

# The role of boundary conditions in the Aharonov–Bohm effect for particles with spin

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The question of the role of boundary conditions in quantum mechanics is considered for the example of spin-1/2 particles possessing a magnetic moment and situated in an Aharonov–Bohm field. The formalism of self-adjoint extensions of operators used in the theory of short-range potentials is analyzed, and the limits of its applicability in the case of the action of an external magnetic field are discussed. The physical consequences of the existence of an anomalous magnetic moment of the particles for this model are investigated.

## 1. INTRODUCTION

The Aharonov–Bohm effect,<sup>1</sup> which was once widely discussed in connection with the role of electromagnetic potentials in quantum mechanics, has now acquired new importance because of interesting analogies—in particular, with the behavior of particles in the vicinity of a cosmic string,<sup>2</sup> and, in general, with the distinctive features of quantum theory for spaces having conic singularities.<sup>3</sup> In the original Aharonov–Bohm model the effect arises when quantum spinless charged particles are scattered by an infinitely thin, infinitely long solenoid containing a finite magnetic flux  $\Phi$ . Since there is no magnetic field outside such a “string,” there are no forces in the classical sense acting on the particle either. We note that, besides the situations listed above, an interaction of a similar “topological” character is also encountered when conduction electrons are scattered by line defects in the crystal lattices of solids—dislocations and disclinations.<sup>4</sup> There are interesting applications of the Aharonov–Bohm effect in the theory of anyons, which is currently being developed with the aim of explaining the phenomenon of high-temperature superconductivity.<sup>5</sup>

The problem of taking spin into account in effects of this kind turns out to be far from simple, and requires a careful analysis of the boundary conditions of the problem. Otherwise, the danger arises that the dynamical evolution of the particles will be incorrectly described as a consequence of violation of the condition that the Hamiltonian be self-adjoint. Attention was first drawn to this in papers devoted to the behavior of fermions in the vicinity of a cosmic string,<sup>6</sup> and in the study of Aharonov–Bohm scattering for relativistic particles with spin 1/2 and  $g=2$  (Ref. 7). The supersymmetric interaction that arises in this scattering permits a considerable simplification of the analysis of the spectrum of the Dirac Hamiltonian: In particular, it is easy to demonstrate the existence of  $N$  modes with zero energy  $E=0$  (one for each quantum of magnetic flux contained in the solenoid).<sup>8</sup> (Here we assume

$f = \Phi/\Phi_0 = N + \delta$  with  $N = [\Phi/\Phi_0]$ , where  $\Phi_0 = 2\pi\hbar c/e_0$  is the quantum of magnetic flux.)

In this paper we analyze the case  $g \neq 2$ . The existence of an anomalous magnetic moment of the particle violates the supersymmetry of the interaction, and, as we shall show below, causes the zero modes to transform into ordinary bound states and an additional energy level to appear. We shall confine ourselves to the nonrelativistic case. In the analysis of the spectrum of the Pauli Hamiltonian and of the boundary conditions imposed on the wave function of the particle in the region of the field source, one uses the method of self-adjoint extensions of operators that has been developed in the theory of  $\delta$ -potentials or short-range potentials.<sup>9</sup> The necessity of introducing a special harmonic is demonstrated, and the influence of characteristics of the singular behavior of this harmonic in different physical situations for particles outside the source is traced. We also investigate the limit  $R \rightarrow 0$  ( $R$  is the radius of the magnetic-field tube), and, thereby, the possibility of using the model of a magnetic “string” for an adequate description of the scattering of fermions in an Aharonov–Bohm field.

## 2. ANALYSIS OF THE BOUNDARY CONDITIONS AND SPECTRUM

We shall consider a nonrelativistic electron with mass  $M$ , charge  $e = -e_0$ , and magnetic moment  $\mu = g\mu_B S$  [ $(g-2)/2 \equiv a_e > 0$ ] in the vicinity of a magnetic string with an Aharonov–Bohm electromagnetic potential

$$\mathbf{A} = \mathbf{e}_\varphi A_\varphi(\rho), \quad A_\varphi(\rho) = \frac{\Phi}{2\pi} \frac{1}{\rho}, \quad \rho > 0$$

and magnetic field

$$\mathbf{H} = \mathbf{e}_z H_z, \quad H_z = \Phi \delta(x) \delta(y).$$

In this case the Pauli equation

$$\left[ \frac{1}{2m} \left( \mathbf{P} + \frac{e_0}{c} \mathbf{A} \right)^2 - (\boldsymbol{\mu} \mathbf{H}) \right] \Psi(\mathbf{r}) = E \Psi(\mathbf{r})$$

can be represented in the form

$$\left[ -\tilde{\Delta} - \frac{2M}{\hbar^2} \left| \mu \right| \Phi \delta(\rho) \right] \varphi(\rho) = \frac{2M}{\hbar^2} E \varphi(\rho), \quad (1)$$

$$\tilde{\Delta} \equiv \left( \hat{\nabla} + i \frac{e_0}{\hbar c} \mathbf{A} \right)^2,$$

where we choose  $p_z = 0$  and  $s_z = \hbar/2$ . (It is easy to see that in the opposite case, when  $\mathbf{S} \uparrow \uparrow \mathbf{H}$ , there will not be any interesting physical consequences.) We shall attempt to avoid the difficulties caused by the  $\delta$ -potential by introducing the operator

$$\hat{H}_0 \equiv -\tilde{\Delta}, \quad D(\hat{H}_0) = \{ \Psi \psi \in L^2(R^2), \quad \psi(0) = 0 \},$$

which is defined only on wave functions regular at the origin. However, if, using the scalar product in  $L^2(R^2)$

$$(g, \hat{H}_0 f) = (\hat{H}_0^* g, f) \Rightarrow \int dr g^* \hat{H}_0 f = \int dr [\hat{H}_0^* g]^* f,$$

we construct the adjoint  $\hat{H}_0^*$  of the original operator  $\hat{H}_0$ , it is easy to show that

$$\hat{H}_0^* = \hat{H}_0, \quad \text{but } D(\hat{H}_0^*) = \{ \Psi \psi \in L^2(R^2) \},$$

i.e., the domain of definition of  $\hat{H}_0^*$  is wider, and, therefore, the operator  $\hat{H}_0$  is not self-adjoint. Following the method of von Neumann, we shall analyze its defect index. For this it is necessary to find all the eigenfunctions corresponding to the complex eigenvalues of  $\hat{H}_0^*$ :

$$\hat{H}_0^* \Psi(\rho) = z^2 \Psi(\rho), \quad z^2 \in \mathbb{C} \setminus \mathbb{R}. \quad (2)$$

Let  $z^2 = \pm ip^2$ , where  $p^2 > 0$  and has the dimensions of energy. Then, expanding the wave function in Fourier harmonics,

$$\Psi(\rho) = \sum_{m=-\infty}^{\infty} C_m e^{im\varphi} R_m(\rho), \quad (3)$$

where the radial wave function satisfies the equation

$$\frac{d^2}{d\rho^2} R_m(\rho) + \frac{1}{\rho} \frac{d}{d\rho} R_m(\rho) - \left[ \left( \frac{\tilde{m}}{\rho} \right)^2 - z^2 \right] R_m(\rho) = 0,$$

$$\tilde{m} = m + f, \quad f = \Phi / \Phi_0,$$

and using the condition that the wave function be square-integrable, we find that solutions of (2) are possible only for the harmonic  $m = -N$  corresponding to the smallest value of the total angular momentum, and can be expressed in the form

$$\Psi_+(\rho) = H_\delta^{(1)}(e^{i\pi/4} p \rho),$$

$$\Psi_-(\rho) = H_\delta^{(2)}(e^{-i\pi/4} p \rho).$$

In this case the defect indices  $(m, n)$  are equal to  $(1, 1)$ , and it is necessary to introduce a one-parameter family of self-adjoint extensions of the original operator  $\hat{H}_0$  only for the harmonic  $m = -N$ :

$$\hat{h}_{f,0} \rightarrow \hat{h}_{f,\alpha},$$

where

$$\hat{h}_{f,\alpha} = -\frac{d^2}{d\rho^2} - \frac{1}{\rho} \frac{d}{d\rho} + \left( \frac{\delta}{\rho} \right)^2,$$

$$\hat{h}_{f,\alpha} \Psi_\pm(\rho) = \pm ip^2 \Psi_\pm(\rho).$$

Here,  $\Psi(\rho) \in D(\hat{h}_{f,\alpha})$  if

$$\Psi(\rho) = \Psi_0(\rho) + C \left[ H_\delta^{(1)} \left( e^{i\pi/4} \frac{\rho}{a_0} \right) + e^{+i\theta} H_\delta^{(2)} \left( e^{-i\pi/4} \frac{\rho}{a_0} \right) \right],$$

where  $\Psi_0(\rho) \in D(\hat{H}_0)$ ,  $C$  is an arbitrary complex constant quantity,  $\theta$  is the parameter that labels the variants of the self-adjoint extensions,  $a_0$  is a dimensional parameter ( $[a_0] \sim \rho$ ) that cannot yet be determined, and  $H_\nu^{(1,2)}(x)$  are Hankel functions of the first and second kind. Using the well known asymptotic behavior of the Bessel functions at small arguments:

$$J_\nu(x) |_{x \rightarrow 0} \cong \left( \frac{x}{2} \right)^\nu \frac{1}{\Gamma(1+\nu)} [1 + o(x^2)],$$

we can describe the sought general behavior of the wave function in the neighborhood of the origin as

$$\Psi(\rho) |_{\rho \rightarrow 0} \cong A \left( \frac{1}{2} \frac{\rho}{a_0} \right)^{-\delta} + B \left( \frac{1}{2} \frac{\rho}{a_0} \right)^\delta + o \left( \frac{\rho}{a_0} \right)^2, \quad (4)$$

where

$$A = C \frac{-2}{\sin(\pi\delta)} e^{i\theta/2} \frac{\sin(\theta/2 + \pi\delta/4)}{\Gamma(1-\delta)},$$

$$B = C \frac{2}{\sin(\pi\delta)} e^{i\theta/2} \frac{\sin(\theta/2 + 3\pi\delta/4)}{\Gamma(1+\delta)},$$

and, hence it is possible to label the variants of the self-adjoint extensions by one real parameter  $\delta$ :

$$\frac{B}{A} = 2\pi\alpha, \quad -\infty < \alpha < +\infty. \quad (5)$$

We shall analyze the spectrum of the Pauli Hamiltonian (1), but now with the correct boundary conditions (4), (5). All nontrivial consequences pertaining to the possible bound states can be obtained by investigating the structure of the resolvent  $\hat{R}$  constructed only for  $\hat{h}_{f,\alpha}$  ( $m = -N$ ). Let

$$\{ \hat{R}(\rho, k) \equiv [\hat{h}_{f,\alpha} - k^2]^{-1} \} h(\rho) = f(\rho), \quad (6)$$

where  $f(\rho) \in D(\hat{h}_{f,\alpha})$ ,  $k^2 \in \mathbb{C}$ .

It is easy to see that for the radial equation the resolvent is an integral operator with kernel  $G(\rho, \rho', k)$ :

$$\hat{L}_\rho \equiv [\hat{h}_{f,\alpha} - k^2] G(\rho, \rho', k) = \delta(\rho - \rho'). \quad (7)$$

It then follows from (6) that

$$\int_0^\infty G(\rho, \rho', k) h(\rho') d\rho' = f(\rho). \quad (8)$$

If  $\rho \neq \rho'$ , then

$$\hat{L}_\rho G(\rho, \rho', k) = \hat{L}_{\rho'} G(\rho, \rho', k) = 0,$$

and we can construct the Green's function  $G(\rho, \rho', k)$  as a superposition of linearly independent eigensolutions of Eq. (7):

$$G(\rho, \rho', k) = \begin{cases} \chi_k^{(1)}(\rho) \chi_k^{(2)}(\rho'), & \rho > \rho' \\ \chi_k^{(2)}(\rho) \chi_k^{(1)}(\rho'), & \rho < \rho' \end{cases} \quad (9)$$

with the normalization condition

$$\int_{\rho-\Delta}^{\rho+\Delta} d\rho' \hat{L}_\rho G(\rho, \rho', k) = 1. \quad (10)$$

The system of relations (9), (10) permits us to determine  $G(\rho, \rho', k)$  uniquely:

$$G(\rho, \rho', k) = \frac{i\pi k}{2} \begin{cases} J_\delta(k\rho) H_\delta^{(1)}(k\rho'), & \rho < \rho' \\ H_\delta^{(1)}(k\rho) J_\delta(k\rho'), & \rho > \rho', \end{cases}$$

and analysis of the boundary condition for  $f(\rho)$  from (8) gives the value  $\alpha = +\infty$ . Thus, we have constructed the resolvent  $\hat{R}^0(\rho, k)$  for the particular case  $\alpha = +\infty$  (the so-called Friedrich variant of self-adjoint extension). For an arbitrary value of  $d$  the resolvent  $\hat{R}(\rho, k)$  can now be constructed using Krein's method:<sup>10</sup>

$$\hat{R}(\rho, k) = \hat{R}^0(\rho, k) + p(k) \int_0^\infty d\rho' H_\delta^{(1)}(k\rho') (\cdot) H_\delta^{(1)}(k\rho),$$

and, analyzing the boundary condition for  $f(\rho)$  from (8), we obtain

$$p(k) = \frac{-(\pi k/2) \sin(\pi\delta) (ka_0)^\delta}{(ka_0)^\delta e^{-i\pi\delta} + 2\pi\alpha (ka_0)^{-\delta} \Gamma(1+\delta) / \Gamma(1-\delta)}.$$

As is well known, the pole of the resolvent makes it possible to determine the bound state. Then

$$p(k) \rightarrow \infty: \quad 2\pi d = -(\kappa a_0)^{2\delta} \frac{\Gamma(1-\delta)}{\Gamma(1+\delta)},$$

or  $k^2 = -\kappa^2 = 2mE/\hbar^2 < 0$ . Thus, we can normalize our scale  $d$  by setting  $\alpha = 1/\kappa$ , where  $\kappa$  characterizes the energy of the bound state, and say that the boundary condition (4), imposed on the wave function ( $\rho \rightarrow 0$ ) for the value

$$2\pi\alpha = -\frac{\Gamma(1-\delta)}{\Gamma(1+\delta)}, \quad (11)$$

corresponds to a bound state. We note here that this method does not permit us to determine the actual magnitude of the energy level and its relationship to the physical parameters  $|\mu|$  and  $\Phi$ .

### 3. REGULARIZATION: MODEL OF A STRING WITH FINITE RADIUS

We now consider a more physical approach—namely, we shall introduce a model of a string of finite radius  $R$  with the magnetic field distributed within it in such a way that the total magnetic flux is equal to  $\Phi$  as before. For this, in order to single out the model-independent physical results we introduce three different magnetic-field distributions that admit exact solutions:

Model I:  $H(\rho) = \Phi/\pi R^2$  (a uniform magnetic field inside the tube).

Model II:  $H(\rho) = \Phi/2\pi R \rho / \rho\theta(R-\rho)$  ("Coulomb"-type behavior).

Model III:  $H(\rho) = \Phi/2\pi R \delta(\rho-R)$  (a cylindrical  $\delta$ -shell of radius  $R$ ).

We rewrite the Pauli equation in the general form

$$\hat{\mathbf{p}}^2 + \frac{e_0}{Mc} (\mathbf{A}\mathbf{p}) + \frac{e_0^2}{2Mc^2} (\mathbf{A})^2 + \frac{\sigma g \mu_B H(\rho)}{2} \psi_\sigma(\mathbf{r}) = E \psi_\sigma(\mathbf{r}).$$

Here,  $\sigma = \pm 1$  indicates that the spin projection is parallel (antiparallel) to the direction of the magnetic field. After the angular dependence has been factored out, in the same way as was done in (3), the radial equation will have the form ( $p_z = 0$ )

$$\left[ -\frac{1}{\rho} \frac{d}{d\rho} \rho \frac{d}{d\rho} + \frac{[m + f a(\rho)]^2}{\rho^2} + \frac{\sigma g f h(\rho)}{2} \right] \psi_{\sigma, m}(\rho) = \varepsilon \psi_{\sigma, m}, \quad (12)$$

where

$$\mathbf{A} = \mathbf{e}_\varphi \frac{\Phi}{2\pi\rho} a(\rho), \quad h(\rho) = \frac{1}{\rho} \frac{d}{d\rho} a(\rho), \quad \varepsilon = \frac{2ME}{\hbar^2}.$$

For us the case  $m = -N$  is the most interesting. We shall consider first the "outer" solutions, i.e., the region  $\rho > R$ . For  $E < 0$  a bound state, described by the wave function

$$\Psi_{-N} = K_\delta(\sqrt{-\varepsilon}\rho), \quad (13)$$

is possible. The logarithmic derivative of this solution is equal to

$$R_{ext}^{(-N)} = \rho \frac{d}{d\rho} \ln \Psi_{-N}(\rho)_{\rho \rightarrow R+0} = (\sqrt{-\varepsilon}R) \frac{K'_\delta(\sqrt{-\varepsilon}R)}{K_\delta(\sqrt{-\varepsilon}R)}. \quad (14)$$

For states in the continuum  $E > 0$  (scattering states), the radial wave function in the general case has the form

$$\Psi_m(\rho) = J_{|\tilde{m}|}(k\rho) + B_m(k) H_{|\tilde{m}|}^{(1)}(k\rho) \quad (15)$$

and its logarithmic derivative is equal to

$$R_{ext}^{(m)} = (\sqrt{\varepsilon}R) \frac{J'_{|\tilde{m}|}(\sqrt{\varepsilon}R) + B_m(k) H_{|\tilde{m}|}^{(1)'}(\sqrt{\varepsilon}R)}{J_{|\tilde{m}|}(\sqrt{\varepsilon}R) + B_m(k) H_{|\tilde{m}|}^{(1)}(\sqrt{\varepsilon}R)}. \quad (16)$$

The expressions (14)–(16) can be analyzed for different values of  $f$ ,  $E$ , and  $R$ . In particular, the limit  $R \rightarrow 0$  for  $E < 0$  gives

$$R_{ext}^{(-N)} = -\delta + o(\varepsilon R^2). \quad (17)$$

Using the explicit solutions of Eq. (12) for the different distributions of the magnetic field inside the tube, we can find the values of the logarithmic derivatives of the "inner" solutions in the same limit for the bound states ( $E < 0$ ).

Model I:

$$R_1^{(-N)} = -\delta + \frac{2 \pm g}{2} f \Phi_1 + o(\varepsilon R^2),$$

$$\Phi_1 \equiv \frac{{}_1F_1((2 \pm g)/4 + 1; 2 + N; f)}{{}_1F_1((2 \pm g)/4; 1 + N; f)}$$

( ${}_1F_1$  is a confluent hypergeometric function).

Model II:

$$R_2^{(-N)} = -\delta + \frac{2 \pm g}{2} f \Phi_2 + o(\varepsilon R^2),$$

$$\Phi_2 \equiv \frac{{}_1F_1((2 \pm g)/4 + 1; 2 + N; 2f)}{{}_1F_1((2 \pm g)/4; 1 + N; 2f)}.$$

Model III:

$$R_3^{(-N)} = -\delta + \frac{2 \pm g}{2} f \Phi_3 + o(\varepsilon R^2),$$

$$\Phi_3 = 1.$$

The magnitude of the energy level for the first two models is determined by the condition for matching at the boundary of the tube:

$$R_{\text{ext}}^{(-N)} = R_i^{(-N)}(\rho = R), \quad i = 1, 2. \quad (18)$$

For model III it is necessary to consider the discontinuity of the first derivative:

$$\frac{d}{d\rho} R_{(-N)}(\rho) \Big|_{R-\varepsilon}^{R+\varepsilon} + \frac{1}{2} g f \frac{1}{R} R_{(-N)}(R) = 0, \quad \varepsilon \rightarrow 0. \quad (19)$$

The solutions (18) and (19) are possible only for  $g > 2$  and  $\sigma = -1$ , i.e., the spin should be antiparallel to the field. The energy level is determined in this case by the transcendental equation

$$\left( \frac{\sqrt{-\varepsilon R}}{2} \right)^{2\delta} = \frac{\Gamma(1+\delta) g - 2 \Phi_i}{\Gamma(1-\delta) 2 \frac{\Phi_i}{2}}, \quad (20)$$

and its magnitude depends on the choice of model. It is easy to show that for this solution the boundary condition (11), predicted by the theory of self-adjoint extensions, is fulfilled. We note that for  $R \rightarrow 0$  the given bound state is preserved only if there is a corresponding "renormalization" of the coupling constant  $a_e$ :

$$a_e \rightarrow (\sqrt{-\varepsilon R})^{2\delta} a_e^{\text{ren}}. \quad (21)$$

This phenomenon is characteristic of the theory of  $\delta$ -potentials, and was first considered by Berezin and Faddeev.<sup>11</sup>

The presence of a bound state also leads to singularities in the scattering of particles with spin. As  $R \rightarrow 0$  and for  $\mathbf{S} \uparrow \mathbf{H}$ , in addition to the ordinary Aharonov-Bohm scattering additional scattering occurs, described by the coefficient  $B_{-N}$  ( $B_m \rightarrow 0$  for  $m \neq -N$ ):

$$B_{-N}(k) = \frac{i \sin(\pi\delta)}{(\kappa/\sqrt{\varepsilon})^{2\delta} - e^{i\pi\delta}}, \quad (22)$$

where  $\kappa$  is the bound-state energy determined by (20). The expression for the scattering cross section in this case has a form analogous to the Breit-Wigner formula.

For a finite value of  $R$  in the case  $g=2$  there exists a level  $E=0$  with degeneracy  $N$ . The outer wave functions in this case have the form

$$R_{\text{ext}}^{(m)}(\rho) = \text{const} \left( \frac{\rho}{R} \right)^{-(N+\delta-|m|)}, \quad 0 < |m| < N-1, \quad (23)$$

and in the limit  $\rho \rightarrow 0$  we should formally discard them because of the requirement of square integrability of the wave functions. Taking the inner structure into account gives the radius  $R$  the meaning of the boundary of existence of the outer solution (23), and eliminates the singularity. This analysis is a particular case of the well known result concerning the number of zero modes in a magnetic field of arbitrary configuration.<sup>8</sup>

For  $g \neq 2$  (to be precise,  $g > 2$ ), the breaking of the supersymmetry lifts the degeneracy, and the additional attraction due to the interaction of the anomalous magnetic moment of the particle and the field of the tube causes the solutions (23) for the zero modes to pass over into wave functions of additional bound states:

$$R_{\text{ext}}^{(m)}(\rho) = K_{N+\delta-|m|} \left( \kappa_m \frac{\rho}{R} \right), \quad 0 < |m| < N-1. \quad (24)$$

A situation analogous to that considered above arises: In the limit  $R \rightarrow 0$ , for formal reasons we must discard these wave functions. Nevertheless, if we take the inner structure into account and make the corresponding "renormalization" of the coupling constant:

$$a_e \rightarrow (\sqrt{-\varepsilon R})^2 a_e^{\text{ren}}, \quad \kappa_m = [a_e f C_m]^{1/2}, \quad (25)$$

it is possible to retain them. We note that the "renormalization" conditions (21) and (25) are incompatible, and, therefore, in the limit  $R \rightarrow 0$  it is possible to consider only either the "quasizero" modes (24) or the "true string" bound state (13).

#### 4. CONCLUSION

We have shown that the method of self-adjoint extensions of operators and the analysis of regularized models give similar results for particles with spin in an Aharonov-Bohm field only for  $N=0$ . Generally speaking, for  $N \neq 0$ , solutions of the Pauli equation arise that are regular in the region  $\rho < R$  but are formally singular outside this region ( $\rho > R$ ) in the limit  $\rho(R) \rightarrow 0$ . We cannot discard them, since they can correspond to real bound states. One way out of this could be a more general mathematical scheme of analysis of the  $\delta$ -potentials than that proposed in Ref. 8 and demonstrated in Sec. 2 of this article.

For real physical situations, when  $a_e$  and  $R$  are small but nonzero (e.g., for the electron,  $a_e = 0.00116$ ), in the sense of the applicability of our analysis [(17), (20), (22)] it is evident that  $1+N$  bound states, corresponding to different energy levels, can exist simultaneously.

Similar conclusions are also valid for real cosmic strings of finite radius with trapped magnetic flux. Generally speaking, it is not correct to attempt to reduce the interaction of such a string with fermions to the choice of some boundary condition for the solution of the corresponding equation describing the motion of the particles in a space with a conic singularity (or to construct a one-parameter family of self-adjoint extensions of the Hamiltonian), since this can lead to the loss of a number of physical effects.

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