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A pragmatic approach to the problem of the self-adjoint extension of Hamilton operators with the Aharonov–Bohm potential

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Abstract. We consider the problem of the self-adjoint extension of Hamilton operators for charged quantum particles in the pure Aharonov–Bohm potential (infinitely thin solenoid). We present a pragmatic approach to the problem based on the orthogonalization of the radial solutions for different quantum numbers. Then we discuss a model of a scalar particle with a magnetic moment which allows us to explain why the self-adjoint extension contains arbitrary parameters and give a physical interpretation.

1. Introduction

The theoretical prediction of the Aharonov-Bohm (AB) effect [1] in 1959 was one of the most intriguing results of quantum theory. Now the AB effect has long been recognized for its crucial role in demonstrating the specific status of electromagnetism in quantum theory. Besides the usual local influence of electric and magnetic fields on charged particles, it manifests non-local quantum effects from electromagnetic fluxes $\Phi = \oint A_i dx_i$ or the corresponding phase factors, $\exp(ie \oint A_i dx_i)$ [15]. By shifting the phases of wavefunctions these gauge-invariant factors influence interference patterns, the energy spectra of quantum particles, and cause other quantum phenomena (for a detailed exposition of theoretical and experimental attempts to investigate the AB effect see [12, 13]). One of these phenomena is the scattering of charged particles by a magnetic string [1] which arises due to distinctive interference of the particle wave. It was shown in [14] that AB scattering is accompanied by electromagnetic radiation, and its angular distribution and polarization were calculated in [14, 4]. A clear example of the AB effect for bound states is the splitting of Landau energy terms for charged particles in a uniform magnetic field [9]. In addition there exist remarkable applications of the AB effect in solid-state physics [10, 11].

The issue of spin appended further peculiarity to the status of the AB effect. It was found that the interaction between the magnetic momentum of a charged particle and the magnetic field of the AB string essentially changes the behaviour of the wavefunctions at the magnetic string [6-8]. In the case of attraction this interaction increases the probability

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of finding the particle near the magnetic string, so that an irregular component inevitably appears in the radial solution. It becomes quite obvious that the Hamilton operator is not self-adjoint in this case. It is the role of the irregular solutions to which we want to draw attention.

Characteristic of the AB effect is the fact that a magnetic field is localized inside a solenoid and vanishing outside. There are many physical realizations for this. But in practice, physical processes, as for example quantum field theoretical processes, can only be studied in detail when reference to a much simpler limiting case is made: the infinitely thin and infinitely long, straight solenoid (the pure AB case). This is therefore the crucial situation to be studied for different matter field equations. For the radial equations in the Schrödinger and Dirac case, irregular solutions cannot be excluded by the normalization condition. Usually at this point the mathematically cumbersome procedure of self-adjoint extension of the respective Hamiltonian is applied [6]. It is the first aim of this paper to point out an equivalent pragmatic approach to the problem, which is quick and transparent.

The resulting self-adjointness conditions do not fix the solutions but still contain open parameters [7,8]. Their appearance reflects the fact that different original physical situations are described by the same pure AB case. To discuss this in detail is the second aim of this paper. We mention that the problem of bound states for quantum particles with magnetic moment in the AB potential is considered in detail in papers [2,3].

This paper is organized as follows. In section 2 we consider radial solutions to wave equations in the presence of the pure AB potential and discuss a mathematical problem which arises due to the singular behaviour of the potential. The problem of self-adjoint extension of the Hamilton operator to wave equations with the AB potential is discussed in section 3. We present the direct approach to the problem based on the orthogonalization of the radial solutions with different quantum numbers. In section 4 the problem of a physically adequate choice of solution is discussed. Then we discuss a model of a scalar particle with a magnetic moment, which allows us to illustrate why the standard method of self-adjoint extension contains an arbitrary parameter.

Throughout we use units such that $\hbar = c = 1$.

2. The pure Aharonov-Bohm case

The pure AB potential [1] which reads in cylindrical coordinates

$$eA_{\varphi} = \frac{e\Phi}{2\pi\rho} = \frac{\Phi}{\Phi_0\rho} = \frac{\phi}{\rho} \tag{1}$$

is realized by an infinitely thin solenoid lying along the z-axis. The related magnetic field is localized on the z-axis

$$H_z = \frac{\phi}{e} \frac{\delta(\rho)}{\rho} \,. \tag{2}$$

Here $\Phi_0 = 2\pi/e$ is the flux quantum. In what follows we decompose the flux ϕ into an integer part N and a fractional part δ with $0 < \delta < 1$, i.e. $\phi = N + \delta$. As we shall see, it is the fractional part δ of the magnetic flux which produces all physical effects.

The corresponding stationary Schrödinger equation reads

$$\frac{1}{2M} \left(-i\nabla - e\mathbf{A}\right)^2 \psi_j(\rho, \varphi, z) = E \ \psi_j(\rho, \varphi, z) \tag{3}$$

where j is a collective index for quantum numbers. After separating the angular and z-dependence with the ansatz

$$\psi_j(\rho,\varphi,z) = e^{ip_3 z} e^{il\varphi} R_l(\rho) \tag{4}$$

we find that the radial part $R_i(\rho)$ of the solution obeys the Bessel equation

$$h_l R_l \equiv R_l'' + \frac{1}{\rho} R_l' - \frac{(l-\phi)^2}{\rho^2} R_l = -p_\perp^2 R_l$$
(5)

where $2ME = p_{\perp}^2 + p_3^2$ and *l* is the angular momentum projection. The general solution of this equation,

$$R_{l} = a_{l} J_{|l-\phi|}(p\rho) + b_{l} J_{-|l-\phi|}(p\rho)$$
(6)

contains regular parts with Bessel functions of positive orders as well as irregular parts with Bessel functions of negative orders. For those l with $|l - \phi| > 1$, i.e. for $l \neq N$ or N + 1 the normalization condition

$$\int_0^\infty R_l(p'\rho) R_l(p\rho) \rho \, \mathrm{d}\rho = \frac{\delta(p-p')}{\sqrt{pp'}} \tag{7}$$

eliminates the irregular parts which diverge at $\rho = 0$. Accordingly we have $a_l = 1$, $b_l = 0$ in this case. But for l = N or N + 1 the Bessel functions of positive and of negative order both are square integrable and we cannot fix the coefficients in this way so that irregular solutions are not excluded. These modes require a separate discussion. In what follows we want to contribute to a clarification of this problem.

A similar situation occurs for the Dirac equation. Here it is also possible to separate variables. One finds for the ρ -dependant part of each spinor component a radial equation of the type

$$\widetilde{h}_{l}R_{l} \equiv R_{l}'' + \frac{1}{\rho}R_{l}' - \frac{(\nu - \phi)^{2}}{\rho^{2}}R_{l} + s\phi\frac{\delta(\rho)}{\rho}R_{l} = -p_{\perp}^{2}R_{l}$$
(8)

where $p_{\perp} = \sqrt{p^2 - p_3^2} = \sqrt{E_p^2 - M^2 - p_3^2}$ is the radial momentum. For different twospinor components s takes the values ± 1 , and $\nu = l$ or l + 1. Note the appearance of the δ -function. It arises from the $\sigma^{\mu\nu}F_{\mu\nu}$ term which is implicitly contained in the Dirac equation. For the pure Aharonov-Bohm potential it reduces to $\sigma^2 B_z \sim \delta(\rho)/\rho$. In the open interval $(0, \infty)$ we find in going back to the full first-order Dirac equation the following solutions for the components of the two-spinors:

$$R_l^1 = a_l J_{l-\phi}(p_\perp \rho) + b_l J_{-l+\phi}(p_\perp \rho)$$
(9)

and

$$R_l^2 = a_l J_{l-\phi+1}(p_\perp \rho) - b_l J_{-l+\phi-1}(p_\perp \rho).$$
⁽¹⁰⁾

The normalization condition here is more complicated, but is of the same type as (7). It shows that for all $l \neq N$ the Bessel functions of negative orders must be removed. For non-negative N for example one finds $b_l = 0$ for l > N and $a_l = 0$ at l < N. Here only one critical mode occurs. For l = N each spinor component contains an irregular part. It is not possible to remove all of them at the same time. Therefore for l = N at least one component of the two-spinors becomes irregular at $\rho = 0$. So in the Dirac case the problem of irregular solutions of the radial equation is even more evident.

Although the radial equations (5) and (8) in the Schrödinger and Dirac cases are essentially the same, one finds different numbers of critical modes and different conditions for the coefficients a and b. This is a consequence of the definition of the respective adjoint operator (see equation (11) below) which depends on the scalar product of the Hilbert space.

3. The self-adjoint extension and a simple equivalent procedure

The fact that the irregular radial solutions of the Schrödinger and Dirac equations cannot be ignored is related to the fact that the respective Hamilton operators h_l and \tilde{h}_l are not self-adjoint. Self-adjointness, however, is needed for a unitary time evolution. Consider the radial equation (5) for l = N or N + 1. The domain of the 'radial Hamilton operator' h_l is given by the set $D(h_l) = \{R_l \in \mathcal{L}^2((0, \infty), \rho \, d\rho) \mid R_l(0) = 0\}$, i.e. the square integrable functions with support away from the origin which have a regular limit for $\rho \to 0$.

The adjoint operator h_i^{\dagger} is constructed in the following way. The domain $D(h_i^{\dagger})$ of h_i^{\dagger} consists of all states S_i for which there exists a state S'_i such that

$$\langle R_l | h_l^{\mathsf{T}} S_l \rangle = \langle R_l | S_l' \rangle \tag{11}$$

for all states $R_l \in D(h_l)$. Then h_l^{\dagger} is defined by $h_l^{\dagger}S_l = S_l^{\prime}$. It turns out that the domains of h_l and h_l^{\dagger} are not the same. $D(h_l^{\dagger})$ also contains the irregular solutions and h_l is therefore not self-adjoint.

A detailed analysis of the operator h_i shows that it is possible to extend its domain in order to make it self-adjoint. This extension essentially consists in the inclusion of irregular solutions in $D(h_i)$. However, because of its mathematical complexity we shall not present this procedure here. For an accurate and mathematically exact treatment of the method of self-adjoint extensions we refer the reader to [16].

For the Schrödinger case this scheme of *self-adjoint extension* leads to the selfadjointness conditions

$$\frac{b_N}{a_N} = \alpha_0 \left(\frac{p}{M}\right)^{2\delta} \tag{12}$$

and

$$\frac{b_{N+1}}{a_{N+1}} = \alpha_1 \left(\frac{p}{M}\right)^{2(1-\delta)} \tag{13}$$

correlating the open parameters in (6) where α_0 and α_1 are arbitrary real numbers called extension parameters. We can express equations (12) and (13) in terms of new boundary conditions replacing $R_l(0) = 0$:

$$\lim_{\rho \to 0} R_l(\rho\rho) \propto (M\rho)^{|l-\delta|} - \tilde{\alpha}(M\rho)^{-|l-\delta|}$$
(14)

where

$$\tilde{\alpha} = 2^{2|l-\delta|} \frac{\Gamma(|l-\delta|)}{\Gamma(-|l-\delta|)} \alpha \,. \tag{15}$$

Therefore, in order to make h_l self-adjoint we have to choose as domain the square integrable functions that satisfy the boundary condition (14) thus allowing an irregularity at $\rho = 0$.

The self-adjoint extension that is constructed in this way depends on the two parameters α_0 and α_1 . It is a characteristic trait of this procedure that they remain open and cannot be determined without any additional information. Because of the relation to boundary conditions it is obvious that they must be connected with the physical details of the flux distribution inside the solenoid of the underlying original model from which the pure AB case was obtained in a limiting procedure.

For the Dirac case the first-order Hamilton operator reads

$$\begin{pmatrix} sM & i\partial_{\rho} + i\frac{l+1-\phi}{\rho} \\ i\partial_{\rho} - i\frac{l-\phi}{\rho} & -sM \end{pmatrix}$$
(16)

for eigenstates of the spin-z operator $S_3 = \gamma^0 \Sigma_3 + \gamma^5 \frac{P_3}{M}$ and the self-adjointness condition for l = N obtained in the same involved mathematical procedure of self-adjoint extension takes the form

$$\frac{b_N}{a_N} = \alpha \frac{M}{E + sM} \left(\frac{p_\perp}{M}\right)^{2\delta} \tag{17}$$

where α is an arbitrary dimensionless number. For example, for a different spin projection, or helicity eigenstates, it differs only by a factor which is independent on p_{\perp} .

We now present an alternative, *pragmatic* approach to the problem of the undetermined parameters in (6) or (9) and (10), respectively. It is simple and quick.

Consider again the Schrödinger case. Because regular and irregular parts are both square integrable, we take as solutions for l = N and N + 1

$$R_N = a_N J_{\delta}(p\rho) + b_N J_{-\delta}(p\rho) \tag{18}$$

and

$$R_{N+1} = a_{N+1}J_{1-\delta}(p\rho) + b_{N+1}J_{-1+\delta}(p\rho).$$
⁽¹⁹⁾

The observation is now that these solutions are not orthogonal for different p and p'

$$\int_0^\infty R_l(p'\rho)R_l(p\rho)\rho \,\mathrm{d}\rho \neq \frac{\delta(p-p')}{\sqrt{pp'}}\,.$$
(20)

This results from the cross terms containing integrals over Bessel functions of opposite orders. Using the well known formula

$$I_{+} = \int_{0}^{\infty} \rho d\rho \ J_{\delta}(p\rho) J_{\delta}(p'\rho) = \frac{1}{\sqrt{pp'}} \delta(p-p')$$
(21)

and the formula developed specifically for our purpose:

$$I_{-} = \int_{0}^{\infty} \rho d\rho \ J_{\delta}(p\rho) J_{-\delta}(p'\rho) = \frac{1}{\sqrt{pp'}} \delta(p-p') \cos \pi \delta + \frac{2\sin \pi \delta}{\pi (p^2 - p'^2)} \left(\frac{p}{p'}\right)^{\delta}$$
(22)

we can calculate the integral (20). To our knowledge the integral (22) has not been solved before. It can be derived from the known indefinite integral (5.53) of [5] by extending the range of integration to $(0, \infty)$ and using the asymptotic form of the Bessel functions. The relation $\lim_{L\to\infty} \frac{\sin(xL)}{x} = \pi \delta(x)$ then leads to (22). It is easy to show that the non- δ terms which arise from (22) are cancelled if the coefficients *a* and *b* fulfil (12) and (13). These conditions can therefore be derived this way. The same procedure can also be applied in the Dirac case and easily leads to (17).

Thus the orthonormality condition lead us directly to the self-adjointness condition, thereby circumventing the mathematically cumbersome procedure of self-adjoint extension. This is of course not just a coincidence but is related to the fact that a self-adjoint operator possesses a complete set of orthonormal eigenstates.

The practical relevance of the pragmatic approach described above is to be seen in the fact that it shortens, for example, the calculations of quantum electrodynamical effects outside thin solenoids. It will be used in a subsequent discussion [17] of the bremsstrahlung emitted by an electron which is scattered by the external Aharonov–Bohm potential.

4. The open parameters α and their physical meaning

The pure AB case is an approximative description of a whole class of real physical situations. All the different configurations which in the limit of vanishing solenoid radius and fixed flux Φ lead to the AB potential (1) are described by it. The appearance of the open extension parameters α in the pure AB case reflects this. Different α correspond to different original situations. Therefore we have to go back to the original situation to find the specific values of α .

All cylindrically symmetric magnetic fields which vanish for $\rho > \rho_0$ so that $A_{\varphi} = \phi/e\rho$ and satisfy

$$\lim_{\rho_0\to 0}\int_0^{\rho_0} H(\rho)\rho \,\mathrm{d}\rho = 0$$

lead in the AB limit $\rho_0 \rightarrow 0$ to the same values of α . This was shown by Hagen [7] for the Dirac case, but applies to spinless and non-relativistic particles as well because the radial equations are identical.

For Schrödinger particles we have

$$\alpha_0 = 0 \qquad \alpha_1 = 0 \tag{23}$$

and for Dirac particles, depending on the mutual interaction of spin and magnetic field,

$$\alpha = \begin{cases} 0 & \text{for } s\phi < 0\\ \infty & \text{for } s\phi > 0 \,. \end{cases}$$
(24)

The Dirac particle carries a magnetic moment $\mu = (e/2M)s$ ($s = \pm 1$) which interacts with the magnetic field resulting in a potential energy $-\mu H$. Therefore it suffers an attractive force if $s\phi > 0$, i.e. if magnetic moment and magnetic field are parallel ($\mu H > 0$), which leads to an enhancement of the wavefunction. For the Schrödinger particle such an interaction is not present and thus the wavefunction always stays regular at $\rho = 0$.

Because the pure AB case allows parameter values different from (23) and (24) it is more general. It also describes physical situations different from the one sketched above[†]. What, therefore, is the physical meaning of the *non-trivial parameters* $0 < \alpha < \infty$? We will give an example.

We saw that the μ -H interaction is responsible for the enhancement of the Dirac wavefunction near $\rho = 0$. Therefore we will consider the influence of an additional interaction of this type for a Schrödinger particle thus modifying the Schrödinger theory. If, in the limit of vanishing solenoid radius, this new model gives the same radial equations as before, the self-adjoint extension procedure will apply here too. This is indeed the case, because the additional interaction is in this limit localized to $\rho = 0$ and the radial equation remains unchanged at $\rho > 0$. Now, in order to fix α we have to return again to the original physical situation and study the limit of vanishing solenoid radius. We will show that it can indeed lead to non-zero values of α .

Let us consider a situation in which the magnetic flux is located on the surface of a cylinder. Then the vector potential and magnetic field are given by

$$eA_{\varphi} = \frac{\phi}{\rho} \Theta(\rho - \rho_0) \qquad eH_z = \frac{\phi}{\rho_0} \delta(\rho - \rho_0). \tag{25}$$

[†] We thank Dr Michael Bordag for fruitful discussions about this problem.

We modify the Schrödinger equation in assuming that the particle carries a magnetic moment μ that couples with the magnetic field H:

$$\left[\frac{1}{2M}\left(-i\nabla - eA\right)^2 - \mu H\right]\psi_j(\rho,\varphi,z) = E \ \psi_j(\rho,\varphi,z) \,. \tag{26}$$

We set $\mu_z = g \frac{e}{2M}$, but do not specify g, and find for the radial equation

$$R_l'' + \frac{1}{\rho}R_l' - \frac{(l-\phi)^2}{\rho^2}R_l + \frac{g\phi}{\rho_0}\,\delta(\rho - \rho_0)R_l + \epsilon R_l = 0$$
(27)

where $\epsilon = 2ME$.

The interior and exterior solutions of the radial equation (27) are given by

$$R_{l} = \begin{cases} c_{l} J_{|l|}(p\rho) & \text{for } \rho < \rho_{0} \\ a_{l} J_{|l-\phi|}(p\rho) + b_{l} J_{-|l-\phi|}(p\rho) & \text{for } \rho > \rho_{0} \end{cases}$$
(28)

and the matching conditions read

$$R_l^{\text{int}}(\rho_0) = R_l^{\text{ext}}(\rho_0) \qquad \rho R_l^{\text{int}'}(\rho_0) = \rho R_l^{\text{ext}'}(\rho_0) + g \phi R_l(\rho_0) \,.$$

They lead to

$$\frac{b_{l}}{a_{l}} = -\frac{J'_{|l-\phi|}(p\rho_{0})J_{|l|}(p\rho_{0}) - J_{|l-\phi|}(p\rho_{0})[J'_{|l|}(p\rho_{0}) - \frac{g\phi}{p\rho_{0}}J_{|l|}(p\rho_{0})]}{J'_{-|l-\phi|}(p\rho_{0})J_{|l|}(p\rho_{0}) - J_{-|l-\phi|}(p\rho_{0})[J'_{|l|}(p\rho_{0}) - \frac{g\phi}{p\rho_{0}}J_{|l|}(p\rho_{0})]}$$
(29)

which fixes a_l and b_l for arbitrary ρ_0 .

Inserting the series representation of the Bessel function, (29) becomes, in the limit of vanishing radius $\rho_0 \rightarrow 0$,

$$\frac{b_l}{a_l} \to \frac{|l-\phi| - |l| + g\phi}{|l-\phi| + |l| - g\phi} \cdot \frac{\Gamma(-|l-\phi|)}{\Gamma(|l-\phi|)} \left(\frac{p\rho_0}{2}\right)^{2|l-\phi|}.$$
(30)

We see that for $\rho_0 = 0$ we have again $b_l = 0$ for all l unless the denominator in (30) becomes zero,

$$|l - \phi| + |l| - g\phi = 0.$$
(31)

For this case we must consider the next term of the series in (29) and find that this can only happen for l = N or N + 1.

The particular physical situation (25) treated by the modified Schrödinger equation (26) can also approximately (limit $\rho_0 \rightarrow 0$) be represented as a particular pure AB case, if the self-adjointness conditions (12) and (13) are fulfilled. Comparison with (30) shows that this is indeed the case if for l = N g satisfies the condition

$$g_N = \frac{1}{N+\delta} \cdot \frac{\Gamma(-\delta) \left(\frac{M\rho_0}{2}\right)^{2\delta} (|N|-\delta) + \alpha_0 \Gamma(\delta)(|N|+\delta)}{\Gamma(-\delta) \left(\frac{M\rho_0}{2}\right)^{2\delta} + \alpha_0 \Gamma(\delta)}$$
(32)

and for l = N + 1 the condition

$$g_{N+1} = \frac{1}{N+\delta} \cdot \frac{\Gamma(-1+\delta) \left(\frac{M\rho_0}{2}\right)^{2(1-\delta)} (|N+1|-1+\delta) + \alpha_1 \Gamma(1-\delta) (|N+1|+1-\delta)}{\Gamma(-1+\delta) \left(\frac{M\rho_0}{2}\right)^{2(1-\delta)} + \alpha_1 \Gamma(1-\delta)}.$$
(33)

Thus we see that the pure AB case may also describe the 'modified' Schrödinger particle that suffers an additional μ -H interaction if its g-factor has the properties (32) and (33).

The extension parameters α_0 and α_1 are then determined by g_N and g_{N+1} and need not to be zero, as is the case of the Schrödinger equation (3).

In general the conditions (32) and (33) are rather exotic, because the g-factor depends on the angular momentum l and on the solenoid parameters ρ_0 and Φ (more precisely on δ). The reason is that we are still dealing with the whole range $0 < \alpha < \infty$ of non-trivial parameters, i.e. with all the parameters which do not fulfil (23). Particular combinations of non-trivial parameters, and this is enough for our purpose, can be combined with reasonable physical situations: For $N \ge 0$ we may for example choose the non-trivial combination $\alpha_0 \ne 0$ and $\alpha_1 = 0$. Then we have that $g_{N+1} = 1$ and g_N still depends on ρ_0 and ϕ , but it approaches the same value ± 1 in the pure AB case as ρ goes to zero:

$$g_N \to 1 + \frac{1}{\alpha_0} \frac{N-\delta}{N+\delta} \frac{\Gamma(-\delta)}{\Gamma(\delta)} \left(\frac{M\rho_0}{2}\right)^{2\delta}$$
 (34)

For $N \leq 0$ we may choose $\alpha_0 = 0$, $\alpha_1 \neq 0$ and find $g_N = -1$ and the same value for g_{N+1}

$$g_{N+1} \to -1 - \frac{1}{\alpha_1} \frac{N+2-\delta}{N+\delta} \frac{\Gamma(-1+\delta)}{\Gamma(1-\delta)} \left(\frac{M\rho_0}{2}\right)^{2(1-\delta)}$$
(35)

in the limit of vanishing solenoid radius ρ_0 . Thus we have obtained the result that in the pure AB case the self-adjoint extension in which one of the parameters is non-zero may describe a 'modified' Schrödinger particle obeying (26). It carries a magnetic moment oriented such that $\mu H > 0$. This model provides one possible physical explanation of non-trivial parameter values which arise from the self-adjoint extension method. The μ -H interaction that we put in by hand here is already present in the Dirac and Pauli equation. Therefore the inclusion of an additional (anomalous) magnetic moment can explain particular parameter values there. This completes our presentation of a physical situation which may be described by the pure AB case with a non-trivial combination of extension parameters.

5. Conclusion

We analysed the problem of the self-adjoint extension for the Hamilton operator containing the pure AB potential. Using a pragmatic approach based on a direct procedure which allowed us to make radial solutions orthogonal at different quantum numbers, we reproduced in a straightforward manner results which follow from the standard method of self-adjoint extension. Regression to the original physical problem leads to definite values for the extension parameter depending on the specific form of the interaction with the magnetic field. In the framework of a simple model of a charged particle with an exotic magnetic moment (modified Schrödinger theory) we explained why the standard extension method contains an arbitrary parameter and gave a physical meaning to non-trivial values of this parameter.

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