The effect of particle identity on a new type of weak localization

E V Orlenko and V V Rumyantsev

Department of Theoretical Physics, Technical University of St Petersburg 195251, Russia

Abstract. In this paper, weak localization of a new kind is studied. Within the framework of the new developing theory, electron exchange is shown to alter the angular distribution of scattered electrons. The range of energies of incident electrons for which exchange effects are important is estimated.

1. Introduction

Weak localization of elastically scattered particles and waves has been the subject of many investigations. There are two ways to investigate the phenomenon of weak localization. Firstly, one can study the conductivity of a disordered system. Secondly, we can measure the current of particles or intensity of light back-scattered from a disordered medium that occupies semispace. The second approach is preferable when we want to deal with the monokinetic beams of particles or with light of a fixed frequency. The existence of weak localization is confirmed in experiments on negative anomalous magnetoresistance and the propagation of light in disordered media.

In back-scattering experiments, the usual weak localization is manifested principally as an increase in the elastic backward scattering. There is experimental evidence of the enhanced back-scattering of light. In the case of electrons, the range of solid angles where back-scattering is enhanced is extremely narrow. This range is of the order λ/l, where λ and l are the wavelength and mean free path of electrons, respectively. This is the reason why experimental observations of enhanced electron back-scattering have not been performed yet. Let us mention that the theory of the lineshape of the angular dependence for electrons scattered from a disordered medium and undergoing localization of the regular kind was developed in [1].

Inelasticity is generally thought to destroy weak localization, which is true for the usual weak localization. However, even in the presence of inelasticity, the coherence survives and produces a new outstanding phenomenon [2]. In this different type of weak localization, electrons scatter from disordered media with a fixed energy loss mainly through angles close to $\pi/2$. In weak localization of the new type, the prevailing scattering angles are of the order $\gamma/\omega = (\lambda/l)(E/\hbar\omega)$, where γ is the electron collision frequency, E is the electron energy $\hbar\omega$ is the energy loss. These statements are equally valid for small numbers of elastic scattering events as for multiple elastic scattering [3].

When electrons undergo the new type of weak localization, they suffer single or multiple elastic scattering and single inelastic scattering, the inelastic scattering being involved in an essential way in the interference process. The energy loss of the electrons in the reflection

beam is due to the same inelastic scattering. There are many sources of inelastic scattering, which provide a clear distinguishable energy loss. Among these are plasmons and various electron transitions in atoms.

Weak localization of the new type could be observed in the reflection of monoenergetic electrons with a fixed energy loss from disordered media. A much wider range of angles than in ordinary localization makes the experimental observation of the new localization much more realistic.

For the usual weak localization, there are many factors which can influence the process; among them are the particle identity effect and spin–orbit interaction. Their role in the new localization has not been studied before, and in this work we shall consider the former factor.

Although the effect of electron interchange could be expected to be weak, we shall show that it has an important part to play, even if the energy of the electrons capable of energy loss is much larger than the energy of electrons bound in the centres of elastic scattering. Owing to this, the Born approximation can work well.

In both electron weak localization of the regular kind and the new type of weak localization, the interference of the electrons is associated with crossed diagrams. For the usual weak localization, there is the only simplest crossed diagram (figure 1) with two crossed broken lines which join an upper line (the retarded-system Green function) and a lower line (the advanced-system Green function). The broken line represents a force-centre correlator. This diagram corresponds to two scattering events and it describes the usual weak localization in its simplest form. Including the maximally crossed diagrams one can describe the usual weak localization in detail.
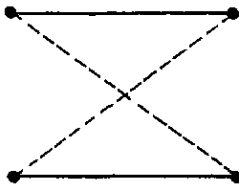

Figure 1. Simplest crossed diagram in the elastic scattering of electrons by atoms.

In the usual weak localization, both crossed lines which connect the upper and lower Green function lines are of the same nature. In the new type of localization, these lines correspond to two different interactions. One (broken) line describes the elastic scattering while the other (wavy) line represents inelastic scattering (figure 2(*b*)). Now we have the two simplest diagrams (figures 2(*b*) and 2(*c*)). There is no need to add more complicated crossed diagrams because they do not change the angular distribution of scattered electrons in an infinite medium [3]. The simultaneous effect of surface and electron exchange on the properties of the new localization will be the subject of a separate study.

The crossed diagrams depicted in figures 2(*b*) and 2(*c*) contribute to the scattering probability factor

$$\sum_q |u(Q-q)|^2 w_i(q,\omega) 2\,\mathrm{Re}\left(\frac{1}{E_p - E_{p-q} - \omega - \mathrm{i}\gamma}\frac{1}{E_p - E_{p-Q+q} + \mathrm{i}\gamma}\right).$$

Here p and E_p are the momentum and energy, respectively, of the incident electron, Q is the total momentum transfer to the medium, q is the momentum transfer to the electrons of
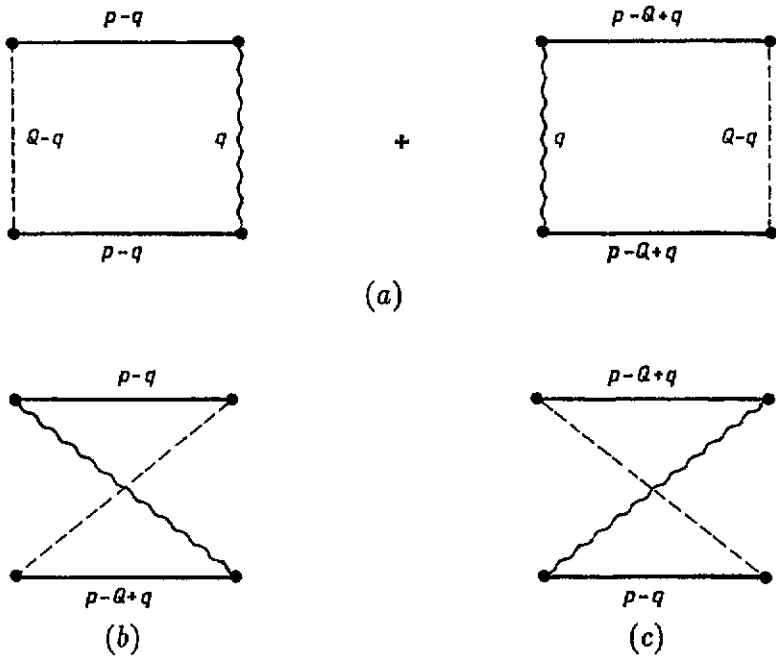
Figure 2. (a) Ladder and (b), (c) crossed diagrams in the elastic scattering of electrons by atoms and inelastic scattering with the excitation of atoms, plasmons or other excitations in solids. The broken lines link one and the same centre of elastic scattering. A wavy line corresponds to a plasmon or other excitation.

the medium, w_i is the probability per unit time of emission of a plasmon with momentum q and energy ω or excitation of an atomic transition. w_i corresponds to the wavy lines in the diagrams. The broken lines linking the upper and lower solid lines in all diagrams give rise to the appearance of the factor $|u(Q-q)|^2$ which corresponds to elastic scattering. Usually one has $Q \gg q$ (even for multiple scattering [3]), and one can omit the momentum q in this expression. Two Green functions $(E_p - E_{p-q} - \omega - i\gamma)^{-1}$ and $(E_p - E_{p-Q+q} + i\gamma)^{-1}$ correspond to the two solid lines in figures 2(b) and 2(c). Summation is carried out over all final states.

Together with the diagrams in figures 2(b) and 2(c) we should take into account the diagrams depicted in figure 2(a). The sum of these diagrams yields

$$|u(Q)|^2 \sum_q w_i(q,\omega)\{[(E_p - E_{p-q} - \omega^2)^2 + \gamma^2]^{-1} + [(E_p - E_{p-Q+q})^2 + \gamma^2]^{-1}$$

$$+ 2\,\mathrm{Re}[(E_p - E_{p-q} - \omega - i\gamma)^{-1}(E_p - E_{p-Q+q} + i\gamma)^{-1}]\}.$$

Neglecting the term of order ω/E, we can rewrite this equation in the form

$$|u(Q)|^2 \sum_q w_i(q,\omega)\left|\frac{1}{q \cdot v - \omega - i\gamma} + \frac{1}{\omega - q \cdot v' - i\gamma}\right|^2.$$

Here $v' = (p - Q)/m$ is the final electron velocity, $\hbar\omega$ is the energy loss, v is the initial electron velocity and γ is the Green function damping.

Let us rewrite this equation as

$$|u(Q)|^2 \frac{1}{(2\pi)^3} \int dq \, q^2 w_i(q,\omega) \mathfrak{G}(q,\omega,\chi)$$

where the factor

$$\mathfrak{G}(q,\omega,\chi) = \int d\Omega_q \left| \frac{1}{v \cdot q - \omega - i\gamma} + \frac{1}{\omega - v'q - i\gamma} \right|^2 \tag{1}$$

accounts for the weak localization. The integration in (1) is carried out over all directions of momentum q transferred to the medium owing to the inelastic scattering.

This function is most significant for the theory of weak localization. The two terms in the bracket are the Green functions whose product will give us the angular dependence on the scattering angle χ.

Equation (1) does not involve electron exchange. We shall rewrite it with new Green functions, so as to take into account the identity principle for electrons in the beam and at the scatterers.

Electron exchange also makes an appearance in the corrections to both the elastic and the inelastic cross sections, which are not always easy to calculate within perturbation theory because of the non-orthogonality of the wavefunctions; the associated difficulties can be overcome by utilizing a special perturbation theory apparatus built for non-orthogonal bases in general [4,5]. However, in this paper we shall omit such calculations, for there is only a vague connection between the pattern that these cross sections make, and the features of the new phenomenon [2,3].

2. The electron Green functions involving electron exchange

In our treatment we shall take into account the identity of incident electrons and those at hydrogen-like scatterers. Hydrogen-doped Zi–Ni alloys have been used as a disordered medium in experiments on ordinary weak localization. Doping the samples with hydrogen has been shown to increase the disorder and to enhance strongly the quantum interference at defects [6–8]. Thus, our mathematically simple approach will also be realistic.

The wavefunction of an incident electron and a hydrogen-like atom, with regard to the exclusion principle and with the force interaction neglected, can be written down conventionally:

$$\Psi(r_1, r_2) = \mathcal{N}[\psi_a(r_1 - R)\psi_p(r_2) \pm \psi_a(r_2 - R)\psi_p(r_1)]. \tag{2}$$

Here

$$\mathcal{N} = [2(1 \pm |\langle \psi_a(r - R)|\psi_p(r)\rangle|^2)]^{-1/2}. \tag{3}$$

In this wavefunction, which is antisymmetric in electron interchange, ψ_a and ψ_p correspond to the bound and incident electrons respectively. The total spin determines the sign of the second term.

The function (2) can be represented in the form of the following series:

$$\Psi(r_1, r_2) = \sum_m f_m(r_2)\psi_{am}(r_1 - R). \tag{4}$$

In the above, R is the position vector of the nucleus, and ψ_{am} refers to the basis of eigenfunctions corresponding to the bound electrons:

$$f_m(r_2) = \mathcal{N}[\langle\psi_{am}(r_1 - R)|\psi_a(r_1 - R)\rangle\psi_p(r_2) \pm \langle\psi_{am}(r_1 - R)|\psi_p(r_1)\rangle\psi_a(r_2 - R)]. \quad (5)$$

Here

$$\psi_p = (2\pi\hbar)^{-3/2}\exp[ip \cdot r/\hbar]$$

$$\psi_{a0} = (\alpha^3/\pi)^{1/2}\exp(-\alpha r).$$

The latter is the wavefunction corresponding to the ground state of the hydrogen-like atom. Finally,

$$f_0 = \mathcal{N}(2\pi\hbar)^{-3/2}\left[\exp\left(\frac{ip \cdot r}{\hbar}\right) \pm \frac{8\alpha^4}{[\alpha^2 + (p/\hbar)^2]^2}\exp\left(\frac{ip \cdot r}{\hbar} - \alpha|r - R|\right)\right]. \quad (6)$$

In this expression the second term is the exchange contribution to the one-electron wavefunction.

In (3) we shall leave out all the terms except for that referring to the ground state of the hydrogen-like atom. All the others are negligible, because the value of overlap integral $\langle\psi_{am}(r - R)|\psi_p(r)\rangle$ is small as a result of the oscillations of ψ_{am} at $m \neq 0$. Given this, the function f can be considered as the wavefunction of one of the indistinguishable electrons in the system.

Now the one-electron Green function that allows for the principle of indistinguishability can be written as follows:

$$G(r, r') = \sum_p \frac{f_0(r)f_0^*(r')}{E - E_p + i\gamma} = \frac{\mathcal{N}^2}{(2\pi\hbar)^3}\sum_p\left(\frac{\exp(ip \cdot (r - r')/\hbar)}{E - E_p + i\gamma} \pm \frac{8}{(1 + (p/\alpha\hbar)^2)^2}\right.$$

$$\times\frac{\exp[i(p/\hbar) \cdot (r - R) - \alpha|r' - R|] + \exp[-i(p/\hbar)\cdot(r' - R)] - \alpha|r - R|)}{E - E_p + i\gamma}$$

$$\left. + \frac{8^2}{[1 + (p/\alpha\hbar)^2]^4}\frac{\exp[-\alpha(|r - R| + |r' - R|)]}{E - E_p + i\gamma}\right). \quad (7)$$

On averaging over randomly distributed scatterers, we obtain

$$G(r, r') = G_0(r, r') \pm G_1(r, r') + G_{aa}(r, r') \quad (8)$$

where G_0 is the same Green function as in [2], which does not include interchange:

$$G_1(p) = \frac{64\pi n}{\alpha^3[1 + (p/\alpha\hbar)^2]^4(E - E_p + i\gamma)}. \quad (9)$$

Here n is the density of scatterers. It is the above expression that accounts for the exchange. In averaging, we shall not take into account that the normalization factor depends on the overlap parameter; otherwise, it would just give us a correction of the second order of $\hbar^2\alpha^2/2mE$.

The third term in (8) is not particularly interesting, as it describes only the electron's motion that begins and ends in one and the same atom.

3. The effect of electron exchange on quantum interference

We shall allow for electron exchange with the aid of the Green functions given by (8), in place of the old functions referred to by the solid lines in figure 2(*b*) and 2(*c*).

Now, instead of (1) we shall have

$$\mathfrak{S} = \int d\Omega_q \, |[G_0(p'+q) \pm G_1(p'+q)] + [G_0(p-q) \pm G_1(p-q)]|^2. \tag{10}$$

Equation (10) can be rewritten as follows:

$$\mathfrak{S} = \mathfrak{S}_0 \mp \mathfrak{S}_{01} + \mathfrak{S}_{11}. \tag{11}$$

Here $\mathfrak{S}_0 = \mathfrak{S}(q, \omega, \chi)$ and $\mathfrak{S}$ is given by (1).

Let us now discuss (11) in more detail. The sign of the second term depends on the total spin of the 'incident electron scatterer' system. However, it is taken for granted that electrons in the beam are unpolarized—the spins can point either way. Therefore, it is necessary to find the average with respect to the total spin. As is known from quantum mechanics, the operator $\hat{D} = \frac{1}{2}(1 + 4\hat{S}_1 \cdot \hat{S}_2)$ has eigenvalues that depend on the total spin $\hat{S} = \hat{S}_1 + \hat{S}_2$ of the system. For instance, if $|s_1| = |s_2| = \frac{1}{2}$ the said operator has two eigenvalues, i.e. $\bar{D} = 1$ at $\bar{S} = 1$, and $\bar{D} = -1$ at $\bar{S} = 0$. This operator can be substituted in (11):

$$\mathfrak{S} = \mathfrak{S}_0 + \tfrac{1}{2}(1 + 4\hat{s}_1 \cdot \hat{s}_2)\mathfrak{S}_{01} + \mathfrak{S}_{11}. \tag{12}$$

Let us calculate the statistical average of this expression over the total spin, with regard to the statistical factors $g_1 = 3$ and $g_0 = 1$ of the two states. The eigenvalues are $\hat{s}_1 \cdot \hat{s}_2 = -\frac{3}{4}$ at $\bar{S} = 0$, and $\overline{\hat{s}_1 \cdot \hat{s}_2} = \frac{1}{4}$ at $\bar{S} = 1$. Accordingly,

$$\langle \hat{s}_1 \cdot \hat{s} \rangle = g_0(-\tfrac{3}{4}) + g_1(\tfrac{1}{4}) = 0. \tag{13}$$

Thus, the spin-average $\mathfrak{S}$ will be

$$\langle \mathfrak{S} \rangle = \mathfrak{S}_0 + \tfrac{1}{2}\mathfrak{S}_{01} + \mathfrak{S}_{11}. \tag{14}$$

Mathematically, electron exchange contributes to the new phenomenon through $\mathfrak{S}_{01}$ and $\mathfrak{S}_{11}$:

$$\mathfrak{S}_{01} = \int d\Omega_q [G_0^*(p'+q)G_1(p-q) + G_1^*(p'+q)G_0(p-q) + G_1^*(p-q)G_0(p'+q)$$

$$+ G_0^*(p-q)G_1(p'+q) + G_0^*(p-q)G_1(p-q) + G_1^*(p-q)G_0(p-q)$$

$$+ G_1^*(p'+q)G_0(p'+q) + G_0^*(p'+q)G_1(p'+q)]. \tag{15}$$

In the above expression the first four terms dominate the new kind of weak localization, while the others contribute only to the background. This is because the scattering angle contains only terms which depend on both the vector p of the initial state of the incident electron and the vector p' of the final state simultaneously. When carried out analytically, (15) gives

$$\mathfrak{S}_{01} = 256\frac{n\pi}{\alpha^3}\left(\frac{\mathfrak{S}_0}{(1 + E_p/E_B)^3} - \frac{8\pi}{E_B^2}\frac{2 + z\ln|(1-z)/(1+z)|}{(1 + E_p/E_B)^5}\right). \tag{16}$$

Here E_B is the Bohr energy, and $z = (\omega + i\gamma)/vq$. $\mathfrak{G}_0$ was first introduced in [2] in the form of an integral, which is found to be equal to

$$
\mathfrak{G}_0 = \frac{4\pi}{qv\gamma} \left[\tan^{-1}\left(\frac{qv+\omega}{\gamma}\right) + \tan^{-1}\left(\frac{qv-\omega}{\gamma}\right) \right.
$$
$$
- \gamma \, \mathrm{Re}(2\omega_c^2(1-\cos\chi) - q^2v^2\sin^2\chi)^{-1/2}
$$
$$
\left. \times \ln\left(\frac{\omega_c^2 - q^2v^2\cos\chi + qv[2\omega_c^2(1-\cos\chi) - q^2v^2\sin^2\chi)^{1/2}}{\omega_c^2 - q^2v^2\cos\chi - qv[2\omega_c^2(1-\cos\chi) - q^2v^2\sin^2\chi]^{1/2}}\right) \right]. \quad (17)
$$

The last term in (14) is

$$
\mathfrak{G}_{11} = \int d\Omega_q \left[|G_1(p'+q)|^2 + |G_1(p-q)|^2 + G_1^*(p'+q)G_1(p-q) + G_1^*(p-q)G_1(p'+q) \right].
$$
$$
(18)
$$

The contribution of this function to the phenomenon is

$$
\mathfrak{G}_{11} = \frac{(64n\alpha^{-3})^2}{18} \left(\frac{36\mathfrak{G}_0}{(1+2mE/\hbar^2\alpha^2)^8} + \frac{24^2 \times 4\pi}{(\hbar^2\alpha^2/2m)^2(1+2mE/\hbar^2\alpha^2)^{10}} \right.
$$
$$
\times \{1 - \cos\chi[2 + z\ln|(1-z)/(1+z)|]\}
$$
$$
\left. - \frac{4\pi(vq)^2(3 \times 4 \times 5)^2}{3(\hbar^2\alpha^2/2m)^2(1+2mE/\hbar^2\alpha^2)^{12}} \right). \quad (19)
$$

4. Conclusion

As seen from (16) and (19), the scattering intensity includes the electron exchange terms varying directly as $\cos\chi$. This additional angular feature appears because the electron hops from one atom to another. Arranging the terms in (14), we finally obtain

$$
\mathfrak{G} = 4 \left[\frac{1}{4} + \frac{201}{(1+E_p/E_B)^3} \frac{n}{\alpha^3} + \frac{80\,770}{(1+E_p/E_B)^8} \left(\frac{n}{\alpha^3}\right)^2 \right] \mathfrak{G}_0(q,\omega,\chi)
$$
$$
- 4 \left[\frac{51\,200}{(1+E_p/E_B)^5} \frac{n}{\alpha^3} + \frac{16.8 \times 10^7}{(1+E_p/E_B)^{10}} \left(\frac{n}{\alpha^3}\right)^2 \right]
$$
$$
\times \frac{2 + z\ln|(1-z)/(1+z)|}{E_B^2} \cos\chi. \quad (20)
$$

Here E_p and E_B are the incident electron energy and the Bohr energy, respectively.

Let us summarize the results obtained. Equation (20) contains two terms. The first is proportional to $\mathfrak{G}_0$. The angular dependence of the intensity of scattered electrons described by this term is the same as for the new type of weak localization withouut electron exchange. The exchange contributions are proportional to n/α^3 or $(n/\alpha^3)^2$. Therefore the exchange only somewhat increases the pre-factor of $\mathfrak{G}_0$.

The second term in (20), proportional to $\cos\chi$, is new and is entirely produced by electron exchange. Thus, the electron exchange enhances the small-angle scattering.

Let us evaluate the relative contribution of the exchange corrections. The relative exchange correction of the pre-factor of $\mathfrak{G}_0$ which contains n/α^3 is equal to 0.3 if E_p/E_B, the incident particle energy in units of the Bohr energy, is given by

$$\frac{E_p}{E_B} \leqslant -1 + \left(\frac{4 \times 201}{0.3}\frac{n}{\alpha^3}\right)^{1/3}. \tag{21}$$

If n/α^3, the concentration of hydrogen-like atoms, equal to unity, equation (21) yields $E_p/E_B \leqslant 13$.

The exchange correction proportional to $(n/\alpha^3)^2$ is smaller than the former by a factor of 3 or 4. At $(n/\alpha^3) \simeq 0.01$ the leading correction is essential for $E_p/E_B \leqslant 2$. Thus, if the concentration of hydrogen-like atoms is small, the exchange correction to the pre-factor of $\mathfrak{G}_0$ in (20) is also small.

The exchange correction to $\mathfrak{G}$ which varies as $\cos\chi$ is important for $E_p/E_B \leqslant 14$ if the concentration is equal to unity. If the concentration is about 0.01, this correction is noticeable for $E_p/E_B \leqslant 5$.

Therefore we see that the effect of electron exchange on the new type of weak localization is manifested in some amplification of the small-angle electron scattering. The corresponding contribution to the scattering cross section is proportional to $\cos\chi$. The range of relative densities of scatterers and the energies of incident electrons in which the effect of electron exchange on the new type of weak localization becomes noticeable is estimated as

$$\frac{51\,200}{(1 + E_p/E_B)^5}\frac{n}{\alpha^3} \geqslant \frac{1}{4}. \tag{22}$$

The above results have been obtained under the assumption of one elastic scattering event and one inelastic scattering event, but they are expected to be valid even for multiple elastic scattering; this suggestion is confirmed by the results of [3].

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