A quantum mechanical description of particle spin rotation in channeling

A. Ya. Silenko

Nuclear Problems Research Institute at Belorussian State University, 220080 Minsk, Republic of Belorussia
(Submitted 7 October 1994; resubmitted 19 December 1994)
Zh. Éksp. Teor. Fiz. **107**, 1240–1246 (April 1995)

Spin rotation of spin-$\frac{1}{2}$ particles involved in planar channeling in straight and bent crystals is described in a consistent quantum mechanical manner. This is done by solving the Dirac equation in the Foldy–Wouthuysen representation, constructing an operator equation of motion for the spin, and calculating the average value of the spin precession frequency. For the case of channeling in bent crystals agreement is observed between the classical and quantum mechanical expressions, provided that the field of the planes is approximated by a harmonic potential. The effect of spin rotation in straight crystals is also examined. © *1995 American Institute of Physics.*

1. INTRODUCTION

This paper is devoted to a quantum mechanical description of spin rotation of spin-$\frac{1}{2}$ particles in planar channeling in crystals. Baryshevskiĭ[1,2] was the first to point to the existence of spin rotation in particles being channeled in bent crystals. The theory of this phenomenon was developed by Lyuboshits[3] and Baryshevskiĭ and Grubich.[4] The existence of spin rotation in particles in straight crystals was predicted in Ref. 4. All these studies[1–4] used a semiclassical approach that employed a classical model of spin; this approach makes it possible to distinguish between the Dirac and anomalous magnetic moments. Using this method, Good,[5] Solomon,[6] and Nyborg[7] (see also Ref. 8) arrived at equations of motion for the spin in an inhomogeneous electromagnetic field that contained terms depending on the variation of the field. This fact distinguishes the equations obtained in Refs. 5–7 from the Bargmann–Michel–Telegdi (BMT) equation,[9] also derived by a semiclassical approach for the case of a homogeneous field.

A consistent quantum mechanical derivation of the equation of motion of the spin was carried out in Refs. 10–12. Ternov *et al.*[10,11] obtained an equation of motion for the spin in a magnetic field that completely corresponded to the BMT equation and contained no terms dependent on the field inhomogeneity. There were also no additional terms in a similar equation derived by Cherkas[12] for the more general case of the presence of both magnetic and electric fields. This fact is very important, because no assumptions about the homogeneity of the field were made in Refs. 10–12. This implies that a meaningful calculation of spin rotation in an external field must be done consistently, in a quantum mechanical manner. The semiclassical and quantum mechanical equations of motion for the spin differ because the classical description of spin motion does not completely correspond to the quantum mechanical (different gyromagnetic ratios for the Dirac magnetic moment and relativistic invariance of the anomalous magnetic moment in QED in contrast to the classical electrodynamics).

2. THE GENERAL THEORY

In contrast to Refs. 10–12, to derive the quantum mechanical equation of motion for the spin in a constant (and, generally, inhomogeneous) electric field we use not the Dirac representation but the Foldy–Wouthuysen (FW) representation, in which the polarization operator has the simpler form $\mathbf{\Pi}=\beta\mathbf{\Sigma}$ (Ref. 11) and there is no need to separate its even part. These matrices are of rank 4 and are specified by the following formulas:

$$\beta=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\quad \mathbf{\Sigma}=\begin{pmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{pmatrix},\quad \mathbf{\Pi}=\begin{pmatrix}\boldsymbol{\sigma} & 0\\ 0 & -\boldsymbol{\sigma}\end{pmatrix},$$

where $\boldsymbol{\sigma}$ are the Pauli matrices, and 0 and ± 1 stand for the respective 2-by-2 matrices. We use the relativistic system of units: $\hbar=c=1$. The Dirac equation for nonrelativistic particles in an electrostatic field in the FW representation has the form

$$H_{\mathrm{FW}}\Psi=\left\{\beta\left(m+\frac{\mathbf{p}^2}{2m}-\frac{\mathbf{p}^4}{8m^3}\right)+e\phi+\frac{1}{4m}(\mu_0+2\mu')\times(\Delta\phi-2\boldsymbol{\sigma}[\mathbf{Ep}])\right\}\Psi, \tag{1}$$

where $\mathbf{p}\equiv -i\nabla$ is the momentum operator, ϕ is the scalar potential of the crystalline field, $\mathbf{E}=-\nabla\phi$, $\mu_0=e/2m$ and μ' are the Dirac and anomalous magnetic moments, and m is the rest mass. In the weak-field approximation when the interaction energy $|W_{\mathrm{int}}|$ is much smaller than m, Suttorp and deGroot[13,14] obtained the relativistic Dirac equation in the FW representation for arbitrary particle energies, without allowing for derivatives of field strength. In the absence of a magnetic field, the equation obtained in Refs. 13 and 14 has the form

$$H_{\mathrm{FW}}\Psi=\left\{\beta\varepsilon'+e\phi-\frac{1}{\varepsilon'}\left(\frac{\mu_0 m}{\varepsilon'+m}+\mu'\right)(\boldsymbol{\sigma}[\mathbf{Ep}])\right\}\Psi, \tag{2}$$

where $\varepsilon'=\sqrt{m^2+\mathbf{p}^2}$. Since in this equation the spinors ψ' and ψ'' entering into the bispinor $\Psi=\binom{\psi'}{\psi''}$ are separated, the Hamiltonian H_{FW} characterizes the FW representation, and a complete quantum mechanical description needs only one spinor. Equation (2), in contrast to Eq. (1), is relativistic. However, in contrast to Eq. (1), in deriving Eq. (2) we did not allow for derivatives of $\mathbf{E}$ (in our case a term propor-

 1063-7761/95/040690-04$10.00

tional to $\Delta\phi = -\nabla\mathbf{E}$), so Eq. (2) can be used only when the absence of terms with derivatives of $\mathbf{E}$ has no effect on the results. The field of the planes is characterized by an even potential: $\phi(x) = \phi(-x)$. In this case the absence in Eq. (2) of a small term even in x and proportional to $\Delta\phi$ has no effect on the results of calculations. We assume that the crystal is bent in such a way that the bending plane is perpendicular to the crystallographic planes, and we denote the radius of curvature by R. We direct the x axis perpendicular to the system of planes in the direction of the bend and the y axis perpendicular to the x axis in the bending plane. The motion of a particle in a bent crystal is equivalent to its motion in a straight crystal, but the particle has an additional potential energy

$$W = -\frac{p_y v_y x}{R} = -\frac{\varepsilon'^2 - m^2}{\varepsilon' R} x, \tag{3}$$

where v is the particle velocity. Stationary states satisfy $H_{\mathrm{FW}}\Psi = \varepsilon\Psi$ ($\varepsilon = \mathrm{const}$). While being channeled, the particles move at small angles to the crystallographic planes, and the total particle energy ε approximates the kinetic energy:

$$\varepsilon \cong \varepsilon' = \sqrt{m^2 + \mathbf{p}^2}.$$

We use Eq. (2) only for the first spinor, ψ', and write it with allowance for W:

$$H'_{\mathrm{FW}}\psi' = \left\{ \varepsilon' + e\phi - \frac{1}{\varepsilon'}\left(\frac{\mu_0 m}{\varepsilon' + m} + \mu'\right)(\boldsymbol{\sigma}[\mathbf{Ep}]) - \frac{\varepsilon'^2 - m^2}{\varepsilon' R} x \right\} \psi'. \tag{4}$$

When only the wave function ψ' is used, the polarization operator of the particle is $\boldsymbol{\sigma}$, and the spin equation of motion has the form (here $[\ldots,\ldots]_-$ stands for a commutator)

$$\frac{d\boldsymbol{\sigma}}{dt} = i[H'_{\mathrm{FW}}, \boldsymbol{\sigma}]_- . \tag{5}$$

The operator of the spin rotation frequency, $\boldsymbol{\omega}$, is determined by the expression

$$\frac{d\boldsymbol{\sigma}}{dt} = \boldsymbol{\omega}\boldsymbol{\sigma}. \tag{6}$$

In accordance with Eqs. (4) and (5) we have

$$\frac{d\boldsymbol{\sigma}}{dt} = \frac{2}{\varepsilon'}\left(\frac{\mu_0 m}{\varepsilon' + m} + \mu'\right)[\boldsymbol{\sigma}[\mathbf{Ep}]] \cong \frac{2}{\varepsilon}\left(\frac{\mu_0 m}{\varepsilon + m} + \mu'\right) \times [\boldsymbol{\sigma}[\mathbf{Ep}]]. \tag{7}$$

The quantum mechanical equation of motion (7) of the spin completely agrees with the BMT equation and contains no terms dependent on field gradients. Thus, as noted in Ref. 12, the conclusion drawn by the classical theory that the spin equation of motion depends on the extent to which the field is inhomogeneous is not supported by the quantum theory. For a particle in a magnetic field, as noted above, this follows from the results obtained in Refs. 10 and 11. If in the classical approach we ignore the inhomogeneity of the field (the BMT equation), the classical and quantum spin equations of motion coincide.

The momentum components in the directions parallel to the crystallographic planes are constants of motion, and the respective operators commute with H'_{FW}. Multiplying both parts of Eq. (4) by the operator ε' and replacing ε' by ε in the small terms, for stationary states we transform this equation to the equivalent form

$$\varepsilon^2\psi' = \left\{ m^2 + \mathbf{p}^2 + 2\varepsilon e\phi - 2\left(\frac{\mu_0 m}{\varepsilon + m} + \mu'\right)(\boldsymbol{\sigma}[\mathbf{Ep}]) - \frac{2(\varepsilon^2 - m^2)}{R} x \right\} \psi'. \tag{8}$$

A relativistic equation that, in contrast to Eq. (8), allows for derivatives of the field strength of all orders is given in Ref. 15. If we add the potential energy (3) to the equation obtained in Ref. 15, the equation becomes

$$\varepsilon^2\psi' = \left\{ m^2 + \mathbf{p}^2 + 2\varepsilon e\phi + \left(\frac{\mu_0 m}{\varepsilon + m} + \mu'\right)\left[\Delta\phi - 2(\boldsymbol{\sigma}[\mathbf{Ep}]) - \frac{2(\varepsilon^2 - m^2)}{R} x\right] \right\} \psi'.$$

Separating the variables in Eq. (8), we write the wave function in the form

$$\psi' = \chi(x)\zeta \exp\{-i\varepsilon t + ip_y y\}, \quad p_y = \mathrm{const},$$

where ζ is the spin function. Since $p_y \cong \sqrt{\varepsilon^2 - m^2}$, the term describing spin–orbit coupling can be transformed as follows:

$$(\boldsymbol{\sigma}[\mathbf{Ep}])\zeta = -\sigma_z\sqrt{\varepsilon^2 - m^2}\frac{d\phi(x)}{dx}\zeta = -\lambda\sqrt{\varepsilon^2 - m^2}\frac{d\phi(x)}{dx}\zeta, \quad \lambda = \pm 1. \tag{9}$$

Since $\varepsilon^2 - m^2 - p_y^2 = \mathrm{const}$ and $p_z = 0$, by taking into account Eq. (9) and introducing the notation $T = (\varepsilon^2 - m^2 - p_y^2)/2\varepsilon$, we arrive at the following equation for the transverse particle motion:

$$T\chi(x) = \left\{ -\frac{1}{2\varepsilon}\frac{d^2}{dx^2} + e\phi(x) + \frac{\lambda}{\varepsilon}\left(\frac{\mu_0 m}{\varepsilon + m} + \mu'\right)\sqrt{\varepsilon^2 - m^2}\frac{d\phi(x)}{dx} - \frac{\varepsilon^2 - m^2}{\varepsilon R} x \right\} \chi(x). \tag{10}$$

Equation (10) is valid for any potential $\phi(x)$ of the planes. It contains no term proportional to $\Delta\phi$, which, being small and even in x, plays no role in further discussions. The projection of the particle spin $\mathbf{s} = \boldsymbol{\sigma}/2$ on the z axis is quantized and is equal to $\lambda/2$. For negatively charged particles, $x = 0$ corresponds to planes, and for positively charged particles, to the midpoint of the distance between the planes. If the crystal is fairly thin, the solutions of the Dirac equation

in the FW representation for a particle inside the crystal (Eq. (10)) and for a particle outside the crystal must be matched.

3. CALCULATION OF PARTICLE SPIN ROTATION IN CHANNELING

The consistent quantum mechanical solution of the problem of particle spin rotation in planar channeling done here has a number of important features. First, the semiclassical spin rotation equation is replaced by the rigorous quantum mechanical equation (7) for the polarization operator $\boldsymbol{\sigma}$. Second, the classical equation of motion is replaced by the quantum mechanical equation (10) for the stationary states of a particle in the field of the planes. Third, instead of the laborious process of integrating $d\mathbf{s}/dt$ over trajectories, we find the average of the operator $\boldsymbol{\omega}$ of the spin precession frequency in given stationary states, $\langle\boldsymbol{\omega}\rangle=\int\psi'^{\dagger}\boldsymbol{\omega}\psi'\,dV$. Here $\langle\omega_i\rangle$ is defined as the average of the spin rotation angle Φ_i of the particle about the ith axis ($i=x,y,z$) per unit time: $\langle\omega_i\rangle=d\Phi_i/dt$. For the case at hand the operators ω_i have the form

$$\omega_x=\omega_y=0,\quad \omega_z=\frac{2}{\varepsilon}\left(\frac{\mu_0 m}{\varepsilon+m}+\mu'\right)\sqrt{\varepsilon^2-m^2}\,\frac{d\phi(x)}{dx}. \tag{11}$$

The last two terms on the right-hand side of Eq. (10) change sign when x is replaced by $-x$, so that the particle trajectory is shifted in relation to the $x=0$ plane. For straight crystals the direction in which the trajectory is displaced is determined by the sign of the projection of the spin on the z axis. Since the operator ω_z is an odd function of x, the displacement of the trajectory leads to a finite average value of this operator. This leads to rotation of the spin of the channeled particles about the z axis in both bent and straight crystals.

The possibility of particle spin rotation in channeling in a straight crystal was predicted in Ref. 4. There, however, the effect was explained by the dependence of the spin equation of motion on the inhomogeneity of the intracrystalline field. Since such dependence exists only in the semiclassical approach and is absent in rigorous quantum theory, the mechanism of spin rotation in a straight crystal described in Ref. 4 is incorrect. The real mechanism of this phenomenon lies in the fact that $(\mathbf{Ep})_z=E_x p_y$ is odd. As a result the quasimagnetic field $(\mathbf{Ep})/\varepsilon$ changes sign under the $x\to -x$ transformation. This mechanism for spin rotation in a straight crystal exists in the classical approach, too.

Let us now obtain the exact expression for $\langle\omega_z\rangle$ in the ordinary approximation of the field of planes by the harmonic potential $\phi(x)=ax^2/2$. Such an approximation is quite admissible for positively charged particles. Equation (10) then assumes the form

$$\left(-\frac{1}{2\varepsilon}\frac{d^2}{dX^2}+\tfrac{1}{2}eaX^2\right)\kappa(x)=(T+\tfrac{1}{2}eax_0^2)\kappa(x), \tag{12}$$

where

$$X=x-x_0,\quad \kappa(X)=\chi(X+x_0),$$

$$x_0=\frac{1}{e\varepsilon}\left[\frac{\varepsilon^2-m^2}{aR}-\lambda\left(\frac{\mu_0 m}{\varepsilon+m}+\mu'\right)\sqrt{\varepsilon^2-m^2}\right], \tag{13}$$

with x_0 the size of the displacement of the particle's path in relation to the channel's center $x=0$. It is known that Eq. (12) can be solved exactly. Since we have $\langle X\rangle=0$, in accordance with Eqs. (11) and (12) the spin precession frequency is the same for all states with the same ε and λ and is given by the expression

$$\langle\omega_z\rangle=\frac{2a}{\varepsilon}\left(\frac{\mu_0 m}{\varepsilon+m}+\mu'\right)\sqrt{\varepsilon^2-m^2}\,x_0. \tag{14}$$

Using the standard notation $\gamma=\varepsilon/m$ and $g=4m(\mu_0+\mu')/e$, we can write Eq. (14) as

$$\langle\omega_z\rangle=a\frac{\sqrt{\gamma^2-1}}{\gamma^2}\left(\frac{1}{\gamma+1}+\frac{g-2}{2}\right)\times\left[\frac{\gamma^2-1}{aR}-\lambda\frac{e}{2m^2}\left(\frac{1}{\gamma+1}+\frac{g-2}{2}\right)\sqrt{\gamma^2-1}\right]. \tag{15}$$

The theory of particle channeling in bent crystals usually gives the relationship between the average spin rotation angle Φ and the average momentum ration angle $\theta=y/R$:

$$\Phi=\frac{R\langle\omega_z\rangle\theta}{v_y}=\frac{\gamma}{\sqrt{\gamma^2-1}}R\langle\omega_z\rangle\theta.$$

If we ignore the second term in Eq. (15), we get

$$\Phi=\left(\frac{\gamma-1}{\gamma}+\frac{g-2}{2}\frac{\gamma^2-1}{\gamma}\right)\theta. \tag{16}$$

This formula coincides with the classical formula obtained by Lyuboshits.[3] Note that in real crystals multiple scattering by nuclei leads to a situation in which different particles in the beam are characterized by different spin rotation angles, and the beam becomes depolarized.[16] The main properties of the particle distribution over the spin rotation angles were studied by Krivosheev.[17]

4. DISCUSSION AND CONCLUSION

The consistent quantum mechanical description of the interaction of spin-$\frac{1}{2}$ particles with a crystal field makes it possible to calculate the angle of spin rotation of particles channeled in straight and bent crystals. The quantum mechanical formula (16), which coincides with the classical formula derived in Ref. 3, is valid only for a harmonic potential. In the presence of strong anharmonicity, which is the case, e.g., in channeling of electrons, deviations from this formula are possible. Calculation of the spin rotation angle for this case can be carried out via Eqs. (10) and (11) and is of considerable interest.

Equation (13) implies that the particle path is displaced in relation to the channel center not only in bent crystals but in straight crystals as well. However, in the latter case this displacement is very small. For $\varepsilon\gg m$ the absolute value of the displacement, $|x_0|$, is approximately $|\mu'/e|$. For both positrons and protons, $|\mu'/e|\sim 10^{-14}$ cm.

Analysis of Eq. (15) shows that the effect of spin rotation for particles channeled in straight crystals ($R\to\infty$) is extremely weak. For instance, for $\gamma\gg 1$ the distance over which the spin rotates through an angle of 2π rad is

$$\Lambda=\frac{2\pi}{|\langle\omega_z\rangle|}=\frac{16\pi m^2}{(g-2)^2 e\alpha}\,. \tag{17}$$

For both positrons and protons this distance amounts to about 10^3 m. At present observing such a weak effect is impossible.

The author would like to express his gratitude to A. O. Grubich, V. V. Tikhomirov, and S. L. Cherkas for their remarks and a discussion of the results.

[1] V. G. Baryshevskiĭ, Pis'ma Zh. Tekh. Fiz. **5**, 182 (1979) [Sov. Phys. Tech. Phys. Lett. **5**, 73 (1979)].
[2] V. G. Baryshevskiĭ, in *Proceedings of the 15th Winter Workshop of the Leningrad Nuclear Physics Institute* (Leningrad, 1979), Leningrad Nucl. Phys. Inst., Leningrad (1980), p. 199 [in Russian].
[3] V. L. Lyuboshits, Yad. Fiz. **31**, 986 (1980) [Sov. J. Nucl. Phys. **31**, 509 (1980)].
[4] V. G. Baryshevskiĭ and A. O. Grubich, Yad. Fiz. **37**, 1093 (1983) [Sov. J. Nucl. Phys. **37**, 648 (1983)].
[5] R. H. Good, Phys. Rev. **125**, 2112 (1962).
[6] A. I. Solomon, Nuovo Cimento **26**, 1320 (1962).
[7] P. Nyborg, Nuovo Cimento **31**, 1209 (1964).
[8] I. M. Ternov and V. A. Bordovitsyn, Usp. Fiz. Nauk **132**, 345 (1980) [Sov. Phys. Usp. **23**, 679 (1980)].
[9] V. Bargmann, L. Michel, and V. L. Telegdi, Phys. Rev. Lett. **2**, 435 (1959).
[10] I. M. Ternov, V. R. Khalilov, and O. S. Pavlova, Izv. Vyssh. Uchebn. Zaved. Fiz. No. 12, 89 (1978).
[11] I. M. Ternov, V. R. Khalilov, and V. N. Rodionov, *Interaction of Charged Particles with an External Electromagnetic Field*, Moscow Univ. Press, Moscow (1982) p. 40 [in Russian].
[12] S. L. Cherkas, Izv. Akad. Nauk Belarusi, Ser. Fiz.-Mat. Nauk, No. 2, 7 (1994).
[13] L. G. Suttorp and S. R. deGroot, Nuovo Cimento A **65**, 245 (1970).
[14] S. R. deGroot and L. G. Suttorp, *Foundations of Electrodynamics*, North-Holland, Amsterdam (1969).
[15] A. Ya. Silenko, in *Abstracts of Reports Presented at the 24th International Conference on Interaction of Charged Particles with Crystals*, Moscow Univ. Press, Moscow (1994), p. 32 [in Russian].
[16] V. G. Baryshevsky (Baryshevskiĭ), Nucl. Instrum. Methods B **44**, 266 (1990).
[17] O. E. Krivosheev, in *Proc. RREPS-93* (Tomsk, 1993), Nucl. Phys. Inst., Tomsk (1993), p. 277.

Translated by Eugene Yankovsky