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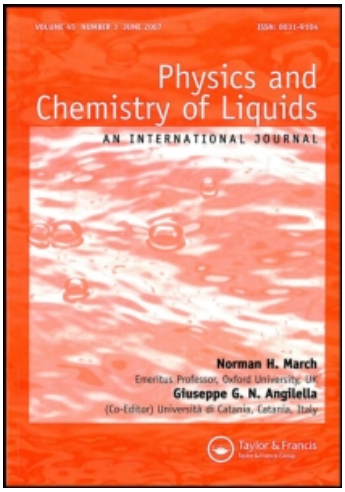

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LETTER
Electron Correlation and the Hall Effect in Liquid Metals

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A formula is proposed for the deviation ΔR_H of the Hall coefficient R_H from 1/nec. Knowledge of the first-order density matrix characterizes the formula. With strong electron correlation, ΔR_H will depend on the discontinuity of the electron momentum distribution at the Fermi surface, as well as on the strength of the electron-ion interaction in the liquid metal.

KEY WORDS: Density matrix, conductivity, thermopower.

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In a recent study, Chapman and March[1] have proposed a formula for the electrical resistivity R of liquid metals in the presence of strong electron-electron interactions. Their result is written in terms of the first-order density matrix describing the electronic structure, by generalizing the independent-electron formula of Rousseau, Stoddart and March[2].

The purpose of the present Letter is to treat the Hall effect. The argument below parallels that of the writer[3] for R, in which the starting point was Huang's formula[4] for impurity resistivity due to scattering from a finite-range spherical potential energy $V(r)$. This is expressed in terms of the phase shifts δ_l of the partial waves. In the present work, use will be made of the single-centre scattering formula for the Hall coefficient R_H given by Szabo[5] in terms of the same phase shifts. This has the form (Szabo's Eq. (11))

$$R_H = \frac{1}{nec}\left(1 + \frac{2}{3\pi n\Omega_0}\frac{\partial}{\partial\mu}\left\{\mu \sum_{l=0}^{\infty} 2(l+1)\sin^2(\delta_{l+1} - \delta_l)\right\}\right) \tag{1}$$

with n the electron density, Ω_0 the atomic volume and μ the chemical potential. The sum appearing in Eq. (1) is simply related to that used by the writer in Ref. 3, namely

$$S = \sum_{l=1}^{\infty} l \sin^2(\delta_{l-1} - \delta_l) \tag{2}$$

which in turn was written in terms of the radial wave functions R_l generated by $V(r)$. This was achieved using the result of Gerjuoy[6], rediscovered by Gaspari and Gyorffy[7], that

$$\int_0^{\infty} r^2 R_{l-1}(r)\frac{\partial V}{\partial r} R_l(r)\, dr = \sin(\delta_{l-1} - \delta_l). \tag{3}$$

Finally, introducing the Dirac idempotent first-order density matrix

$$\rho(\mathbf{r}_1\mathbf{r}_2\mu) = \sum_i^{\mu} \psi_i^*(\mathbf{r}_1)\psi_i(\mathbf{r}_2) \tag{4}$$

where the ψ's are merely products of R_l and the spherical harmonics, one can show that S in Eq. (2) is simply related to the force-force correlation function $F(\mu)$, which in terms of V and ρ is given by

$$F(\mu) = \int \frac{\partial V}{\partial \mathbf{r}_1} \cdot \frac{\partial V}{\partial \mathbf{r}_2} \left| \frac{\partial \rho(\mathbf{r}_1\mathbf{r}_2\mu)}{\partial \mu} \right|^2 d\mathbf{r}_1\, d\mathbf{r}_2. \tag{5}$$

The burden of the remaining argument is to eliminate the one-body elements in Eq. (5) in favour of the density matrix which has a ready many-electron generalization. This is done by Chapman and March[1] by utilizing the equation of motion of the Dirac density matrix ρ, which in coordinate representation reads

$$\nabla_{\mathbf{r}_1}^2 \rho - \nabla_{\mathbf{r}_2}^2 \rho = \frac{2m}{\hbar^2} [V(\mathbf{r}_1) - V(\mathbf{r}_2)]\rho. \tag{6}$$

Dividing both sides by ρ and writing the difference in Laplacian operators as $\Delta L \equiv \nabla_{\mathbf{r}_1}^2 - \nabla_{\mathbf{r}_2}^2$ we find, with $\hbar^2/2m$ conveniently incorporated in the definition of L:

$$\mathrm{grad}_1 V(\mathbf{r}_1) = \mathrm{grad}_1 \left(\frac{\Delta L \rho}{\rho} \right) \tag{7}$$

Hence Eq. (5) becomes

$$F(\mu) = -\int \mathrm{grad}_1 \left(\frac{\Delta L \rho}{\rho} \right) \cdot \mathrm{grad}_2 \left(\frac{\Delta L \rho}{\rho} \right) \left| \frac{\partial \rho(\mathbf{r}_1\mathbf{r}_2\mu)}{\partial \mu} \right|^2 d\mathbf{r}_1\, d\mathbf{r}_2 \tag{8}$$

as in Ref. 1. The final postulate in the present work is that one can replace the one-body idempotent density matrix ρ in Eq. (8) by the many-electron first-order density matrix γ satisfying now the matrix inequality $\gamma^2 < \gamma$ to obtain F_{e-e} in the presence of electron-electron interactions as

$$F_{e-e}(\mu) = -\int \mathrm{grad}_1 \left(\frac{\Delta L \gamma}{\gamma} \right) \cdot \mathrm{grad}_2 \left(\frac{\Delta L \gamma}{\gamma} \right) \left| \frac{\partial \gamma(\mathbf{r}_1\mathbf{r}_2\mu)}{\partial \mu} \right|^2 d\mathbf{r}_1\, d\mathbf{r}_2. \tag{9}$$

Since the sum in Eq. (1) is proportional to $F(\mu)$, it is now clear that the deviation ΔR_H of the Hall coefficient from 1/nec is characterized by the first-order density matrix γ.

In summary, a formula for ΔR_H has been proposed for liquid metals with strong electron-electron interactions; e.g. the expanded alkali metals discussed in Refs. 1 and 8, in terms of the first-order density matrix. Given this formula, the following consequences arise:

(i) Insertion of any translationally invariant $\gamma = \gamma(|\mathbf{r}_1 - \mathbf{r}_2|)$ whatsoever leads, as in Ref. 1, to $F_{e-e}(\mu) = 0$ and to the simple result $R_H = 1/nec$.

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(ii) Assuming, as in Ref. 1 for R, that $\gamma(\mathbf{r}_1\mathbf{r}_2) \doteq f(\mathbf{r}_1 - \mathbf{r}_2)g(\mathbf{r}_1 + \mathbf{r}_2)$, one must expect ΔR_H to depend on the discontinuity, q say, of the electronic momentum distribution of the liquid metal at the Fermi surface; see especially Ref. 8.

(iii) Though further work is clearly required on the many-electron derivation of the formula for ΔR_H proposed in this Letter, this formula does motivate the suggestion that, even in the presence of strong electron-electron interactions, ΔR_H may be closely correlated with measured conductivity and thermopower. However quantitative numerical studies are required on this last point and it is intended to report further on this aspect of the problem later.

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