved iteratively for $J^z_{\vec{k}s\vec{k}'s'}(u)$ in terms of $J^z_{\vec{k}ss'}(u)$ and the result substituted into (6), obtaining simultaneous integral equations for the quantities $J^z_{\vec{k}ss'}(u)$. Carrying out this procedure to leading order in W (proceeding naively to higher order in W would yield inconsistent results[1,5]) one finds

$$uJ^z_{\vec{k}ss'}(u) = j^z_{\vec{k}s}\delta_{ss'} - \frac{1}{\hbar}\sum_{\substack{\vec{k}''\\ s'''}} \left(\frac{W_{\vec{k}s\vec{k}''s''} W_{\vec{k}''s''\vec{k}s'''} J^z_{\vec{k}s'''s'}(u) - W_{\vec{k}s\vec{k}''s''} W_{\vec{k}''s'''\vec{k}s'} J^z_{\vec{k}''s'''s''}(u)}{\hbar u - iE_{\vec{k}''} + iE_{\vec{k}}} \right.$$
$$\left. - \frac{W_{\vec{k}s\vec{k}''s'''} W_{\vec{k}''s''\vec{k}s'} J^z_{\vec{k}''s'''s''}(u) - W_{\vec{k}s'''\vec{k}''s''} W_{\vec{k}''s''\vec{k}s'} J^z_{\vec{k}ss'''}(u)}{\hbar u - iE_{\vec{k}} + iE_{\vec{k}''}} \right). \tag{9}$$

Taking the limit $u \to 0^+$ and making the usual assumption that $\omega_L(|\vec{k} - \vec{k}'|)$ and $\langle \vec{k} | \omega_{NL} | \vec{k}' \rangle$ are real and symmetric in $\vec{k}$ and $\vec{k}'$, one finds that the equations (9) have a solution such that

$$J^z_{\vec{k}ss}(0^+) = J^z_{\vec{k}-s-s}(0^+) \tag{10}$$

and

$$J^z_{\vec{k}s-s}(0^+) = 0 . \tag{11}$$

The vanishing, in the leading approximation (9), of matrix elements $J^z_{\vec{k}s-s}(0^+)$ which are nondiagonal in the spin index s is a consequence of the fact that for real, symmetric ω_L and ω_{NL},

$$\sum_{s''} \langle \vec{k}s \,|\, W \,|\, \vec{k}''s'' \rangle \langle \vec{k}''s'' \,|\, W \,|\, \vec{k}s' \rangle = 0 \quad \text{if } s \neq s', \tag{12}$$

even though $\langle \vec{k}s \,|\, W \,|\, \vec{k}''s'' \rangle$ and $\langle \vec{k}''s'' \,|\, W \,|\, \vec{k}s' \rangle$ may be nonvanishing.

The result (11) can also be understood in terms of the absence of "interference terms" in van Hove's $\lambda^2 t$ limit[6] for systems possessing the diagonal singularity property.

It is now straightforward to solve the Boltzmann equation to which (9) reduces for $J^z_{\vec{k}ss}(0^+)$ and to evaluate ρ_R to leading order in the scattering by the procedure given in I. One finds that the SO interaction contributes a new term

$$\rho_{SO} = \frac{3\pi\Omega_0}{2j^2_{k_F}\hbar} \int_{-1}^{1} dx(1-x)(\lambda_p + \lambda_d k_F^2 x)^2 k_F^4 \times (1-x^2) I(\sqrt{2}\, k_F (1-x)^{1/2}) \tag{13}$$

to the resistivity, where Ω_0, j_{k_F} and the interference function I are as defined in Ref. 1.

The expression (13) can also be obtained quite simply from a conventional Boltzmann equation. That approach was adopted by Animalu[7] in his calculations using model pseudopotentials. However, the conventional Boltzmann equation arguments rely on the use of the "repeated random-phase assumption" whose validity is uncertain. The argument given above depends instead on the property (12) of the spin-orbit interaction.

In the case of Cd, inserting the Stark-Falicov[2] parameters λ_p, λ_d into (13) and using the same values for the remaining variables as in I, ρ_{SO} is positive and equal to 0.7% of the experimental value 34 $\mu\Omega$ cm of the resistivity. This is a smaller effect than the effective-mass correction to the Ziman formula discussed in I, and probably also smaller than the uncertainty introduced into the resistivity calculation by the interpolation procedure[1,8] used to obtain $\omega_L(q)$ over the range $0 \leq q \leq 2k_F$. The contribution ρ_{SO} to the resistivity is expected to be more important for metals heavier than Cd.

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