Self-adjoint extensions of the Hamiltonian for a charged particle in the presence of a thread of magnetic flux

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Self-adjoint extensions of the usual Hamiltonian are studied for a charged particle moving in the x-y plane in the presence of an infinitely thin thread of magnetic flux along the z axis. This is done by starting with a square-well potential and taking its zero-range limit. The wave function for such an extended Hamiltonian is, although square integrable, singular at the origin. There are interesting differences between the cases with and without the magnetic flux.

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Let us start with a standard problem discussed in quantum-mechanics textbooks: a nonrelativistic particle moving in a central potential in two or three dimensions. The Schrödinger equation has regular and irregular solutions. In an S state, the irregular solution is, although singular at the origin, square integrable. We usually assume that the wave function is finite and discard the irregular solution, but there is no *a priori* reason why the latter is not admissible. Such an irregular solution is associated with a self-adjoint extension of the usual Hamiltonian. Including Kato's seminal paper of 1951 [1], there is vast literature on this subject, which can be traced through Ref. [2]. There are physical situations in which irregular solutions may emerge, as we will discuss later.

The purpose of this note is to examine self-adjoint extensions of the Hamiltonian for a nonrelativistic particle moving in the x-y plane in the presence of an infinitely thin thread of magnetic flux along the z axis. This note is a sequel to a recent paper [3], in which a similar problem, but in the absence of magnetic flux, was discussed. We will see some interesting differences between the cases with and without magnetic flux. This note also supplements Ref. [4], in which a similar aspect of a relativistic particle has been examined. In constructing the self-adjoint extensions, we assume an attractive potential of a finite range and take its zero-range limit. We prefer this pedestrian approach rather than the more sophisticated mathematical methods expounded in Refs. [1,2] because we can study the mechanism more closely in this way.

Consider a particle of mass m and charge e, which is free to move in the x-y plane, except that it is under the influence of a thread of magnetic flux Φ along the z axis. We choose the vector potential due to the magnetic flux as

$$\mathbf{A}=\left[-\frac{\Phi y}{2\pi r^2},\frac{\Phi x}{2\pi r^2},0\right]. \tag{1}$$

When the angular part of the wave function is separated, the radial part of the Hamiltonian becomes

$$H_0=\frac{\hbar^2}{2m}\left[-\frac{d^2}{dr^2}-\frac{1}{r}\frac{d}{dr}+\frac{\nu^2}{r^2}\right],\quad \nu=n+\alpha\ , \tag{2}$$

where $r=(x^2+y^2)^{1/2}$, n is the (integral) angular momentum, and α is related to the magnetic flux Φ by $\alpha=-e\Phi/(2\pi c\hbar)$. Unless otherwise stated, ν should be understood as a noninteger in the following. The H_0 is the Hamiltonian examined by Aharonov and Bohm [5]. This system is also referred to as an "anyon" in the literature [6]. The Schrödinger equation $H_0\phi(r)=E\phi(r)$ has regular and irregular solutions, which are given by the Bessel functions $J_{|\nu|}(kr)$ and $N_{|\nu|}(kr)$, respectively, where $k^2=2mE/\hbar^2$. The standard boundary condition dictates that $\phi(r)$ be finite at the origin. If $|\nu|<1$, however, $N_{|\nu|}(kr)$ is square integrable (locally around the origin). In this case H_0 admits a one-parameter family of self-adjoint extensions [7]. For such extensions of H_0, $\phi(r)$ is singular at the origin. In this sense the boundary condition is a nonstandard one. We assume that $|\nu|<1$ in the following.

We construct self-adjoint extensions of H_0 using the following procedure. We first replace the infinitely thin magnetic flux with a uniform flux of a finite radius R. We do this by modifying the vector potential $\mathbf{A}$ as

$$\mathbf{A}=\left[-\frac{\Phi y}{2\pi R^2},\frac{\Phi x}{2\pi R^2},0\right]\quad \text{for } r<R\ . \tag{3}$$

The $\mathbf{A}$ for $r>R$ is the same as that of Eq. (1). In addition, we assume a potential $V(r)$, which, together with the magnetic interaction, forms an attractive square-well potential of radius R and depth D, that is

$$V(r)-\frac{enB}{2mc}+\frac{e^2B^2}{8mc^2}r^2=-D\quad \text{for } r<R\ , \tag{4}$$

where $B=\Phi/(\pi R^2)$. *When $R\neq 0$, we require that the*

wave function satisfies the standard boundary condition at the origin [8]. Then, we let $R \to 0$ and $D \to \infty$. The wave function obtained in this limit is subject to a nonstandard boundary condition. The structure of the flux that we assumed is *ad hoc*. As it turns out, however, the self-adjoint extensions that emerge in the limit of $R \to 0$ are insensitive to the details of the potential within the flux.

The radial part of the Schrödinger equation reads

$$\left[\frac{\hbar^2}{2m}\left[-\frac{d^2}{dr^2}-\frac{1}{r}\frac{d}{dr}+\frac{n^2}{r^2}\right]-D\right]\phi=E\phi \quad \text{for } r<R \ , \tag{5}$$

$$\frac{\hbar^2}{2m}\left[-\frac{d^2}{dr^2}-\frac{1}{r}\frac{d}{dr}+\frac{\nu^2}{r^2}\right]\phi=E\phi \quad \text{for } r>R \ . \tag{6}$$

Since n and ν appear only in the form of n^2 and ν^2 in Eqs. (5) and (6), we will only consider non-negative values of n and ν. In relating results to α, however, we have to remember $\nu=n+\alpha$ and incorporate appropriate signs of ν and n. The wave function $\phi(r)$ for the bound (ground) state is given in terms of Bessel functions

$$\phi(r)=\begin{cases} J_n(k_0 r), & r<R \\ K_\nu(\kappa r), & r>R \ , \end{cases} \tag{7}$$

where $k_0^2=2m(D+E)/\hbar^2$ and $\kappa^2=-2mE/\hbar^2$. We have not included the irregular solution $N_n(k_0 r)$ for $r<R$ for the reason stated following Eq. (4). The eigenvalue E can be determined from the continuity of $(r/\phi)(d\phi/dr)$ at $r=R$. Let us define $F(k_0R)$ by

$$F(k_0R)=\left.\frac{r}{\phi}\frac{d\phi}{dr}\right|_{r=R-0}=\frac{R}{J_n(k_0R)}\frac{dJ_n(k_0R)}{dR} \ , \tag{8}$$

and also $G(\kappa R)$ by

$$G(\kappa R)=\left.\frac{r}{\phi}\frac{d\phi}{dr}\right|_{r=R+0}=\frac{R}{K_\nu(\kappa R)}\frac{dK_\nu(\kappa R)}{dR} \ . \tag{9}$$

The matching condition for $\phi(r)$ at $r=R$ is

$$F(k_0R)=G(\kappa R) \ . \tag{10}$$

We now let $R \to 0$ and $D \to \infty$, but keep κ fixed at a finite value, which we can choose at will. Then $\kappa R \to 0$, and the limit of $k_0R \simeq [(2mD/\hbar^2)]^{1/2}R$ is determined by the matching condition (10). In the limit of $R \to 0$, the square-well potential becomes a δ-function potential, which is characterized by parameter κ. Let us emphasize that Eq. (2) defines H_0 only "formally." When it is complemented by the δ-function potential (specified with κ), the H_0 is completely defined. When $R \to 0$, the part of the wave function (for $r<R$) that is given by $J_n(k_0 r)$ disappears, and $\phi(r)$ is represented by $K_\nu(\kappa r)$ in the entire region of $r>0$. Recall that $K_\nu(\kappa r) \to \infty$ as $r \to 0$. This is how a wave function subject to a nonstandard boundary condition emerges. Note also that although the irregular solution is square integrable, it leads to an *infinite probability density* at the origin. This is a reflection of the underlying singular interaction.

When $\nu=0$, the choice of $\kappa=0$ leads to the standard boundary condition (without the δ-function potential) [3]. This can be understood as follows. In two dimensions with $\nu=0$, any globally attractive potential supports a bound state, no matter how weak the potential [9]. For the square-well potential, therefore, $\kappa=0$ (zero binding energy) implies $D=0$. When $\nu \neq 0$, however, $\kappa=0$ does not imply $D=0$. In order to have a bound state at threshold in this case, there has to be an attractive potential that counteracts the repulsive term proportional to ν^2/r.

If $\kappa R \ll 1$, we obtain

$$G(\kappa R)=-\nu-\frac{2\Gamma(1-\nu)}{\Gamma(\nu)}\left[\frac{\kappa R}{2}\right]^{2\nu}+\cdots \ , \tag{11}$$

where $\Gamma(\nu)$ is the gamma function. In the special case of $\nu=\frac{1}{2}$ ("semion"), $G(\kappa R)$ is exactly given by

$$G(\kappa R)=-\tfrac{1}{2}-\kappa R \ . \tag{12}$$

Note that $G(\kappa R) \to -\nu$ when $\kappa R \to 0$. The limit of k_0R has to be tuned such that Eq. (10) is satisfied for a given value of κ. Since $G(\kappa R)$ is finite, the limit of k_0R has to be finite. This situation is in a sharp contrast to that of $n=\nu=0$ [3]. In the latter case, if we take a finite value for the limit of k_0R, the binding energy becomes infinite ($\kappa \to \infty$). If $\nu=0$ and $\kappa R \to 0$, then $G(\kappa R) \to 1/\ln(\kappa R)$. In order for the bound state not to collapse (i.e., κ remains finite) the depth D of the potential has to be regulated. This is done by choosing the limit of k_0R as $k_0R \sim [(2mD/\hbar^2)]^{1/2}R \to [-2/\ln(\kappa R)]^{1/2}$. When $\nu>0$, however, the repulsive ν^2/r^2 term of H_0 prevents the bound state from collapsing.

Once the δ-function potential (specified with κ) is implemented, the scatting problem can be done. The scattering wave function for $r>R$ can be written as

$$\phi(r)=\cos\eta_\nu J_\nu(kr)-\sin\eta_\nu N_\nu(kr) \ , \tag{13}$$

where $k^2=2mE/\hbar^2$ and η_ν is the "phase shift." We define $\mathcal{G}(kR)$ by

$$\mathcal{G}(kR)=\left.\frac{r}{\phi}\frac{d\phi}{dr}\right|_{r=R+0} \ , \tag{14}$$

where ϕ is the $\phi(r)$ of Eq. (13). We equate this $\mathcal{G}(kR)$ with $F(k_0R)$, where $k_0^2=2m(D+E)/\hbar^2=(2mD/\hbar^2)+k^2$. Finally, we let $R \to 0$. In this limit, $D \to \infty$ and $k_0^2 \to 2mD/\hbar^2$. The $F(k_0R)$ for scattering becomes indistinguishable from that for the bound state and hence $\mathcal{G}(kR)$ can be equated with $G(\kappa R)$, which was defined for the bound state. Recall that $G(\kappa R) \to -\nu$ as $\kappa R \to 0$. In this way, we are led to

$$\tan\eta_\nu=-\sin(\nu\pi)(k/\kappa)^{2\nu} \ . \tag{15}$$

Note that $F(k_0R)$ plays only an intermediary role; the details of $F(k_0R)$ are unimportant. This aspect reminds us of the boundary condition model of the nucleon-nucleon interaction [10]. The above phase shift can be compared with $\tan\eta_0=\pi/[2\ln(k/\kappa)]$ for $\nu=n=0$; see Eq. (18) or Ref. [3]. There is a gap between $\eta_{\nu\neq 0}$ and η_0. The usual partial-wave phase shift δ_n for $n=\nu-\alpha$ can be

obtained by adding η_ν to the standard Aharonov-Bohm phase shift [11,7]. The δ_n for $n \neq \nu - \alpha$ is not affected.

So far we have considered a particle that is free apart from the interaction with the thread of magnetic flux. Next let us consider a model that contains an additional harmonic-oscillator potential. Such a model has been used as a means of calculating the second virial coefficient of an anyon gas [12]. The Hamiltonian is

$$H = H_0 + \tfrac{1}{2} m\omega^2 r^2 . \tag{16}$$

We try to obtain self-adjoint extensions of this H again by using a square-well potential. We assume the same Schrödinger equation (5) for $r < R$. For $r > R$, we replace Eq. (6) with

$$\left[\frac{\hbar^2}{2m} \left[-\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{\nu^2}{r^2} \right] + \tfrac{1}{2} m\omega^2 \right] \phi = E\phi \quad \text{for } r > R , \tag{17}$$

which can be reduced to Kummer's equation [13]. Hence the wave function for $r > R$ is given by

$$\phi(r) = (\lambda r)^{-\nu} e^{-(\lambda^2 r^2/2)} U\left[\frac{1}{2}\left[1 - \nu - \frac{E}{\hbar\omega} \right], 1-\nu, \lambda^2 r^2 \right] , \tag{18}$$

where $\lambda^2 = m\omega/\hbar$ and U is the Kummer function.

When $\nu \to 0$, the above $\phi(r)$ is reduced to Eq. (20) of Ref. [3]. If we put $\nu = 0$ and $E = (2N+1)\hbar\omega$, where N is a non-negative integer, the above Kummer function turns out to be a Laguerre polynomial

$$U = (-1)^N N! L_N^{(0)}(\lambda^2 r^2) \quad \text{for } \nu = 0 \text{ and } E = (2N+1)\hbar\omega . \tag{19}$$

This is nothing but the case of the usual two-dimensional harmonic oscillator (with angular momentum $n = 0$). The $\phi(r)$ of this case of course conforms to the standard boundary condition.

Another simple case is

$$U = 2^{-N} H_N(\lambda r) \quad \text{for } \nu = \tfrac{1}{2} \text{ and } E = (N + \tfrac{1}{2})\hbar\omega , \tag{20}$$

where H_N is the Hermite polynomial of order N [14]. There is a subtle point to be noted here regarding the possible values for N. The U of Eq. (20) with any non-negative integer N furnishes $\phi(r)$, which satisfies Eq. (17). However, as eigenstates of the Hamiltonian H, we have to choose either even N's or odd N's, but not both. If we require the standard boundary condition, only odd N's are allowed. If we take a nonstandard boundary condition such that even N's are allowed and $\phi(r)$ becomes singular at the origin, we have to reject odd N's. Note that the two different (standard and nonstandard) boundary conditions are associated with two different Hamiltonians.

There is yet another case in which the U is reduced to a simple form

$$U = \sqrt{\pi} e^{\lambda^2 r^2} \operatorname{erfc}(\lambda r) \quad \text{for } \nu = \tfrac{1}{2} \text{ and } E = -\tfrac{1}{2}\hbar\omega . \tag{21}$$

Unlike Eqs. (19) and (20), the U of Eq. (21) is not a polynomial, but it leads to $\phi(r)$, which converges as $r \to \infty$ such that it is square integrable [15].

The examples discussed above may give a false impression that the choice of the values for E is quite restricted. As shown below, however, self-adjoint extensions of the Hamiltonian can accommodate any value of E other than those of Eqs. (19)–(21). For the $\phi(r)$ of Eq. (18), we obtain

$$\left. \frac{r}{\phi}\frac{d\phi}{dr} \right|_{r=R+0} = -\nu - \lambda^2 R^2 + \frac{R}{U}\frac{dU}{dR} . \tag{22}$$

When $R \to 0$, the above can be reduced to

$$\left. \frac{r}{\phi}\frac{d\phi}{dr} \right|_{r=R+0} \sim -\nu - \frac{2\Gamma(1-\nu)\Gamma[1-(E/\hbar\omega)]}{\Gamma(\nu)\Gamma[1-\nu-(E/\hbar\omega)]} (\lambda R)^{2\nu} . \tag{23}$$

If the self-adjoint extension of H_0 has already been fixed in terms of parameter κ before the harmonic-oscillator potential is added, the right-hand side of Eq. (23) can be equated with $G(\kappa R)$ of Eq. (11). Then, by letting $R \to 0$, we obtain

$$\frac{\Gamma[1-(E/\hbar\omega)]}{\Gamma[1-\nu-(E/\hbar\omega)]} = \left[\frac{\kappa}{2\lambda} \right]^{2\nu} , \tag{24}$$

which determines E for a specified κ, or κ for any given value of E. If $\nu = 0$, Eq. (24) is an identity that is not particularly interesting. If $\nu \neq 0$, however, Eq. (24) is a nontrivial equation, no matter how small ν is.

Let us mention two cases in which the relation between κ and E is very simple. First, Eq. (24) is satisfied by

$$E = (N+1-\nu)\hbar\omega, \quad \kappa = 0 . \tag{25}$$

This E is a generalization of the E of Eq. (20). It turns out that the U in this case is a polynomial of degree N; in particular, $U = 1$ if $N = 0$. It is interesting that this energy spectrum coincides with that of Wigner's generalized harmonic oscillator [16]. The second case is

$$\nu = \tfrac{1}{2}, \quad E = -\tfrac{1}{2}\hbar\omega, \quad \kappa = \sqrt{\pi}\lambda , \tag{26}$$

which corresponds to Eq. (21). The energies of the excited states of this case are not equally spaced.

For E other than those of Eqs. (19), (20), and (25), U is an infinite series, but $\phi(r)$ converges as $r \to \infty$ sufficiently fast. The wave function that emerges in the limit of $R \to 0$ is subject to a nonstandard boundary condition at the origin. Let us emphasize that there is no *a priori* reason why the special values of E examined above should be preferred instead of other possible values.

Finally let us discuss possible physical implications of the self-adjoint extensions. The aspect that the value of κ and hence the bound-state energy can be chosen arbitrarily may give the impression that the extensions are a mere mathematical artifact. This is not necessarily so. Consider the (ordinary) hydrogen atom. We know that the standard solutions of the Schrödinger equation are in good agreement with experiment. Next consider a hadronic hydrogen atom such as those of $\pi^- p$, $K^- p$, or $\bar{p}p$.

It is known that the S-state levels are shifted from the pure Coulombic levels. This is due to the hadronic interaction at short distances ($r \lesssim 1$ fm). This short-range interaction can be simulated by a square-well potential [17]. Then the resulting S-state wave functions (subject to the standard boundary condition) behave differently for $r \lesssim 1$ fm as compared with the corresponding wave functions in the absence of the short-range interaction. If one takes the zero-range limit of the square-well potential, the wave function in the limit obtains an irregular component. In the sense that 1 fm is almost zero as compared with the relevant Bohr radius, the wave functions obtained in the zero-range limit would not be very different from the real wave functions. A similar situation will arise if the magnetic flux has a structure at very short distances.

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