Scattering of electrons by impurities in a magnetic field

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The differential scattering cross section for electrons by impurity atoms may acquire a right-left asymmetry linearly proportional to an applied magnetic field. If this were true, there would arise a new contribution to the Hall coefficient. The Boltzmann transport equation ordinarily used in magneto-transport theory requires that each one-electron wave function be described in its own time-dependent gauge. In order to calculate quantum mechanically the differential scattering cross section, the ingoing and outgoing wave functions must be transformed into a common gauge. When this is done the scattering matrix element has no contribution linear in the magnetic field for an isotropic scattering potential. Consequently, there will not be a new contribution to the Hall coefficient.

I. INTRODUCTION

In a magnetic field the differential scattering cross section for electrons by impurity atoms may acquire a right-left asymmetry linearly proportional to the applied magnetic field. If this were true, it would produce a new contribution to the Hall coefficient.

This intriguing idea was first suggested by Chambers,[1] who argued that this effect would occur for free electrons scattered by a central potential. Chambers applied his theory to the Hall effect in liquid transition metals. A rough calculation indicated that the effect was of the right order of magnitude to explain some of the experimental results.

In this paper we reexamine the theory of this effect. We show that the differential scattering cross section for free electrons is unchanged to first order in the applied magnetic field if the scattering potential is isotropic. Consequently there will not be a new contribution to the Hall coefficient.

Several sources of a right-left asymmetry in the differential scattering cross section are known.[2] For example, if the scattering potential includes the spin-orbit interaction between the electron and the impurity, there will be a right-left asymmetry linearly proportional to the spin of the electron, which yields a contribution to the Hall coefficient.[3] This asymmetry is caused by the spin-orbit interaction.

In this paper our sole concern is the possible asymmetry due to the effect of the applied magnetic field on the scattering. In order to avoid any confusion between this and other sources, we assume that the scattering potential depends only on the position of an electron relative to an impurity. Since the spin of the electron is irrelevant, the electrons may be imagined as spinless.

We consider a system of free electrons scattered by random impurities in a uniform magnetic field. We assume that the magnetic field is sufficiently weak that the motion of an electron between collisions may be treated classically. Each electron state corresponds to a classical trajectory $\vec{r}(t)$ of an electron in a magnetic field.

The Boltzmann equation for the momentum distribution is

$$\frac{\partial f_{\vec{k}}}{\partial t} - \frac{e}{\hbar c}(\vec{v}_{\vec{k}} \times \vec{B}) \cdot \frac{\partial f_{\vec{k}}}{\partial \vec{k}} = C(f_{\vec{k}}), \tag{1a}$$

with the collision operator

$$C(f_{\vec{k}}) = N \sum_{\vec{k}'} [w_{\vec{k}\vec{k}'} f_{\vec{k}}(1 - f_{\vec{k}}) - w_{\vec{k}'\vec{k}} f_{\vec{k}'}(1 - f_{\vec{k}'})]. \tag{1b}$$

$f_{\vec{k}}(t)$ is the number of electrons whose mean momentum is $\vec{p} = \hbar\vec{k}$; $\vec{v}_{\vec{k}}$ is the velocity of an electron with momentum $\vec{p} = \hbar\vec{k}$. $w_{\vec{k}'\vec{k}}$ is the transition rate between electron states due to scattering by a single impurity and N is the total number of impurities.

Although the motion of an electron between collisions may be treated classically, the scattering probability must be calculated quantum mechanically. In order to take into account the effect of the magnetic field on the scattering, the electron wave functions corresponding to the classical trajectories in a magnetic field are required.

In a magnetic field, the physical interpretation of an electron wave function Ψ depends upon the gauge. The mean velocity of an electron is

$$\langle \vec{v} \rangle = \left\langle \Psi \middle| \frac{1}{m}\left(\vec{p} + \frac{e}{c}\vec{A}\right) \middle| \Psi \right\rangle. \tag{2}$$

In order for the simple relation $m\langle \vec{v} \rangle = \langle \vec{p} \rangle$ to hold, the gauge must be chosen so that $\langle \vec{A} \rangle = 0$.[4] In a uniform magnetic field this may be accomplished by choosing a time-dependent vector potential

$$\vec{A} = \tfrac{1}{2}\vec{B} \times (\vec{r} - \langle \vec{r} \rangle), \tag{3}$$

which is different for each classical trajectory $\vec{r}(t)=\langle\vec{r}\rangle$. With this choice, the wave packet

$$\Psi=\sum_{\vec{k}}\alpha_{\vec{k}}(t)e^{i\vec{k}\cdot\vec{r}} \tag{4}$$

describes an electron with (Jones-Zener gauge)

$$\langle\vec{v}\rangle=(\hbar/m)\langle\vec{k}\rangle. \tag{5}$$

Since the motion of a free electron is classical, the rate of change of its mean velocity is proportional to the Lorentz force so that (Jones-Zener gauge)

$$\hbar\frac{d\langle\vec{k}\rangle}{dt}=\frac{-e}{c}(\langle\vec{v}\rangle\times\vec{B}). \tag{6}$$

If instead of choosing the Jones-Zener gauge, we had chosen the symmetric gauge, with

$$\vec{A}=\tfrac{1}{2}\vec{B}\times\vec{r}, \tag{7}$$

then the wave packet (4) would describe an electron with (symmetric gauge)

$$\langle\vec{v}\rangle=(\hbar/m)\langle\vec{k}\rangle+(e/2mc)\vec{B}\times\langle\vec{r}\rangle \tag{8}$$

and (symmetric gauge)

$$\hbar\frac{d\langle\vec{k}\rangle}{dt}=\frac{-e}{2c}(\langle\vec{v}\rangle\times\vec{B}), \tag{9}$$

which is one-half the Lorentz force.

Thus the Boltzmann Equation (1) with $\vec{v}_{\vec{k}}=\hbar\vec{k}/m$, which is ordinarily used in magneto-transport theory, requires that each electron wave function be described in its own time-dependent gauge, the Jones-Zener gauge (3). When there is no magnetic field, the momentum $\vec{p}=\hbar\vec{k}$ has the physical meaning of being proportional to the velocity $\vec{v}$, i.e., $\vec{p}=m\vec{v}$. The Jones-Zener gauge is the only gauge which preserves this physical meaning.

In a magnetic field there is, in general, a distinction between the dynamical momentum $\vec{p}$ and the kinematic momentum $m\vec{v}=\vec{p}+(e/c)\vec{A}$. The rate of change of the kinematic momentum is equal to the Lorentz force; the rate of change of the dynamical momentum depends on the vector potential and is, in general, not equal to the Lorentz force. For a classical system the momentum distribution satisfies the Boltzmann equation (1) provided that what is meant by the momentum is the kinematic momentum $m\vec{v}$. In order that the mean dynamical momentum $\langle\vec{p}\rangle$ of an electron wave function be equal to its mean kinematic momentum $m\langle\vec{v}\rangle$, the Jones-Zener gauge must be chosen.[5]

II. ELECTRON WAVE FUNCTIONS IN A MAGNETIC FIELD

Let $\vec{r}(t)$ and $\vec{v}(t)$ be the classical position and velocity of an electron in a uniform magnetic field, whose initial position and velocity are $\vec{r}(0)$ and $\vec{v}(0)$. To find the electron wave function corresponding to this classical motion, we choose the Jones-Zener gauge with the vector potential

$$\vec{A}=\tfrac{1}{2}\vec{B}\times[\vec{r}-\vec{r}(t)]. \tag{10}$$

The scalar potential Φ is determined by

$$\vec{E}=-\vec{\nabla}\Phi-\frac{1}{c}\frac{\partial\vec{A}}{\partial t}=0, \tag{11}$$

so that

$$\vec{\nabla}\Phi=\frac{-1}{c}\frac{\partial\vec{A}}{\partial t}=\frac{-1}{2c}[\vec{v}(t)\times\vec{B}]. \tag{12}$$

It is convenient to choose

$$\Phi=(-1/2c)[\vec{v}(t)\times\vec{B}]\cdot[\vec{r}+\vec{r}(t)]. \tag{13}$$

Substituting into the Schrödinger equation,

$$i\hbar\frac{\partial\Psi}{\partial t}=\left[\frac{1}{2m}\left(\vec{p}+\frac{e}{c}\vec{A}\right)^2-e\Phi\right]\Psi, \tag{14}$$

we obtain

$$i\hbar\frac{\partial\Psi}{\partial t}=\left(\frac{p^2}{2m}+\frac{e}{2mc}(\vec{p}\times\vec{B})\cdot[\vec{r}-\vec{r}(t)]+\frac{e^2}{8mc^2}|\vec{B}\times[\vec{r}-\vec{r}(t)]|^2+\frac{e}{2c}[\vec{v}(t)\times\vec{B}]\cdot[\vec{r}+\vec{r}(t)]\right)\Psi. \tag{15}$$

If the electron is described by a wave packet, then for small magnetic fields the center of the wave packet follows the classical trajectory. Thus, the term proportional to B^2 will be small in the region where the wave function is not zero. Neglecting this term, the solution for Ψ is

$$\Psi=\exp\{i[\vec{k}(t)\cdot\vec{r}-\omega_{\vec{k}}t]\}. \tag{16}$$

$\vec{k}(t)$ is related to the classical velocity by $\hbar\vec{k}(t)=m\vec{v}(t)$; $\hbar\omega_{\vec{k}}=\hbar^2k^2(t)/2m=\hbar^2k^2(0)/2m$ is the classical energy.

A wave packet may be formed by combining the solutions (16) corresponding to the classical trajectories whose initial positions are all $\vec{r}(0)$ and whose initial velocities are centered about $\vec{v}(0)$. Since there is a different gauge associated with each classical trajectory, the wave functions must all be transformed into the same gauge, the gauge associated with the classical trajectory whose initial position and velocity are $\vec{r}(0)$ and $\vec{v}(0)$, before being combined. It can be shown that this wave packet corresponds to the classical trajectory. Its mean position and momentum are $\langle\vec{r}\rangle=\vec{r}(t)$ and $\langle\vec{p}\rangle=\hbar\langle\vec{k}\rangle=m\vec{v}(t)$.

III. SCATTERING IN A MAGNETIC FIELD

We now consider the scattering of an electron in a magnetic field by a potential $V(\vec{r})$ centered at the origin. The scattering potential causes transitions between the electron wave functions in a magnetic field. In order to calculate the transition rate $w_{\vec{k}\vec{k}'}$, the electron wave functions $\Psi_{\vec{k}}$ between which transitions occur must be identified.

In the Boltzmann equation the collisions are treated as instantaneous. The transition rate $w_{\vec{k}\vec{k}'}$ in the collision operator describes transitions between electron states whose momenta at the instant of the collision are $\vec{p}=\hbar\vec{k}$ and $\vec{p}'=\hbar\vec{k}'$. On the other hand, the effect of the applied magnetic field on an electron between collisions, which is described by the Lorentz force drift term in the Boltzmann equation, is treated as continuous.

If the collision is not instantaneous, then during the collision the electron's momentum will be changing due to the combined effects of the scattering potential and the Lorentz force. In order to avoid overcounting the effect of the magnetic field, the change in momentum due to the Lorentz force that an electron would experience during the collision, if it were free, must be subtracted from the total change in momentum during the collision.[6]

This may be accomplished by choosing $\Psi_{\vec{k}}$ to be the electron wave function in a magnetic field corresponding to the classical trajectory whose position and velocity at $t=0$ are $\vec{r}(0)=0$ and $\vec{v}(0)=\hbar\vec{k}/m$. Letting $\vec{r}_{\vec{k}}(t)$ and $\vec{v}_{\vec{k}}(t)$ be the classical position and velocity of this trajectory, the electron wave function $\Psi_{\vec{k}}$ is

$$\Psi_{\vec{k}}=(1/\sqrt{\Omega})\exp\{i[\vec{k}(t)\cdot\vec{r}-\omega_{\vec{k}}t]\} \tag{17}$$

in the Jones-Zener gauge with

$$\begin{aligned}\vec{A}_{\vec{k}}&=\tfrac{1}{2}\vec{B}\times[\vec{r}-\vec{r}_{\vec{k}}(t)],\\ \Phi_{\vec{k}}&=(-1/2c)[\vec{v}_{\vec{k}}(t)\times\vec{B}]\cdot[\vec{r}+\vec{r}_{\vec{k}}(t)].\end{aligned} \tag{18}$$

In these equations, the subscript $\vec{k}$ labels the classical trajectory in a magnetic field with $\vec{r}(0)=0$ and $\vec{v}(0)=\hbar\vec{k}/m$. The wave function $\Psi_{\vec{k}}$ is normalized in the volume Ω of the system.

For $\vec{k}\neq\vec{k}'$, the gauges (18) associated with $\Psi_{\vec{k}}$ and $\Psi_{\vec{k}'}$ are not equal. Thus, during the collision, the electron wave functions (17) of the initial and final states are defined in different gauges. It is mandatory that the transition rate be calculated between wave functions defined in the same gauge.

Having identified the electron wave functions between which transitions occur, each defined in its own gauge, we may now transform them to a common gauge in order to calculate the transition rate. Introducing a gauge transformation $\Lambda_{\vec{k}}$ from the Jones-Zener gauge (18) to the symmetric gauge,

$$\vec{A}'=\tfrac{1}{2}\vec{B}\times\vec{r},\quad \Phi'=0, \tag{19}$$

the wave function (17) is transformed into

$$\Psi'_{\vec{k}}=\exp[-(ie/\hbar c)\Lambda_{\vec{k}}(\vec{r},t)]\Psi_{\vec{k}}. \tag{20}$$

The gauge transformation $\Lambda_{\vec{k}}$ is determined by

$$\begin{aligned}\vec{\nabla}\Lambda_{\vec{k}}&=\vec{A}'-\vec{A}_{\vec{k}}=\tfrac{1}{2}\vec{B}\times\vec{r}_{\vec{k}}(t),\\ \frac{\partial\Lambda_{\vec{k}}}{\partial t}&=-c(\Phi'-\Phi_{\vec{k}})=-\tfrac{1}{2}[\vec{v}_{\vec{k}}(t)\times\vec{B}]\cdot[\vec{r}+\vec{r}_{\vec{k}}(t)].\end{aligned} \tag{21}$$

From (21), $\Lambda_{\vec{k}}$ may be expressed as

$$\Lambda_{\vec{k}}(\vec{r},t)=\tfrac{1}{2}[\vec{B}\times\vec{r}_{\vec{k}}(t)]\cdot\vec{r}+\lambda_{\vec{k}}(t), \tag{22}$$

with

$$\frac{d\lambda_{\vec{k}}}{dt}=-\tfrac{1}{2}[\vec{v}_{\vec{k}}(t)\times\vec{B}]\cdot\vec{r}_{\vec{k}}(t). \tag{23}$$

The classical position $\vec{r}_{\vec{k}}(t)$ satisfies

$$\vec{v}_{\vec{k}}(t)-\vec{v}_{\vec{k}}(0)=(e/mc)\vec{B}\times[\vec{r}_{\vec{k}}(t)-\vec{r}_{\vec{k}}(0)]. \tag{24}$$

Setting $\vec{v}_{\vec{k}}(t)=\hbar\vec{k}(t)/m$, $\vec{k}(0)=\vec{k}$, and $\vec{r}_{\vec{k}}(0)=0$,

$$\vec{k}(t)-\vec{k}=(e/\hbar c)[\vec{B}\times\vec{r}_{\vec{k}}(t)]. \tag{25}$$

From (22) and (25), the transformed wave function (20) may be expressed as

$$\Psi'_{\vec{k}}=\frac{1}{\sqrt{\Omega}}\exp\left[i\left(\tfrac{1}{2}[\vec{k}(t)+\vec{k}]\cdot\vec{r}-\omega_{\vec{k}}t-\frac{e}{\hbar c}\lambda_{\vec{k}}(t)\right)\right]. \tag{26}$$

The wave vector $\vec{k}(t)$ rotates about the direction of the magnetic field $\vec{B}$ at the cyclotron frequency $\omega_c=eB/mc$. Thus, for $\vec{k}\neq\vec{k}'$, the states $\Psi'_{\vec{k}}$ and $\Psi'_{\vec{k}'}$ will be orthogonal as long as $\omega_c|t|\ll 1$. If the duration of the collision is much less than the cyclotron period, the initial and final states in the symmetric gauge will be orthogonal during the transition.

We treat the scattering between the electron states $\Psi'_{\vec{k}}$ by the method of variation of constants.[7] We put

$$\Psi'_{\vec{k}}=\psi'_{\vec{k}}e^{-i\omega_{\vec{k}}t}. \tag{27}$$

From (26)

$$\psi'_{\vec{k}}=\frac{1}{\sqrt{\Omega}}\exp\left[i\left(\tfrac{1}{2}[\vec{k}(t)+\vec{k}]\cdot\vec{r}-\frac{e}{\hbar c}\lambda_{\vec{k}}(t)\right)\right]. \tag{28}$$

We expand the electron wave function in the states $\psi'_{\vec{k}}$,

$$\Psi'=\sum_{\vec{k}}c_{\vec{k}}(t)\psi'_{\vec{k}}e^{-i\omega_{\vec{k}}t}. \tag{29}$$

Substituting into the Schrödinger equation in the symmetric gauge,

$$i\hbar\frac{\partial\Psi'}{\partial t}=\left[\frac{1}{2m}\left(\vec{p}+\frac{e}{c}\vec{A}'\right)^2+V(\vec{r})\right]\Psi', \tag{30}$$

and neglecting terms of order B^2 as before, we obtain the equations of motion of the expansion coefficients,

$$i\hbar \frac{\partial c_{\vec{k}}}{\partial t} = \sum_{\vec{k}'} V_{\vec{k}\vec{k}'} c_{\vec{k}'} e^{i\omega_{\vec{k}\vec{k}'} t}, \tag{31}$$

with $V_{\vec{k}\vec{k}'} = \langle \psi'_{\vec{k}} | V | \psi'_{\vec{k}'} \rangle$ and $\omega_{\vec{k}\vec{k}'} = \omega_{\vec{k}} - \omega_{\vec{k}'}$. The dependence of the transition rate on the magnetic field is contained in the matrix element $V_{\vec{k}\vec{k}'}$.

Expanding $\psi'_{\vec{k}}$ to first order in the magnetic field,

$$\psi'_{\vec{k}} = [1 - (ie/2mc)(\vec{k} \times \vec{B})\, t \cdot \vec{r}\,]\, \psi^{(0)}_{\vec{k}}, \tag{32}$$

with

$$\psi^{(0)}_{\vec{k}} = (1/\sqrt{\Omega}) e^{i\vec{k}\cdot\vec{r}} \tag{33}$$

being the free electron wave function in the absence of a magnetic field. Taking $\vec{B} = B\hat{z}$, (32) may be expressed as

$$\psi'_{\vec{k}} = (1 - \tfrac{1}{2} i\omega_c t\, l_z)\psi^{(0)}_{\vec{k}}. \tag{34}$$

$\vec{l} \equiv \vec{r} \times (1/i)\vec{\nabla}$ is the orbital angular momentum operator. $\psi'_{\vec{k}}$ may be interpreted as the state obtained from $\psi^{(0)}_{\vec{k}}$ by an infinitesimal rotation of angle $\frac{1}{2}\omega_c t$ about the direction of the magnetic field. Thus, to first order in the magnetic field,

$$V_{\vec{k}\vec{k}'} = \langle \psi^{(0)}_{\vec{k}} | V' | \psi^{(0)}_{\vec{k}'} \rangle, \tag{35}$$

with

$$V' = V + \tfrac{1}{2} i\omega_c t [l_z, V]. \tag{36}$$

V' is the transformation of V under an infinitesimal rotation of angle $-\frac{1}{2}\omega_c t$ about the direction of the magnetic field.

If $V = V(r)$ is a central potential, $[l_z, V] = 0$ so that the matrix element $V_{\vec{k}\vec{k}'}$ is unchanged to first order in the applied magnetic field. From the equations of motion (31) of the expansion coefficients, the same will be true of the transition rate $w_{\vec{k}\vec{k}'}$ (to all orders in the potential V). Thus the differential scattering cross section is unchanged to first order in the applied magnetic field. Consequently, there will not be a new contribution to the Hall coefficient.

IV. DISCUSSION

It is instructive to examine this problem in the limit of classical scattering. During a collision, the electron's velocity is changing due to the combined effects of the Lorentz force and the scattering potential. There will be a magnetic field correction to the transition rate if either the change due to the Lorentz force is modified by the scattering potential or the change due to the scattering potential is modified by the Lorentz force.

Since the Lorentz force is proportional to the velocity, it may appear at first sight that the electron's velocity will be rotated by the magnetic field during a collision by a different amount than if it were free. If this were true, the difference would have to be included in the transition rate. However, since the cyclotron frequency does not depend on the electron's velocity, the angle of rotation of the electron's velocity is the same whether or not the electron experiences a collision. Thus the change in velocity due to the Lorentz force is not modified by the scattering potential.

As a result of the deflection of an electron by the magnetic field, the path of an electron through the scattering region will be different than if there were no magnetic field. Thus, the change in velocity due to the scattering potential may be modified by the magnetic field. Our result implies that there will be no change to first order in the magnetic field if the scattering potential is isotropic.

Our conclusion disagrees with Chambers's.[1] During a collision the velocity of an electron will be rotated by the Lorentz force about the direction of the magnetic field. If this change of velocity is included in the calculation of the transition rate, there will arise a left-right asymmetry in the differential scattering cross section, as noted by Chambers. However, this velocity rotation caused by the magnetic field is *already* included in the Boltzmann equation by the Lorentz-force drift term; it must not be included a second time in the collision operator.

In most applications of the Boltzmann equation, the effect of the applied magnetic field on the scattering is neglected. Then the free-electron wave functions in the absence of a magnetic field may be used to calculate the transition rate. If the effect of the applied magnetic field on the scattering is not neglected, the electron wave functions in a magnetic field must be used.

In order to identify the correct initial and final states, it is essential to realize that each electron wave function is described in its own time-dependent gauge, the Jones-Zener gauge (3). Quantum-theoretic scattering rates can then be calculated only after initial and final states have been transformed to a common gauge.

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