Weak Localization in Two and Three Dimensions: Dephasing by Zero-Point Motion

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(Received 6 July 1987)

A mechanism leading to a temperature-independent dephasing time, τ_ϕ, in the weakly localized regime is discussed. It is shown that the time-reversed complementary scattering paths which lead to weak localization experience a relative phase shift due to the zero-point motion of the ions in the material. By use of a simple model it is shown that this mechanism can explain the saturation of τ_ϕ which is seen at low temperatures in a wide variety of systems.

PACS numbers: 71.55.Jv, 72.10.−d, 72.15.Cz, 73.50.Bk

The theory of weak localization has been extremely successful in explaining many features of low-temperature electron transport in highly disordered conductors, especially the magnetoconductivity of thin metallic films and bulk amorphous metals.[1,2] The effects of weak localization result from the interference between two complementary electron waves, which can be modeled semiclassically as Boltzmannian trajectories traversing a given multiple-scattering path in opposite directions.[3] One of the key parameters entering the theory is the time over which the electron wave amplitudes along the two trajectories maintain relative phase coherence. Generally this dephasing time, τ_ϕ, is determined by inelastic-scattering processes which, in changing the electron's energy, eventually cause a sufficient accumulation of relative phase shift between the two trajectories to destroy the coherence. Indeed most authors show a temperature dependence of τ_ϕ between 4 and 20 K which varies as T^{-2}, characteristic of inelastic electron-phonon scattering,[1] or as T^{-1}, characteristic of electron-electron scattering.[4] However, below 4 K it is observed in a wide variety of disordered conductors that τ_ϕ saturates, to a value between 10^{-9} and 10^{-12} s, depending on the system. The saturation has been generally ascribed to scattering by residual magnetic impurities[4] or to decoupling of the electron gas from the thermal bath.[5] However, these explanations cannot cover all cases,[2,6] and furthermore ignore not only the generality of the effect but also some of its systematics, viz., that the saturation value generally increases with the mobility of the carriers.[4,5,7]

In the present Letter we offer a more general explanation of the phenomenon: dephasing of the two complementary wave amplitudes through the zero-point motion of the ions. A simple model calculation of the effect gives results in general agreement with what is observed.

Figure 1 shows two complementary Boltzmannian trajectories whose interference contributes to weak localization. Traditionally the scatterers are assumed (at low temperatures) to be fixed in space. In reality, however, they vibrate because of zero-point motion. Since the two trajectories visit a given ion at different times, they will find it at different and random positions (provided that $1/\tau_\phi$ is less than the Debye frequency). Thus a random relative phase shift accumulates between the two trajectories, providing an additional, temperature-independent, dephasing mechanism. It should be stressed that the effect does not involve inelastic scattering.

To estimate the size of the effect we use a simple Debye model for the vibration of the ions. In the ground state, zero-point motion leads to a mean square displacement, $\langle \delta R^2 \rangle$, of each ion given by

$$\langle \delta R^2 \rangle = 3\hbar/2M\omega_D, \tag{1}$$

M being the mass of the ion and ω_D the Debye frequency. For a scattering event, i, which leads to a momentum transfer $\mathbf{q}_i$, there is a phase shift due to zero-point motion of $\Delta\phi_i = \mathbf{q}_i \cdot \delta\mathbf{R}_i$. Over the dephasing time τ_ϕ, the number of scattering events is τ_ϕ/τ_e, where τ_e is the elastic-scattering time. Since the phases $\Delta\phi_i$ are random, the total mean square accumulated phase difference between the two trajectories is

$$\langle \Delta\phi^2 \rangle = (\tau_\phi/\tau_e) 8 k_F^2 \langle \delta R^2 \rangle \langle \sin^2\theta/2 \rangle, \tag{2}$$

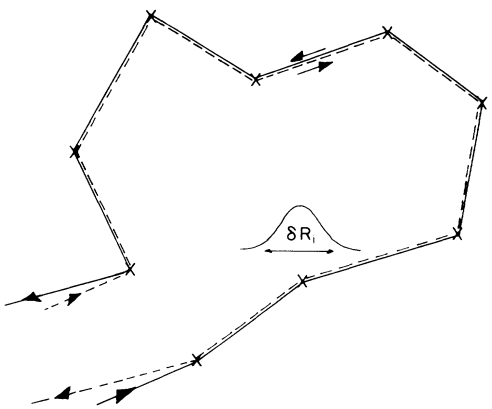

FIG. 1. Coherent backscattering from a pair of time-reversed complementary paths, shown as Boltzmannian trajectories. Each scatterer is assumed to be executing zero-point motion leading to positional dispersion as indicated at a typical site in the figure.

where $\langle \delta R^2 \rangle$ is the mean square zero-point displacement of the ions at each scattering event, and where $\langle \sin^2\theta/2 \rangle$ is taken over the scattering angle θ, as shown in Fig. 2. The saturation value for τ_ϕ as a result of zero-point motion (which we will denote by τ_ϕ^0) is now given by the condition that $\langle \Delta\phi^2 \rangle \approx 1$.[8,9]

We now evaluate τ_ϕ^0 in two extreme limits. In the first we assume each scatterer to be strong, such as may be expected in amorphous transition metals. In this case each scattering event becomes localized at one site and $\langle \delta R^2 \rangle$ is simply given by Eq. (1). In the second case we assume a high density of very weak scatterers, such as should be appropriate for an amorphous s,p metal like Mg-Zn. In this case scattering is spread over a large number of scatterers, and therefore δR_i must be replaced by a coarse-grain average displacement over a volume of linear dimension ξ, where ξ is approximately the lesser of the phonon coherence length and the distance traveled by the electron in the Debye time, $(D/\omega_D)^{1/2}$. If we replace, for simplicity, the Debye spectrum by a δ function at ω_D, this averaging reduces δR by the factor $f(\lambda)$ where

$$f(\lambda) = \frac{3}{4\pi\xi^3} \int_{r<\xi} e^{i\boldsymbol{\lambda}\cdot\mathbf{r}} d^3r, \tag{3}$$

with $\lambda = \pi/a$, a being the interatomic spacing. With this factor included, we find the following simple expression for τ_ϕ^0:

$$\tau_\phi^0 \approx \frac{M}{m}\frac{\theta_D}{T_F}\frac{D}{D_0}\frac{\hbar}{E_F}\left(\frac{\xi}{a}\right)^4, \tag{4}$$

where D is the electron diffusivity, m is the electron mass, $D_0 = \hbar/m$, θ_D is the Debye temperature, T_F is the Fermi temperature, and E_F is the Fermi energy. The strong-scattering form of Eq. (4) may be approximated by our letting $\xi/a \to 1$.

Equation (4) leads to the following general conclusions. If we take, for a typical metal, $M/m \approx 10^5$, $\theta_D/T_F \approx 3\times10^{-3}$, and $E_F \approx 8$ eV, then the value of τ_ϕ^0 in the strong-scattering limit is about 0.02 ps, whereas in the weak-scattering limit this value could be as high as 15 ns. For specific examples Eq. (4) gives $\tau_\phi^0 = 22$ ps for $Y_{60}Al_{40}$, whereas the experimental value is 26 ps,[2] and $\tau_\phi^0 = 3$ ns for $Mg_{70}Zn_{30}$, whereas experiment finds 1.5 ns.[10] In view of the crudeness of the approximations we used in reaching Eq. (4) such agreement must be considered fortuitous. Nonetheless it does indicate that the model is giving the right order of magnitude. Furthermore, it has a simple prediction: If one takes a system where the scattering may be progressively altered from weak to strong, then one should observe a drastic reduction in the saturation value for τ_ϕ^0. Such a system is $Ca_{70}(Mg,Al)_{30}$, which we are currently investigating.

Alternatively the effect of changing the scattering may be seen in the behavior of thin Cu films,[7] where there is again clear evidence for the saturation of τ_ϕ. In addition to the relatively weak scattering in the bulk, there is strong, large-scale scattering by the surface. We accommodate the latter by noting that there are approximately v_F/t surface scattering events per unit time (t being the thickness of the film). These give an additional mean square relative phase shift (in time τ_ϕ^0) of $(\tau_\phi^0 v_F/t) \times (2k_F\delta R)^2$, where the scattering angle has been set equal to π. Thus for the film

$$\frac{1}{\tau_\phi^0} \approx \left(\frac{1}{\tau_\phi^0}\right)_{\text{bulk}} + 12\frac{v_F}{t}\frac{T_F}{\theta_D}\frac{m}{M}, \tag{5}$$

where the first term on the right-hand side comes from Eq. (4). We thus find that $1/\tau_\phi^0$ should vary as $1/t$, and this is consistent with what is seen experimentally (Fig. 3).

We conclude that zero-point motion of the ions gives rise to a temperature-dependent dephasing time in weak localization. A simple estimate leads to values which are

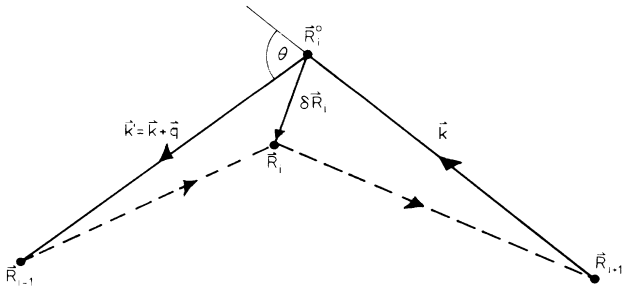

FIG. 2. Path length difference due to motion of one of the scatterers in Fig. 1.

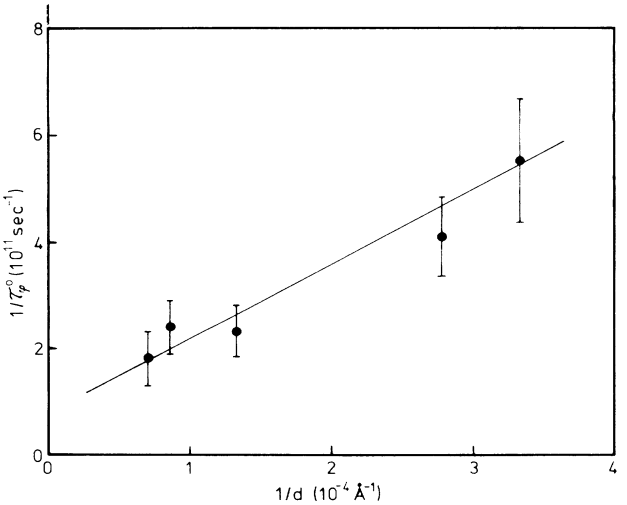

FIG. 3. Dependence of τ_ϕ^0 on the thickness of thin Cu films. Data are taken from Fig. 2 of Ref. 7. The solid line is a guide to the eye.

in agreement with values of τ_ϕ^0 found experimentally at low temperatures.

This work was supported by the Natural Sciences and Engineering Research Council of Canada under Grants No. A8439 and No. IS-0331.

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[1]G. Bergmann, Phys. Rep. **107**, 1 (1984).

[2]M. Olivier, J. O. Strom-Olsen, Z. Altounian, R. W. Cochrane, and M. Trudeau, Phys. Rev. B **33**, 2799 (1986).

[3]S. Chakravarty and A. Schmid, Phys. Rep. **140**, 184 (1986).

[4]J. J. Lin and N. Giordano, Phys. Rev. B **35**, 1071 (1987).

[5]D. J. Bishop, R. C. Dynes, and D. C. Tsui, Phys. Rev. B **26**, 773 (1982).

[6]R. P. Peters, G. Bergmann, and R. M. Mueller, Phys. Rev. Lett. **58**, 1964 (1987).

[7]D. Abraham and R. Rosenbaum, Phys. Rev. B **27**, 1413 (1983).

[8]B. L. Altshuler and A. G. Aronov, in *Electron-Electron Interaction in Disordered Systems,* edited by A. L. Efros and M. Pollak (North-Holland, Amsterdam, 1985).

[9]Equation (2) may be obtained rigorously within the framework of the quasiclassical theory of electrons in a random potential (Ref. 3), starting with the Lagrangean for the electron

$$L = \tfrac{1}{2} m(d\mathbf{r}/dt)^2 + V_R(\mathbf{r} - \mathbf{u}(\mathbf{r},t)),$$

where V_R is the random potential, $\mathbf{r}$ the electron coordinate, and $\mathbf{u}$ the lattice displacement field. The transformation $\mathbf{r} \rightarrow \mathbf{r} + \mathbf{u}$ gives a term $(d\mathbf{r}/dt)\cdot(d\mathbf{u}/dt)$ (which was neglected in Ref. 3), which leads directly to the phase shift of Eq. (2). Although the quasiclassical approach has been justified for weak localization in Ref. 3, a full quantum-mechanical calculation would be more satisfactory. We are currently working on such an approach.

[10]R. Richter, David V. Baxter, and J. O. Strom-Olsen, unpublished. Similar values for τ_ϕ^0 at low temperatures have been seen in thick quench-condensed films of amorphous Mg by J. Kästner and R. Mölleken, in *Proceedings of the International Conference on Localization, Interaction and Transport Phenomena in Impure Metals,* edited by L. Schweitzer and B. Kramer (Physikalisch-Technische Bundesanstalt, Braunschweig, Federal Republic of Germany, 1984), Suppl. PTB-PG-1.