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Polarization effects in penetration of a barrier with a magnetic field applied

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The spin polarization of an electron moving nonrelativistically through a potential barrier $V(z)$, with also a constant uniform magnetic field $(0,0,B)$ applied, is calculated using the WKB approximation for the z dependence of the wave function. It is found that, in a classically allowed region, the polarization precesses at fixed angle θ about the magnetic field, with phase angle the same as a classical particle with a magnetic dipole moment. The particle penetrates through the barrier with no change in the phase of the precession but with a discontinuity in θ.

I. INTRODUCTION

Several groups have recently made measurements of the spin polarization of electrons that are field emitted from magnetic materials in the presence of an external magnetic field.[1–4] This type of experiment gives new and valuable information about surface and bulk properties of the material.

Some aspects of the theoretical background for the experiment are still under development. The change of polarization as the electron moves through the external electric and magnetic fields after leaving the material is reasonably well understood. Eckstein and Müller[5] made a numerical analysis of that problem for electrons initially polarized parallel to the magnetic field with consideration of off-axis variation of the magnetic field. Also Schmit and Good[6] treated that problem analytically for arbitrary initial polarization but neglecting the off-axis variation of the field. What happens to the polarization as the electron passes through the surface is not so well established; this is the subject of the present paper.

As a reasonable model for first investigation of the problem, one can picture the electron with a definite polarization emerging from the bulk of the material and impinging on a potential barrier at the surface. There is thus a barrier penetration problem in the presence of the external magnetic field. As shown below, this situation can be analyzed completely using the WKB approximation for the dependence on the coordinate normal to the metal.

The results are as follows: In an allowed region the electron polarization precesses at constant angle θ about the magnetic field, with phase angle the same as that of a classical magnetic dipole. The barrier penetration takes place with no change in phase angle but with a discontinuity in θ. With the electric and magnetic fields typically used in field-emission experiments the discontinuity in θ is small and the electron jumps through the barrier with very little change of polarization.

II. HAMILTONIAN

The Hamiltonian for the electron in potential V and magnetic field $\vec{B}$ is

$$H=\tfrac{1}{2}\vec{\pi}\cdot\vec{\pi}+V+\tfrac{1}{4}ge\vec{\sigma}\cdot\vec{B}\ , \tag{1}$$

where $\vec{\pi}=\vec{p}+e\vec{A}$, $g=2.0023...$, and $\vec{\sigma}$ are the Pauli matrices. Units are chosen in such a way that factors of m, c, and $\hbar$ do not appear.The symbol e indicates a positive number so the electron charge is $-e$.

The scalar potential is considered to be a function of z, the coordinate normal to the metal, only and to have the form indicated in Fig. 1. The magnetic field is constant in space and time and is perpendicular to the surface. It is of the form $(0,0,B)$, where B may be positive or negative, and a convenient vector potential is $(-\frac{1}{2}By,\frac{1}{2}Bx,0)$. With these specializations the Hamiltonian becomes

$$H=\tfrac{1}{2}\vec{p}\cdot\vec{p}+\tfrac{1}{2}eB(xp_y-yp_x)+\tfrac{1}{8}e^2B^2(x^2+y^2)+V(z)+\tfrac{1}{4}geB\sigma_z\ . \tag{2}$$

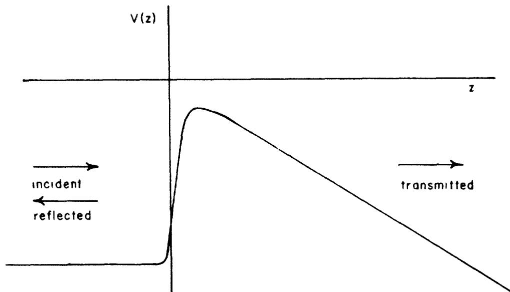

FIG. 1. Potential model for the surface of the material.

III. INTEGRALS OF THE MOTION

The operators

$$x_0 = \tfrac{1}{2}x - p_y/eB \quad , \tag{3a}$$

$$y_0 = \tfrac{1}{2}y + p_x/eB \tag{3b}$$

commute with the Hamiltonian of Eq. (2) and lead to a separation of the variables in the problem. These operators were originally introduced by Johnson and Lippmann[7] and their usefulness in constant-magnetic-field problems is well known.[8] We will also make use of the operators

$$R_0^2 = x_0^2 + y_0^2 \quad , \tag{4}$$

$$\bar{A} = \pi[(x - x_0)^2 + (y - y_0)^2] \quad , \tag{5}$$

$$L_z = xp_y - yp_x \quad . \tag{6}$$

They commute with H and are connected by the rule

$$\bar{A} = \pi R_0^2 + (2\pi/eB)L_z \quad . \tag{7}$$

The classical interpretation of these operators is as follows: Consider the XY projection of the orbit of a classical particle governed by the Hamiltonian of Eq. (2), the spin term disregarded. All the above quantities are constants of the motion. The projection is a circle with center at (x_0, y_0) and with area $\bar{A}$. If $L_z = 0$ the circle passes through the origin, if $L_z/eB > 0$ the origin is inside the circle, if $L_z/eB < 0$ it is outside.

The Hamiltonian has an especially simple form in terms of the area operator

$$H = (e^2B^2/2\pi)\bar{A} + \tfrac{1}{2}p_z^2 + V(z) + \tfrac{1}{4}geB\,\sigma_z \quad . \tag{8}$$

The operators H, R_0^2, L_z, and σ_z all commute with each other so we can consider simultaneous eigenfunctions of all of them. Let

$$H\psi = E\psi \quad , \tag{9a}$$

$$R_0^2\psi = [(2n+1)/e|B|]\psi \quad , \tag{9b}$$

$$L_z\psi = \bar{m}(B/|B|)\psi \quad , \tag{9c}$$

$$\sigma_z\psi = \pm\psi \quad . \tag{9d}$$

By introducing cylindrical coordinates (r, ϕ, z) in Eqs. (9b) and (9c), one establishes the ranges of the quantum numbers

$$n = 0, 1, 2, \ldots, \tag{10a}$$

$$\bar{m} = -n, -n+1, -n+2, \ldots, \tag{10b}$$

and finds that the r, ϕ dependence of the wave function is of the form

$$\psi \sim \rho^{\bar{m}/2} e^{-\rho/2} L_n^{(\bar{m})}(\rho) e^{i\bar{m}\phi} \quad , \tag{11}$$

where $\rho = \frac{1}{2}e|B|r^2$ and $L_n^{(\bar{m})}$ is the associated Laguerre polynomial in the notation of Magnus, Oberhettinger, and Soni.[9] All that remains is to get the z dependence and for it Eqs. (7), (8), and (9a) lead to

$$\frac{\partial^2\psi}{\partial z^2} + 2[E - V(z) - e|B|(n + \bar{m} + \tfrac{1}{2}) \mp \tfrac{1}{4}geB]\psi = 0 \quad , \tag{12}$$

where the upper (lower) sign is for spin up (down).

IV. BARRIER PENETRATION

The standard WKB result, connecting a wave incident from the left to a wave transmitted to the right (as in Fig. 1) is[10]

$$\frac{1}{\sqrt{p}}\exp\left(-i\int_z^a p(z')\,dz'\right) \to \frac{1}{\sqrt{p}}\exp\left(-\int_a^b |p(z')|\,dz'\right) \times \exp\left(\int_b^z p(z')\,dz'\right) \quad . \tag{13}$$

In this application p is given by

$$p(z) = \{2[E - V(z) - e|B|(n + \bar{m} + \tfrac{1}{2}) \mp \tfrac{1}{4}geB]\}^{1/2} \quad , \tag{14}$$

the positive root to be taken in the classically allowed regions. Here a and b are the left and right turning points, such that $p(a) = p(b) = 0$. There is also a reflected wave on the left-hand side which is disregarded in Eq. (13).

An expansion for small values of $\mp\frac{1}{4}geB$ will be made in order to isolate the spin effects in the problem. One finds, for example, to first order that

$$\int_b^z p\,dz' = \int_{\bar{b}}^z \bar{p}\,dz' \mp \tfrac{1}{4}geB\int_{\bar{b}}^z \frac{dz'}{\bar{p}} \quad , \tag{15}$$

where $\bar{p}$ is defined by

$$\bar{p}(z) = \{2[E - V(z) - e|B|(n + \bar{m} + \tfrac{1}{2})]\}^{1/2} \quad (16)$$

and $\bar{b}$ is the turning point for $\bar{p}$, such that $\bar{p}(\bar{b}) = 0$. Although p, a, b are different for different spin orientations and might be given a $\pm$ subscript, $\bar{p}$, $\bar{a}$, $\bar{b}$ are independent of spin eigenvalue. The above expansion is justified because, in the present units and for a field of 10^4 G, $\frac{1}{4}geB$ is about 10^{-10}, whereas $E - V(z)$, corresponding to an energy of a few eV, is about 10^{-5}. This kind of expansion of $p(z)$ itself would not be valid near the turning points but Eq. (15) applies well as long as z is far from the turning points since then the expansion is governed by the ratio of $\frac{1}{4}geB$ to a representative value of $\bar{p}^2$ far from the turning points. With this type of expansion made for all the integrals Eq. (13) becomes

$$\frac{1}{\sqrt{\bar{p}}}\exp\left[\int_z^{\bar{a}}\bar{p}\,dz' \pm i\tfrac{1}{4}geB\int_z^{\bar{a}}\frac{dz'}{\bar{p}}\right] \rightarrow \frac{1}{\sqrt{\bar{p}}}\exp\left[\int_{\bar{a}}^{\bar{b}}|\bar{p}|\,dz' \mp \tfrac{1}{4}geB\int_{\bar{a}}^{\bar{b}}\frac{dz'}{|\bar{p}|}\right] \times\exp\left[i\int_{\bar{b}}^{z}\bar{p}\,dz' \mp i\tfrac{1}{4}geB\int_{\bar{b}}^{z}\frac{dz'}{\bar{p}}\right] . \quad (17)$$

The difference between p and $\bar{p}$ is disregarded in the $p^{-1/2}$ factor.

This result holds for spin-up and spin-down states, $\binom{1}{0}$ and $\binom{0}{1}$, say. A state of arbitrary polarization but definite energy E and quantum numbers n, $\bar{m}$ can be formed by taking a linear combination of the spin-up and -down results with coefficients α and β. The connection for such a state is evidently

$$\frac{1}{\sqrt{\bar{p}}}\exp\left[-i\int_z^{\bar{a}}p\,dz'\right]\begin{bmatrix}\alpha\exp\left[i\tfrac{1}{4}geB\int_z^{\bar{a}}\frac{dz'}{\bar{p}}\right]\\ \beta\exp\left[-i\tfrac{1}{4}geB\int_z^{\bar{a}}\frac{dz'}{\bar{p}}\right]\end{bmatrix}$$

$$\longrightarrow \frac{1}{\sqrt{\bar{p}}}\exp\left[-\int_{\bar{a}}^{\bar{b}}|\bar{p}|\,dz'\right]\exp\left[i\int_{\bar{b}}^{z}\bar{p}\,dz'\right]\begin{bmatrix}\alpha\exp\left[-\tfrac{1}{4}geB\int_{\bar{a}}^{\bar{b}}\frac{dz'}{|\bar{p}|}\right]\exp\left[-i\tfrac{1}{4}geB\int_{\bar{b}}^{z}\frac{dz'}{\bar{p}}\right]\\ \beta\exp\left[\tfrac{1}{4}geB\int_{\bar{a}}^{\bar{b}}\frac{dz'}{|\bar{p}|}\right]\exp\left[i\tfrac{1}{4}geB\int_{\bar{b}}^{z}\frac{dz'}{\bar{p}}\right]\end{bmatrix} \quad (18)$$

For the complete wave function one must also include as overall factors, e^{-iEt} and the function of r and ϕ given in Eq. (11).

V. CONNECTION BETWEEN POLARIZATIONS

As is well known, any two-component state

$$\psi = \begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix} \quad (19)$$

is polarized in a specific direction $\hat{s}$ where the spherical polar angles (θ, ϕ) of the unit vector $\hat{s}$ are given by

$$\tan\tfrac{1}{2}\theta e^{i\phi} = \psi_2/\psi_1 \ . \quad (20)$$

The state is polarized in the sense that

$$\hat{s}\cdot\vec{\sigma}\psi = \psi \ . \quad (21)$$

From the ratio of the components in Eq. (18) one can find the direction of polarization on the two sides of the barrier.

As a convenient notation, let (θ_i, ϕ_i) and (θ_t, ϕ_t) be the polarization directions of the incident and transmitted beams and let

$$\beta/\alpha = \tan\tfrac{1}{2}\theta_0 e^{i\phi_0} \ . \quad (22)$$

The results for the polarization are

$$\theta_i = \theta_0 \ , \quad (23a)$$

$$\phi_i = \phi_0 - \tfrac{1}{2}geB\int_z^{\bar{a}}\frac{dz'}{\bar{p}} \ , \quad (23b)$$

$$\tan\tfrac{1}{2}\theta_t = \tan\tfrac{1}{2}\theta_0\exp\left[\tfrac{1}{2}geB\int_{\bar{a}}^{\bar{b}}\frac{dz'}{|\bar{p}|}\right] \ , \quad (24a)$$

$$\phi_t = \phi_0 + \tfrac{1}{2}geB\int_{\bar{b}}^{z}\frac{dz'}{\bar{p}} \ . \quad (24b)$$

Interpretation of these results is as follows: As the electron moves in the positive z direction in an allowed region, the polarization keeps a constant angle θ with the magnetic field and precesses in the right-hand sense about the field with phase angle ϕ given by

$\frac{1}{2}geB\int dz'/\bar{p}$. In the transition through the barrier the phase angle does not change, $\phi_t(\bar{a})=\phi_t(\bar{b})$, but the angle with the field changes according to Eq. (24a).

VI. DISCUSSION

The precession of the polarization in a classically allowed region coincides with the precession of a classical electrically charged magnetic dipole. For such a system the internal angular momentum varies according to

$$\frac{d\vec{\sigma}}{dt}=-\frac{1}{2}ge\,\vec{\sigma}\times\vec{B}. \tag{25}$$

This means that $\vec{\sigma}$ keeps a constant angle θ with the magnetic field and precesses in the right-hand sense about $\vec{B}$ with phase angle

$$\phi=\frac{1}{2}geBt\ . \tag{26}$$

The position of the dipole is determined by the equations

$$\ddot{x}=-e\dot{y}B\ , \tag{27a}$$

$$\ddot{y}=e\dot{x}B\ , \tag{27b}$$

$$\ddot{z}=-\frac{dV}{dz}\ . \tag{27c}$$

First integrals of the system are

$$\dot{x}=-eB(y-y_0)\ , \tag{28a}$$

$$\dot{y}=eB(x-x_0)\ , \tag{28b}$$

$$\frac{1}{2}(\dot{x}^2+\dot{y}^2+\dot{z}^2)+V=E\ , \tag{29}$$

where x_0, y_0, E are the integration constants. Evidently $\dot{x}^2+\dot{y}^2$ is also an integral and

$$\dot{x}^2+\dot{y}^2=e^2B^2[(x-x_0)^2+(y-y_0)^2]$$
$$=e^2B^2\bar{A}/\pi\ , \tag{30}$$

where $\bar{A}$ is the area of the XY projection of the orbit. Equations (29) and (30) combine to give

$$\dot{z}^2=\bar{p}^2\ , \tag{31}$$

where $\bar{p}(z)$ is defined as in Eq. (16) except with $\bar{A}$ in place of the eigenvalue $(2\pi/e|B|)(n+\bar{m}+\frac{1}{2})$. The time is therefore given by $\int dz/\bar{p}$ and the phase angle by

$$\phi=\frac{1}{2}geB\int\frac{dz}{\bar{p}} \tag{32}$$

in agreement with the quantum-mechanical result.

An estimate of the importance of the discontinuity in θ can be made by considering the triangular barrier

$$V(z)=\begin{cases}-V_0 & \text{for } z<0\ ,\\ -e\epsilon z & \text{for } z>0\ .\end{cases} \tag{33}$$

Here ϵ is the size of the electric field applied outside the metal surface. The integral is found immediately to be

$$\int_{\bar{a}}^{\bar{b}}\frac{dz'}{|\bar{p}|}=\frac{(2\Phi)^{1/2}}{e\epsilon}\ , \tag{34}$$

where $\Phi=-E$ and the B term inside $\bar{p}$ is disregarded. The exponent in Eq. (24a) amounts to $(B/\epsilon)(2\Phi)^{1/2}$. Typically in a field emission experiment B, ϵ, and Φ correspond to 10^4 G, 10^7 V/cm, and 5 eV, in which case the exponent is about 10^{-3}. The formula

$$\theta_t=\theta_i+\frac{1}{2}geB\sin\theta_i\int_{\bar{a}}^{\bar{b}}\frac{dz'}{|\bar{p}|} \tag{35}$$

is the first-order approximation to Eq. (24a) when the exponent is small.

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[10]See, for example, E. Merzbacher, *Quantum Mechanics* (Wiley, New York, 1961), pp.121 and 122. Our equation (13) corresponds to his equations (7.29) and (7.30) with $G=0$ and $(2\theta)^{-1}$ neglected compared to 2θ.