RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 34, NUMBER 2 15 JULY 1986

Destruction of phase coherence by electron-phonon interactions in disordered conductors

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(Received 24 March 1986)

We present a novel formalism for calculating the destruction of phase coherence in weak localization and apply it to the case of electron-phonon interactions. The calculation demonstrates that in the present case quasielastic collisions are negligible, leading to the result that the phase-breaking rate due to electron-phonon interactions is identical to the inelastic collision rate.

There are moderately disordered conductors where localization of the electronic wave function has only a weak though measurable influence on conductivity. This weak-localization effect can be understood in terms of quantum-mechanical interference within a quasiclassical theory,[1-3] as follows. The set of classical electronic paths which return to the starting point in a given time t_0 includes pairs of paths which differ only in that they are traversed in the opposite direction of time and so interfere constructively in case of time-reversal invariance. In correspondence to this enhanced localization, there is a decrease in conductivity which can be calculated according to[2]

$$\Delta\sigma = -\frac{2e^2}{\pi\hbar} D \int_\tau dt_0 \tilde{W}_{t_0} \ , \tag{1}$$

where D is the diffusion constant and τ the elastic collision time, and where $\tilde{W}_{t_0}$ is the interference term between pairs of paths, as referred to above.

In case of time-reversal invariance, $\tilde{W}_{t_0}$ is equal to the classical probability W_{t_0} that an electron at the Fermi level returns to its starting point in time t_0. If this invariance is broken, a phase difference between pairs of time-reversed paths appears, and the constructive interference is partially destroyed. This destruction of phase coherence leads to an extra factor $[\exp(-t_0/\tau_\varphi)]$ in the expression for $\tilde{W}_{t_0}$, where $1/\tau_\varphi$ may be called the phase-breaking rate. The purpose of this Rapid Communication is to present a calculation of the phase-breaking rate due to electron-phonon interactions using the simple interference picture outlined above.

We start from the one-electron Lagrangian which is given by

$$L = \tfrac{1}{2} m\mathbf{v}^2 - e\phi - V_{\rm imp} \ , \tag{2}$$

where $V_{\rm imp}$ is the impurity potential. Furthermore, the deformation potential

$$e\phi = \frac{n}{2N_0} \nabla\cdot\mathbf{u} \ , \tag{3}$$

where $\mathbf{u}=\mathbf{u}(\mathbf{r},t)$ denotes the lattice displacement field, and where (we assume one electron per ion) n and N_0 are the electronic density and density of states per spin, respectively.

It is important to note that the impurities move in phase with the distorted lattice; hence, the impurity potential has the form $V_{\rm imp}(\mathbf{r}) = \sum_i v(\mathbf{r}-(\mathbf{R}_i^0+\mathbf{u}))$ where $\mathbf{R}_i^0$ denotes the equilibrium position of the ith impurity. Consequently, the impurity scattering is only elastic in the reference frame that locally moves along with the lattice. Therefore, we shift to this moving reference frame by changing the electronic coordinate according to $\mathbf{r}\rightarrow\mathbf{r}+\mathbf{u}$ and the impurity scattering then becomes static.[4]

Neglecting terms of relative order m/M (m the electronic mass, M the ionic mass), the transformed Lagrangian may be written as $L = L_0 + L_1$, where

$$\begin{aligned} L_0 &= \frac{m}{2}\mathbf{v}^2 - V_{\rm imp} \ , \\ L_1 &= m\mathbf{v}\cdot(\mathbf{v}\cdot\nabla)\mathbf{u} - \tfrac{1}{3} m\mathbf{v}^2 \nabla\cdot\mathbf{u} \ . \end{aligned} \tag{4}$$

Note that in the last line we have expressed $e\phi$ according to (3) and that we have used the relation $n/2N_0 = mv_F^2/3$.

The quantity of interest is the phase difference between pairs of time-reversed paths. According to Feynman, each path carries a phase factor $\exp(iS[\mathbf{r}_t]/\hbar)$, where

$$S[\mathbf{r}_t] = \int_{-t_0/2}^{t_0/2} dt\, L(\mathbf{r}_t, \dot{\mathbf{r}}_t, t) \tag{5}$$

is the action. In the expression above we have for convenience chosen the path to start at time $-t_0/2$ and end at $t_0/2$. Therefore, this phase difference is equal to $\varphi[r_t] = \{S[\mathbf{r}_t] - S[\mathbf{r}_{-t}]\}/\hbar$. Note that a substantial cancelation occurs in this phase difference since L_0 is an even function of the velocity and independent of time. Hence, it is a small quantity given by[2]

$$\varphi[\mathbf{r}_t] = \frac{1}{\hbar}\int_{-t_0/2}^{t_0/2} [L_1(\mathbf{r}_t, \dot{\mathbf{r}}_t, t) - L_1(\mathbf{r}_t, -\dot{\mathbf{r}}_t, -t)] \ , \tag{6}$$

where, in the last term, we have replaced the integration variable t by $-t$. *We recognize that L_1, though small, plays an important role here since it breaks the time reversal symmetry.* Considering the specific form L_1 as given by (4), we obtain the phase difference

$$\varphi[\mathbf{r}_t] = \frac{m}{\hbar}\int_{-t_0/2}^{t_0/2} dt [\nabla^\beta u^\alpha(\mathbf{r}_t,t) - \nabla^\beta u^\alpha(\mathbf{r}_t,-t)] \times [\dot{r}_t^\alpha \dot{r}_t^\beta - \tfrac{1}{3}\delta_{\alpha\beta}\dot{\mathbf{r}}_t^2] \ , \tag{7}$$

where summation over repeated Cartesian indices is implied.

In case of random impurity positions, there will be many classical paths that return to the starting point. Therefore, we introduce the probability $w_{t_0}[\mathbf{r}_t]$ that an electron at the Fermi level returns in time t_0 to its starting point for any realization of the impurity positions. Then

$$\tilde{W}_{t_0}=\sum_{\{\mathbf{r}_t\}} w_{t_0}[\mathbf{r}_t]\exp(i\varphi[\mathbf{r}_t]) \ , \tag{8}$$

where the summation includes all possible paths. Evidently, W_{t_0} is obtained from Eq. (8) by putting $\varphi=0$.

It is necessary to average $\tilde{W}_{t_0}$ as given in Eq. (8) with respect to the lattice vibrations. Since the Lagrangian of the lattice vibrations is a quadratic form and $\varphi[\mathbf{r}_t]$ is a linear form in $\mathbf{u}(\mathbf{r},t)$, the phonon average can be computed according to

$$\langle\exp(i\varphi[\mathbf{r}_t])\rangle_{\rm ph}=\exp\{-\tfrac{1}{2}\langle(\varphi[\mathbf{r}_t])^2\rangle_{\rm ph}\} \ .$$

Concerning the summation with respect to the classical paths, we will resort to an approximation which can be expressed as follows:

$$\tilde{W}_{t_0}=W_{t_0}\exp\left[-\frac{1}{2W_{t_0}}\sum_{\{\mathbf{r}_t\}} w_{t_0}[\mathbf{r}_t]\langle(\varphi[\mathbf{r}_t])^2\rangle_{\rm ph}\right] \ . \tag{9}$$

Since the exponential is a convex function, the approximation (9) is of the form of an inequality where the right side is less than or equal to the left side.

It can be shown[2] that for most problems of weak localization, adequate expressions for the probabilities above are obtained by considering the classical paths as realizations of Brownian motion. Presently, however, the phase difference (7) depends very sensitively on the velocity, which is a meaningless quantity in Brownian motion. This makes it necessary for us to consider paths which are realizations of Boltzmannian motion. By this we mean motion along straight lines which happen to be terminated by random scattering events.

At a given time, a Boltzmannian path is completely specified by its position and by its velocity (of which only the direction of $\mathbf{v}$ is important since the scattering is elastic). Since we are dealing with a Markovian process, a basic quantity is the conditional probability[5] $F(\mathbf{r},\mathbf{v},t;\mathbf{r}',\mathbf{v}',t')\,d^3r\,d\Omega_{\mathbf{v}}$ that there are paths having final position $\mathbf{r}$ and velocity $\mathbf{v}$ in the indicated range for given initial conditions. In case of isotropic scattering, this quantity obeys the inhomogeneous Boltzmann equation

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{r}}+\frac{1}{\tau}\right)F-\frac{1}{\tau}\int\frac{d\Omega_{\mathbf{v}}}{4\pi}F =\delta(t-t')\delta(\mathbf{r}-\mathbf{r}')\tilde{\delta}(\mathbf{v}-\mathbf{v}') \ , \tag{10}$$

where $\tilde{\delta}$ is a spherical δ function. The Fourier transform of the solution of (10) is given by[5]

$$F(\mathbf{v},\mathbf{v}';\mathbf{k},\omega)=\frac{1}{-i\omega+i\mathbf{v}\cdot\mathbf{k}+1/\tau} \times\left(\frac{1/\tau}{-i\omega+i\mathbf{v}'\cdot\mathbf{k}+1/\tau}L(k,\omega)+\tilde{\delta}(\mathbf{v}-\mathbf{v}')\right) \ . \tag{11}$$

In the expressions above, $|\mathbf{v}|=|\mathbf{v}'|=v_F$ is the Fermi velocity and

$$L(k,\omega)=\{1-(kl)^{-1}\arctan[kl(1-i\omega\tau)^{-1}]\}^{-1} \ ,$$

where $l=v_F\tau$ is the mean free path. In the region kl, $\omega\tau\lesssim 1$ we have $L(k,\omega)=\tau^{-1}(-i\omega+Dk^2)^{-1}$, where $D=\frac{1}{3}v_F l$ is the diffusion constant. In the following, we will also make use of the notion that an angular average of F with respect to one of its velocities is indicated by a bar. For instance, we have $W_{t_0}=\bar{F}(\mathbf{r}=0,t_0;\mathbf{r}'=0,0)$, and one finds from Eq. (11) that $W_{t_0}=(4\pi Dt_0)^{-3/2}$ for $t_0>>\tau$.

Concerning the argument of the exponential in (9), we note that

$$\tfrac{1}{2}\langle(\varphi[\mathbf{r}_t])^2\rangle_{\rm ph}=\frac{m^2}{\hbar^2}\int_{-t_0/2}^{t_0/2}dt\,dt'\left[\sum_{\pm}\pm D^{\alpha\beta\gamma\delta}(\mathbf{r}_t-\mathbf{r}_{t'},t\mp t')\right] \times[v_t^{\alpha}v_t^{\beta}-\tfrac{1}{3}\delta_{\alpha\beta}\mathbf{v}_t^2][v_{t'}^{\gamma}v_{t'}^{\delta}-\tfrac{1}{3}\delta_{\gamma\delta}\mathbf{v}_{t'}^2] \ , \tag{12}$$

where the phonon correlator

$$D^{\alpha\beta\gamma\delta}(\mathbf{r},t)=\langle\nabla^{\beta}u^{\alpha}(\mathbf{r},t)\nabla^{\delta}u^{\gamma}(0,0)\rangle_{\rm ph}$$

is an even function of t. On account of the Markovian property, the four-point correlation function (two end points and two intermediate points) required in (9)—see also (12)—may be expressed as a product of three conditional probabilities of the type (11). Furthermore, it will be convenient to chose a definite sequence of times, say $-t_0/2<t'<t<t_0/2$, which can be done by supplying an extra factor of 2. Since we expect that only thermally excited phonons contribute, we conclude that $D^{\alpha\beta\gamma\delta}(\mathbf{r},t\pm t')$ is essentially zero for $|t\pm t'|\geq\hbar/k_BT$. This allows us to extend to infintiy the domain of the integration with respect to $t\pm t'$ provided that $t_0>>\hbar/k_BT$. If this is the case, we obtain

$$\tilde{W}_{t_0}=W_{t_0}\exp\left[-\frac{2m^2}{\hbar^2W_{t_0}}\int\frac{d^3k\,d^3k'\,d\omega\,d\omega'}{(2\pi)^8}\int\frac{d\Omega_{\mathbf{v}_1}d\Omega_{\mathbf{v}_2}}{(4\pi)^2}\bar{F}(\mathbf{v}_1;\mathbf{k},\omega)F(\mathbf{v}_1,\mathbf{v}_2;\mathbf{k}+\mathbf{k}',\omega+\omega')\right.$$
$$\left.\times[\bar{F}(\mathbf{v}_2;\mathbf{k},\omega)e^{-i\omega t_0}-\bar{F}(\mathbf{v}_2;\mathbf{k},\omega+2\omega')e^{-i(\omega+\omega')t_0}]\,D^{\alpha\beta\gamma\delta}(-\mathbf{k}',-\omega')[v_1^{\alpha}v_1^{\beta}-\tfrac{1}{3}\delta_{\alpha\beta}v_1^2][v_2^{\gamma}v_2^{\delta}-\tfrac{1}{3}\delta_{\gamma\delta}v_2^2]\right] \ . \tag{13}$$

We expect that the argument of the exponential above increases linearly in t_0 for $t_0\to\infty$. Since $W_{t_0}^{-1}\propto t_0^{3/2}$, this means that the integral above should not decrease faster than $t_0^{-1/2}$. Such a slow decrease is obtained from the $(\mathbf{k},\omega)$ integration

only from the combination $\bar{F}(\mathbf{v}_1;\mathbf{k},\omega)\bar{F}(\mathbf{v}_2;\mathbf{k},\omega)$ which features a singular behavior $\simeq(-i\omega+Dk^2)^{-2}$ for small $(\mathbf{k},\omega)$. In fact, it is easy to see that it is just this combination which leads to a time dependence proportional to $t_0^{-1/2}$. Compared to that, all other contributions may be neglected. Therefore, we are allowed to approximate $F(\mathbf{v}_1,\mathbf{v}_2;\mathbf{k}+\mathbf{k}',\omega+\omega')$ by $F(\mathbf{v}_1,\mathbf{v}_2;\mathbf{k}',\omega')$. In addition, the second term in the square bracket may be omitted, as we show in a moment. Thus, $\tilde{W}_{t_0}=W_{t_0}\exp(-t_0/\tau_\varphi)$, where

$$\frac{1}{\tau_\varphi}=\frac{2m^2}{\hbar^2}\int\frac{d^3k'\,d\omega'}{(2\pi)^4}\int\frac{d\Omega_{\mathbf{v}_1}d\Omega_{\mathbf{v}_2}}{(4\pi)^2}F(\mathbf{v}_1,\mathbf{v}_2;\mathbf{k}',\omega')\times D^{\alpha\beta\gamma\delta}(\mathbf{k}',\omega')(v_1^\alpha v_1^\beta-\tfrac{1}{3}\delta_{\alpha\beta}\mathbf{v}_1^2)\times(v_2^\gamma v_2^\delta-\tfrac{1}{3}\delta_{\gamma\delta}\mathbf{v}_2^2)\ . \tag{14}$$

In order to proceed further, we have to specify details of the lattice vibrations. For simplicity, we take an isotropic model without dispersion which is specified by the density n and the mass M of the ions, and by the longitudinal c_L and the transverse c_T sound velocities. In case of longitudinal vibrations, the representation in normal modes is of the form

$$\mathbf{u}(\mathbf{r},t)=iN^{-1/2}\sum_{\mathbf{k}}\hat{\mathbf{k}}Q_{\mathbf{k}}(t)\exp(i\mathbf{k}\cdot\mathbf{r})\ ,$$

where $\hat{\mathbf{k}}=\mathbf{k}/k$ and N is the number of ions in the normalization volume. Observe now that

$$\langle Q_{\mathbf{k}}(t)Q_{\mathbf{k}'}(t')\rangle_{\rm ph}=\delta_{\mathbf{k},-\mathbf{k}'}(\hbar/M\omega_k)H(\omega_k)\cos[\omega_k(t-t')]\ ,$$

where $\omega_k=c_Lk$. Thus, we obtain for the Fourier transform of the phonon correlator

$$D_L^{\alpha\beta\gamma\delta}(\mathbf{k},\omega)=\frac{\pi\hbar k^2}{nM\omega_k}\hat{k}^\alpha\hat{k}^\beta\hat{k}^\gamma\hat{k}^\delta H(\omega_k)\times[\delta(\omega-\omega_k)+\delta(\omega+\omega_k)]\ . \tag{15}$$

Strictly speaking, we have $H(\omega)=N(\omega)+\frac{1}{2}$, where N is the Bose distribution function. However, the present single-electron theory does not take into account the Pauli principle which forbids scattering of electrons into occupied states. General considerations lead to the conclusion that the Pauli principle can be incorporated by the replacement $H(\omega)=N(\omega)+f(\hbar\omega)=1/\sinh(\hbar\omega/k_BT)$, where f is the Fermi function.

Upon inserting (15) into the expression (14) for $1/\tau_\varphi$, we encounter directional averages involving expressions of the type

$$\hat{k}^\alpha\hat{k}^\beta(v^\alpha v^\beta-\delta_{\alpha\beta}\mathbf{v}^2/3)=k^{-2}[(\mathbf{k}\cdot\mathbf{v})^2-(\mathbf{k}^2)(\mathbf{v}^2)/3]\ .$$

Altogether, these averages appear in the combination

$$\phi_L(kl)=\frac{18}{\pi v_F^3k^3}\left\{L(k)\left[\int\frac{d\Omega_{\mathbf{v}}}{4\pi}\frac{(\mathbf{k}\cdot\mathbf{v})^2-(\mathbf{k}^2)(\mathbf{v}^2)/3}{-i\omega+i\mathbf{v}\cdot\mathbf{k}+1/\tau}\right]^2+\int\frac{d\Omega_{\mathbf{v}}}{4\pi}\frac{[(\mathbf{k}\cdot\mathbf{v})^2-(\mathbf{k}^2)(\mathbf{v}^2)/3]^2}{-i\omega+i\mathbf{v}\cdot\mathbf{k}+1/\tau}\right\}=\frac{2}{\pi}\left[\frac{kl\arctan(kl)}{kl-\arctan(kl)}-\frac{3}{kl}\right]\ , \tag{16}$$

where the result in the last line is obtained since $\omega=c_Lk\ll v_Fk$. Using this result, we obtain the phase-breaking rate due to longitudinal phonons

$$\frac{1}{\tau_{\varphi L}}=\frac{\pi\hbar^2}{6mMc_L}\int_0 dk\,k^2\phi_L(kl)\frac{1}{\sinh(\hbar c_Lk/k_BT)}\ . \tag{17}$$

In limiting cases, this rate is equal to

$$(7\pi\zeta(3)/12)(k_BT)^3/(\hbar mMc_L^4)$$

for

$$\hbar c_Lk_D\gg k_BT\gg\hbar c_L/l$$

and

$$(\pi^4/30)l(k_BT)^4/(\hbar^2mMc_L^5)$$

for $k_BT\ll\hbar c_L/l$. We note that the result (17) for the phase-breaking rate is identical to the inelastic electron-phonon collision rate.[6,7]

The expression (16) for ϕ_L demonstrates in a direct way the important compensation that takes place in the case of longitudinal phonons between the two mechanisms contained in L_1. First, the term $(\mathbf{k}\cdot\mathbf{v})^2$ corresponds to $m\mathbf{v}\cdot(\mathbf{v}\cdot\nabla)\mathbf{u}$ and represents the coupling of the electrons to the vibrating impurities. Second, the term $-\frac{1}{3}(\mathbf{k}^2)(\mathbf{v}^2)$ is connected with $-\frac{1}{3}m\mathbf{v}^2\nabla\cdot\mathbf{u}$ and originates from the interaction of the electrons with the lattice vibrations. Without this compensation, each of these mechanisms would appear to be enhanced in an impure metal and would lead to an enhanced phase-breaking rate proportional to $(k_BT)^2/(mMc_L^3l)$. It may be worthwhile to mention that there exist several papers where such enhanced rates have been proposed. Such statements, however, are merely an indication of an incomplete analysis of the problem.

The physical meaning of the second term in the square bracket of Eq. (13) is as follows. It is appreciable only if the lattice deformation stays approximately constant during the time the electron spends on its path and leads, in this case, to a cancellation of the first term. This effect can be incorporated quantitatively in the present threory if we introduce a lower cut-off $k_0=1/c_L\tau_\varphi$ in the integral of Eq. (17). This is of importance in the case of electron-electron interactions.[8] In the present case, however, there are no realistic models of phonon spectra where this effect is of importance.

In case of transverse vibrations, we should note that $D_T^{\alpha\beta\gamma\delta}$ is of similar form (15) where, however, $\hat{k}^\alpha\hat{k}^\gamma$ has to be replaced by $(\delta_{\alpha\gamma}-\hat{k}^\alpha\hat{k}^\gamma)$ with an additional factor of 2 which accounts for the multiplicity. Eventually, we obtain a phase-breaking rate $1/\tau_{\varphi T}$ which is similar to Eq. (17) with c_L and ϕ_L replaced by c_T and

$$\phi_T(kl)=3\pi^{-1}(kl)^{-4}[2(kl)^3+3kl-3(k^2l^2+1)\arctan(kl)],$$

respectively. In limiting cases, this rate is equal to $(\pi^2/2)(k_BT)^2/(mMc_T^3l)$ for $\hbar c_Tk_D\gg k_BT\gg\hbar c_T/l$ and $(\pi^4/20)l(k_BT)^4/(\hbar^2mMc_T^5)$ for $k_BT\ll\hbar c_T/l$. Again, we have the expected identity with the inelastic collision rate.[6,7] Note that in the high-temperature region, the transverse contribution is negligible in comparison with the longitudinal one if $c_T\sim c_L$. On the other hand, the transverse rate dominates in the case where the transverse sound velocity is much smaller than the longitudinal one. Such a situation may quite well be realized in some amorphous metals;[9] then, it is possible to observe $1/\tau_\varphi\propto T^2/l$ at intermediate temperatures.[10]

In conclusion, we have developed a formalism that allows a transparent calculation of the phase-breaking rate in the case of electron-phonon interactions. This is of importance in view of the present disagreement[10] between theory and experiment and the formalism will therefore be a valuable tool in further theoretical investigations on phase-breaking rates.

This work has been initiated during a stay of one of the authors (A.S.) at the Ørsted Institute and at NORDITA. Therefore, he wishes to express his gratitude for their hospitality. Both authors have benefited from valuable and stimulating discussions with W. Eiler, P. E. Lindelof, and H. Smith. Financial support from the Deutsche Forschungsgemeinschaft is also acknowledged.

[1]D. E. Khmelnitskii, Physica B **126**, 235 (1984); Yu. V. Sharvin, *ibid.* **126**, 288 (1984).

[2]S. Chakravarty and A. Schmid, Phys. Rep. (to be published).

[3]For a general review, see also G. Bergmann, Phys. Rep. **107**, 1 (1984).

[4]A. B. Pippard, Philos. Mag. **46**, 1106 (1955).

[5]A. Schmid, Z. Phys. **243**, 346 (1971).

[6]A. Schmid, Z. Phys. **259**, 421 (1973); B. Keck and A. Schmid, J. Low Temp. Phys. **24**, 611 (1976).

[7]A. Schmid, in *Localization, Interaction and Transport Phenomena,* edited by B. Kramer, G. Bergmann, and Y. Bruynseraede, Springer Series in Solid-State Sciences, Vol. 61 (Springer-Verlag, New York, 1985).

[8]B. L. Altshuler, A. G. Aronov, and D. E. Khmelnitskii, J. Phys. C **15**, 7367 (1982); W. Eiler, J. Low Temp. Phys. **56**, 481 (1984). The lower cutoff can also be understood in terms of the uncertainty principle which implies that the electronic energy is a meaningful quantity only on a scale of order $\hbar/\tau_\varphi$.

[9]W. Dietsche, H. Kinder, J. Mattes, and H. Wühl, Phys. Rev. Lett. **45**, 1332 (1980).

[10]See also the discussion in Sec. 6 of Ref. 3.