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Backscattering of high-energy electrons from disordered media: Antienhancement due to the spin-orbit interaction

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We propose that high-energy electrons when scattered from random media reveal a backscattered peak similar to that found recently for optical waves. However, unlike electromagnetic waves, an antibackscattered peak will appear when spin-orbit scattering is strong. The antienhancement of the backscattered electrons is unique to three-dimensional systems and is absent for two-dimensional systems where a reduced backscattered peak is predicted. Possible experimental realizations are proposed.

Recently, weak localization of classical waves has attracted much interest. In particular, it has been demonstrated¹⁻⁵ that when light is scattered from a random medium, the scattered wave exhibits a narrow backscattered peak of width $\sim \lambda/l$, where λ is the photon wavelength and *l* is the elastic transport mean-free path. In random solids, this peak is hidden due to the optical intensity fluctuations (speckle)^{4,5} and is recovered^{4,5} only after an ensemble average of the intensity is performed. Thus, the backscattered peak is a general phenomenon which results⁶ from interference between a multiple-scattering path and its time-reversal path. This always leads to constructive interference which enhances the backscattered peak near the backward direction ($\theta = \pi$). Effect of polarization on the backscattered peak was also intensively studied.⁷

The problem we address in this Rapid Communication is whether it is possible to observe antibackscattered peak due to the destructive interference. We argue that this can be realized for scattering of high-energy electrons, in the energy range of $\sim 200 \text{ eV}$, from amorphous semiconductorlike Ge or Si. The backscattered intensity will possess a narrow backscattered peak of width $\lambda/l \approx 0.01$ rad. When the semiconductor is doped or alloyed with large valence atoms (for example, Si:Sb or $Si_{1-x}Nb_x$), we predict that an antibackscattered peak will be revealed. The antibackscattered peak results from antilocalization, a phenomenon known from studies of transport properties of disordered materials. However, surprisingly, we find that the effect of the spin-orbit interaction on the backscattered peak depends strongly on the dimensionality of the system.

The antibackscattered peak appears only for threedimensional systems. For strictly two-dimensional systems, we find that the effect of the spin-orbit interaction leads only to a reduced backscattered peak which never turns into an antipeak. Crossover effects from three dimensional systems to quasi two dimensional systems are also of great interest. We hope that our predictions will motivate an experimental search in the area of scattering of high-energy electrons from disordered materials.

We consider an electron of wave vector \mathbf{K}_i and spin S that is injected into a random material at point *n* undergoing elastic multiple scattering and is emitted at point *m*

with a final wave vector \mathbf{K}_f and spin S' (see Fig. 1). A time-reversal trajectory exists in which the electron is injected at point m and emitted at point n, with a different final spin state S'' due to the spin-orbit interaction. We calculate the intensity which results from the interference between these two trajectories. The initial electron wave function is $\psi_i = |\mathbf{K}_i, \mathbf{S}\rangle$, where S is the initial spinor. At point *m*, the final wave function is $\psi_f = |\mathbf{K}_f, \mathbf{S}'\rangle$ in which both the K state and the spinor S of the electron are changed due to multiple-elastic scattering. The spinor is changed due to rotations⁸ caused by spin-orbit interactions. The final electron state in the reversed trajectory is $\psi_f(\mathrm{TR}) = |\mathbf{K}_f, \mathbf{S}''\rangle$. Thus, although the electron is emitted with the same final wave vector, its final spinor S'' is *different* from S' due to lack of time-reversal symmetry in the spin-orbit interaction Hamiltonian

$$H_{\rm so} = C_0 \boldsymbol{\sigma} \cdot \mathbf{L} \ , \tag{1}$$

where $C_0 = (2m^2C^2r)^{-1}(dV/dr)$ and V is the scattering potential.

The scattering amplitude in the Born approximation is



FIG. 1. The two-electron time-reversed multiple-scattered trajectories which contribute to the interference which results in a backscattered intensity peak.

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given by

$$A_{ba} = \langle \mathbf{S}_b, \mathbf{K}_b | H_{so} | \mathbf{K}_a, \mathbf{S}_a \rangle \tag{2}$$

which can be rewritten⁸ as

$$A_{ba} = V_{K_a, K_b} \langle \mathbf{S}_b | I + i\epsilon (\mathbf{K}_a \times \mathbf{K}_b) \cdot \boldsymbol{\sigma} | \mathbf{S}_a \rangle , \qquad (3)$$

where $V_{\mathbf{K}_{a},\mathbf{K}_{b}}$ and ϵ depend on the explicit form of the potential V(r). As pointed out by Bergmann⁸ this term has the effect of rotating the initial spinor. The final spinor $|S_{b}\rangle$ is related to the initial spinor by a rotational matrix <u>R</u>

$$|\mathbf{S}_b\rangle - \underline{R} |\mathbf{S}_a\rangle . \tag{4}$$

For *n* multiple scatterings, <u>R</u> can be written as a product $R = R_n \cdot R_{n-1} \dots R_2 \cdot R_1$. The rotational matrix can be expressed⁸ in terms of Euler angles (θ, ϕ, Φ) in the follow-

ing way:

$$\underline{R} = \begin{bmatrix} \cos\theta/2 \ e^{i(\phi+\Phi)} \ i \sin\theta/2 \ e^{-i(\phi-\Phi)} \\ i \sin\theta/2 \ e^{i(\phi-\Phi)} \ \cos\theta/2 \ e^{-1(\phi+\Phi)} \end{bmatrix} .$$
(5)

For a given trajectory, we may write

$$\psi_{f} = |\mathbf{K}_{f}\rangle(\underline{R} |\mathbf{S}\rangle) ,$$

$$\psi_{f}(\mathbf{TR}) = |\mathbf{K}_{f}\rangle(\underline{R}^{-1} |\mathbf{S}\rangle) ,$$
(6)

where \underline{R}^{-1} is the inverse matrix of \underline{R} . The intensity of the electron backscattered wave for a particular trajectory is given by

$$I_j(\mathbf{K}_i, \mathbf{K}_f) \propto |\psi_{f,j}(\mathrm{TR}) + \psi_{f,j}|^2 .$$
(7)

Using Eq. (6) and summing over all trajectories that start at point *n* and end at point *m* (within a distance $\sim l$ from the scattered boundary) we get

$$I(\mathbf{K}_{i},\mathbf{K}_{f}) = I_{0} \sum_{j} \sum_{n,m} |P_{nmj} \exp[i(\mathbf{K}_{i} \cdot \mathbf{r}_{n} - \mathbf{K}_{f} \cdot \mathbf{r}_{m} + \phi_{nmj})] \underline{R}_{nmj} |\mathbf{S}\rangle + P_{mnj} \exp[i(\mathbf{K}_{i} \cdot \mathbf{r}_{m} - \mathbf{K}_{f} \cdot \mathbf{r}_{n} + \phi_{nmj})] \underline{R}^{\dagger_{nmj}} |\mathbf{S}\rangle|^{2}, \quad (8)$$

where ϕ_{nmj} is the phase acquired during the trajectory *j* between points *n* and *m*. By using Eq. (8) we take only the "diagonal"⁵ terms: namely, interference of a given trajectory with the time-reversed trajectory. For random solids, however, the off-diagonal terms lead to interference between different trajectories which produces intensity fluctuations.⁵ Thus, Eq. (8) may be understood as the ensemble-averaged backscattered intensity which removes the off-diagonal terms (speckle).⁵ Using the relations

$$\langle \mathbf{S} | (\underline{R}^{\dagger})^2 | \mathbf{S} \rangle = (\langle \mathbf{S} | R^2 | \mathbf{S} \rangle)^*, \langle \mathbf{S} | R^2 | \mathbf{S} \rangle = Ae^{i\delta}$$

and $\phi_{mnj} = \phi_{nmj}$ the final expressions for the backscattered intensity is

$$I(\mathbf{q}) = I_0 \left(1 + \sum_{j,nm} A_j | P_{nmj} |^2 \cos[\mathbf{q} \cdot (r_n - r_m) + \delta_j] \right) , \quad (9)$$

where $|P_{nmj}|^2$ is the probability for an electron that is first scattered at point n to be emitted at point m in a trajectory j. The scattering vector **q** is given by $\mathbf{q} = \mathbf{K}_i + \mathbf{K}_f$. The second term in Eq. (9) leads to the backscattered peak due to interference. Whether this term is positive or negative (destructive interference) depends on the values of A_j and δ_j which are due to the spin-orbit interaction. For $A_i = 1$ and $\delta_i = 0$ we get the usual enhancement^{5,6} for scalar spinless waves which, as seen from Eq. (9), leads to a maximum peak of factor of 2 at q = 0 which corresponds to the backscattered angle $\theta = \pi$. This will be approximately the case for a weak spin-orbit interaction. If we define the diffusion spin-orbit length L_{so} as the distance an electron diffuses in a spin-orbit scattering time, then for a sample of size $L < L_{so}$, one always expects an enhanced backscattering peak as in the case for light scattering. However, for $L \gg L_{so}$ and $L_{so} \ll L_i$ (L_i is the inelastic scattering length) the second term in Eq. (9) is usually negative for large trajectories where the size of the trajectories W_j is much larger than L_{so} . For such long trajectories, the angle between $|S\rangle$ and $|S'\rangle$ is random and unrelated and the sum over all possible (large) trajectories is

equivalent to an average over all Euler angles which leads to

$$\langle\langle S | R^2 | S \rangle\rangle_{\theta, \Phi, \theta} = -\frac{1}{2}, \ W_j \gg L_{so}$$
 (10)

Thus for trajectories for which $W_j \gg L_{so}$, we may take in Eq. (9) the values $A_i = -\frac{1}{2}$, $\delta_i = 0$. This is the origin of the antipeak of the backscattered electrons in a disordered system undergoing spin-orbit scattering. Since long trajectories correspond to small backscattered angles, the width of the antipeak will be of order $\theta \approx 2\lambda/L_{so}$. For short trajectories for which $W_j < L_{so}$, which correspond to $\theta \gg \lambda / L_{so}$, the spin-orbit effect is negligible and we get the normal enhancement backscattered tail. Thus in the presence of strong spin-orbit scattering, the backscattered peak is split into two peaks separated by an antipeak. In Fig. 2, we plot our calculated backscattered peak for a three-dimensional system in the presence of spin-orbit scattering. We used the diffusion approximation^{5,6} for $|P_{nmj}|$ with an absorbing boundary, which was very successful^{6,9} in accounting for the backscattered peak of light.

The dashed curve is the backscattered peak for $l/\lambda = 2$ without spin-orbit scattering. The solid curve corresponds to the backscattered antipeak. The two maxima correspond to the crossover from short trajectories ($W_j \leq L_{so}$) to long trajectories ($W_j \geq L_{so}$).

We now turn to the calculation of the backscattering of electrons from a disordered strictly two-dimensional system. For light scattering from a two-dimensional system it was shown¹⁰ that the line shape of the backscattered peak is identical to that for three-dimensional systems (except near $\theta \approx \pi$ where strong localization rounds off the peak). By contrast it turns out that the effect of spinorbit scattering on the backscattered peak is very sensitive to the dimensionality of the system. For two dimensions, the fact that the orientation of the z component of the spin is unchanged due to spin-orbit scattering affects the backscattered peak. The matrix $\langle S | R^2 | S \rangle$ in two dimensions

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FIG. 2. Backscattered intensity as a function of backscattered angle. The solid curve corresponds to the case of spinorbit scattering and the dashed curve is the enhanced peak without spin-orbit scattering.

depends only on ϕ and Φ and for long trajectories, $W_j \gg L_{so}$, we obtain

$$\langle\langle S | R^2 | S \rangle\rangle_{\phi,\phi} = 0 . \tag{11}$$

Long trajectories will *not* contribute to the backscattered peak since according to Eq. (11) on the average there is no interference between the time-reversal trajectories and the second term in Eq. (9) vanishes. Thus there is no antipeak for backscattering of electrons from a two-dimensional system, although the peak is much reduced since for $\theta < \lambda/L_{so}$ there is no constructive interference. In Fig. 3, we plot the backscattered peak of electrons from a two-dimensional system for $l/\lambda = 2$. The dashed curve is the backscattered peak without spin-orbit scattering. The solid curve is due to spin-orbit scattering. The crossover between the curves occurs at $\theta = \pm \lambda/L_{so}$; for $|\theta| > \lambda/L_{so}$, the effect of the spin-orbit interaction is negligible and both curves nearly coincide.

For a *quasi*-two-dimensional system where the component of the spin **S** in the z direction is not strictly conserved, we expect interesting crossover effects from Fig. 2 to Fig. 3 as the width of the layer is reduced.

Very recently, it was proposed¹¹ that strong spin-flip scattering of neutrons may lead to an antibackscattered peak. These calculations were carried out only to second order which is justified for neutrons which possess a long



FIG. 3. Backscattered intensity as a function of backscattered angle for a two-dimensional system. The dashed curve is the backscattered peak without spin-orbit scattering and the solid curve is due to spin-orbit scattering.

mean-free path. We have carried out a similar calculation on the effect of spin-flip on electron scattering which includes all higher orders and find that the antibackscattering peak is much reduced that it will be hard to observe experimentally. Therefore, the only realistic possibility of observing an antibackscattered peak for electrons is via the spin-orbit interaction. For electron energies of ~ 200 eV in amorphous Ge or Si, the elastic mean-free path is about¹² 500 Å which allows for many multiple scatterings. A strong electron spin-orbit interaction can be obtained when these semiconductors are doped, for example, with Sb. This suggestion is supported by the fact that recently it was found¹³ that spin-orbit scattering dominates the low-temperature transport of Si:Sb. Other materials which may exhibit strong spin-orbit effects are $Si_{1-x}Nb_x$ and $Si_{1-x}Au_x$.

In summary, we have shown that the scattering of high-energy electrons from random systems leads to a sharp backscattered peak. When spin-orbit interactions are strong, we predict an antibackscattered peak for three-dimensional systems and a reduced backscattered peak for two-dimensional systems.

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