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On the Hermitian of Hamiltonians of Radial Equations

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The Hamiltonian of a radial equation is defined on a half-line, and there is an intimate relation between its hermitian and the boundary conditions of the wave functions at the origin. If the wave functions are nonvanishing and convergent at the origin, the Hamiltonian has a one-parameter family of self-adjoint extensions which are related to the condition for the vanishing radial probability current at the origin. In this paper the problem on the hermitian of the Hamiltonian of a radial equation is studied systematically. Some methods for determining the parameter for the fermion moving in a magnetic monopole field are discussed.

1. INTRODUCTION

There is an intimate relation between the hermitian of an operator defined in a half-line and the boundary conditions of its eigenfunctions. A Hamiltonian of a radial equation is defined in a half-line, $0 \le r < \infty$, then, when its eigenfunction is neither vanishing nor divergent at the origin, the hermitian of the Hamiltonian depends on the boundary conditions which the wave-functions should satisfy, so does the orthogonality of the energy eigenfunctions. This problem with this kind of operators has been studied clearly in mathematics[1]. In the terminology of Weyl and von Neumann, this kind of Hamiltonian is of limit circle type at the origin and of limit point type in infinity, hence the Hamiltonian has a one-parameter family of self-adjoint extensions[1-3]. In recent years this problem has drawn more attention of physicists, in the research on fermions moving in a magnetic monopole field or in a strong Coulomb field. In the viewpoint of physics, Hamiltonian must

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be hermitian and no undetermined parameter is allowed.

In physics, Kazama-Yang-Goldhaber[4] were the pioneers to discuss the problem of determining this parameter. Because the difficulty of Lipkin-Weisberger-Peshkin[5] exists in the origin of the monopole field, they introduced an infinitesimal extra magnetic moment which makes the eigenfunctions vanishing at the origin. The essence of this method is to introduce an additional potential that takes effect only near the origin and determines the parameter. Dai and Ni[6] pointed out that the hermitian of a Hamiltonian is related to the condition for the vanishing radial probability current of wave functions which are non-vanishing at the origin. They raised a principle which was called "principle of orthogonality and variation" for determining the parameter. Unfortunately, they did not really use this principle to determine the parameter, instead, they put by hand an assumption that there is a zero energy solution. Under this assumption they obtained the same results as that by Kazama-Yang-Goldhaber. Yamagishi[7] further discussed the problem of fermions moving in a magnetic monopole field, and discovered that the vacuum fractional charge depends on the parameter. Thus, for a given constant parameter, the magnetic monopole becomes a dyon, and the parameter is related to the θ vacuum parameter in terms of Witten's formula[8]. Up to now, the magnetic monopole has not yet been definitely discovered in experiments , and the θ vacuum parameter is not determined by experiments, so it is to depend on further experiments to prove which one of the two methods in determining the parameter is better.

In this paper the hermitian of a Hamiltonian of a radial equation is discussed systematically, the source and the meaning of the undetermined parameter are discussed from the physical point of view. For the interactive system of a fermion and a monopole, a few methods for determining the parameter are compared to each other.Especially, in comparison with the exact solution of a fermion moving in the analytic magnetic monopole field of the nonabelian gauge theory,the meaning of the parameter will be clearer.

The paper is organized as follows. In sec.2, we explain the method of self-adjoint extensions of a singular Hamiltonian of a radial equation of Schrödinger equation, and demonstrate the source of an undetermined parameter. In sec.3, we discuss the problem of fermions moving in a magnetic monopole field to demonstrate the general mathematical methods of self-adjoint extensions of a singular Hamiltonian, and the physical method for determining the parameter. A new method for determining is also proposed here. In Sec.4, in comparison with the exact solution of a fermion moving in the fundamental magnetic monopole field of the SU(5) grand unified model, we explain the meaning of the undetermined parameter.

Another interesting physical problem which is related to the problem of the hermitian of the Hamiltonian is the energy level of a fermion moving in a strong Coulomb field, that we will discuss elsewhere.

2. THE HERMITIAN OF A HAMILTONIAN IN THE SCHRÖDINGER RADIAL EQUATION

In fact, the relation between the hermitian of a Hamiltonian and the boundary condition of wavefunctions already existed in the Schrödinger radial equation, but that did not draw enough attention to Physicists.

The Schrödinger radial equation ($\hbar = c=2m = 1$) is as follows:

$$u'' + \left[E - V(r) - \frac{l(l+1)}{r^2}\right]u = 0 \tag{1}$$

where the spherically symmetric potential V(r) is assumed to be vanishing fast enough at the origin and in infinity. The definition of the hermitian of a Hamiltonian is as follows:

$$\int u_1^* H u_2 dr - \int (Hu_1)^* u_2 dr = 0 \tag{2}$$

If u_1 and u_2 are the eigenfunctions of the Hamiltonian, we have

$$(E_2 - E_1)\int u_1^* u_2 dr = 0 \tag{3}$$

so the hermitian of the Hamiltonian guarantees the orthogonality of the energy eigenfunctions. For the real solutions of the radial equation(1), in terms of the integration by parts, the hermitian condition of the Hamiltonian becomes

$$(u_1 u_2' - u_1' u_2)\big|_0^\infty = 0 \tag{4}$$

When $E < 0$, the physical wavefunctions vanish in infinity; when $E > 0$, the energies of u_1 and u_2 are both positive but different, the left-hand-side of (4) oscillates rapidly and vanishes in average; when u_1 and u_2 are two different solutions with the same positive energy, Wronskian makes the left-hand-side of (4) vanishing. Therefore, the hermitian condition (4) becomes

$$(u_1 u_2' - u_1' u_2)\big|_{r=0} = \left[u_1 u_2\left(\frac{u_2'}{u_2} - \frac{u_1'}{u_1}\right)\right]_{r=0} = 0 \tag{5}$$

When the angular momentum l is larger than zero, equation (5) holds for the solutions convergent at the origin, $u(r)\big|_{r\sim 0} \sim r^{l+1} \sim 0$. For S wave, both solutions are finite, and the general solution goes to a finite constant at the origin. The probability at a small volume near the origin for the solutions is finite although the total wavefunctions of Schrödinger equation (see (9)) are singular at the origin. Now, the hermitian condition for a Hamiltonian becomes that the logarithmic derivative of wavefunctions at the origin is a constant independent of the energy

$$u'/u\big|_{r=0} = \text{const.} \tag{6}$$

It is also the condition for the orthogonality of the energy eigenfunctions.

The radial probability current at the origin for the complex combination of two energy eigenfunctions, $u = c_1 u_1 + c_2 u_2$, is proportional to the following quantity:

$$-i[u^* u' - u^{*\prime} u]_{r=0} = Im(c_1^* c_2)[u_1 u_2' - u_2 u_1']_{r=0} \tag{7}$$

Therefore, when the wavefunction u is neither vanishing nor infinite at the origin, the hermitian condition (5) is equivalent to that for the vanishing radial probability current of wavefunctions at the origin.

In mathematics, the constant in (6) is a one-parameter family of self-adjoint extensions of the Hamiltonian. A different choice of the constant corresponds to different phase shifts for scattering states and different energy levels for bound states, which can be measured in experiments. Therefore, it is not allowed in physics to choose the constant arbitrarily. A usual choice of the constant is $C \sim \infty$, i.e., the wavefunctions are vanishing at the origin. This choice can be understood by the following physical model. Assume that the angular momentum in "S wave" tends to be zero but is not equal to zero exactly, that is, there is an additional infinitesimal centrifugal potential $\varepsilon(\varepsilon+1)/r^2$, where ε is a positive infinitesimal quantity. This centrifugal potential is of no effect on the finite r, but important near the origin: it makes one solution divergent and the other vanishing at the origin. This physical model is, in fact, similar to that of introducing an infinitesimal "extra" magnetic moment by Kazama-Yang-Goldhaber[4].

Schrödinger equations have their own characteristics. The radial equation (1) comes from the three-dimensional Schrödinger equation

$$\nabla^2\psi + [E - V(r)]\psi = 0 \tag{8}$$

$$\psi = \frac{1}{r} u_l(r) Y^l_m(\theta, \varphi) \tag{9}$$

If $u(r) \sim$ const. at the origin, because

$$\nabla^2 \frac{1}{r} = -4\pi\delta(\boldsymbol{r}) \tag{10}$$

this solution does not satisfy (8) in which there is no potential of δ function. Therefore, the solution u(r) which tends to be a nonvanishing constant should be ruled out for Schrödinger equation (8), but it seems to be an admissible one for the radial equation (1) in the mathematical viewpoint.

3. FERMIONS MOVING IN A MAGNETIC MONOPOLE FIELD

If a spherically symmetric potential V(r) of Dirac equation has a good asymptotic behaviour at the origin, the solutions are vanishing at the origin, and then there is no singular problem for the Hamiltonian. However, the singular problem occurs when a fermion moving in a magnetic monopole field or a strong Coulomb field is studied. In these cases the hermitian of the Hamiltonian is related to the boundary conditions of wavefunctions at the origin. In this paper we discuss the case with a magnetic monopole field, but leave the case with a strong Coulomb field elsewhere.

The Dirac equation for a fermion moving in a magnetic monopole field is as follows

$$[\boldsymbol{\alpha} \cdot (-i\nabla - e\boldsymbol{W}) + \beta M]\psi = E\psi \tag{11}$$

For the Wu-Yang U(1) magnetic monopole solution W(r), the wavefunctions with the lowest angular momentum j = 0 may not be vanishing at the origin. In the section of gauge[10] the wavefunction ψ (r) can be expressed as follows

$$\psi(r) = \frac{1}{r}\begin{pmatrix} if(r) & \eta(\theta,\varphi) \\ g(r) & \eta(\theta,\varphi) \end{pmatrix}, \quad \eta(\theta,\varphi) = \frac{1}{\sqrt{2}}\begin{pmatrix} Y_{\frac{1}{2}-\frac{1}{2}}(\theta,\varphi) \\ Y_{\frac{1}{2}\frac{1}{2}}(\theta,\varphi) \end{pmatrix} \tag{12}$$

where Y is the monopole harmonics[10]. The radial equation becomes

$$f' = -(E+M)g, \quad g' = (E-M)f \tag{13}$$

when |E| > M we obtain the scattering solutions

$$\begin{aligned} f &= \sqrt{E+M}\,\sin(kr+\delta_0), \quad g = -\sqrt{E-M}\,\cos(kr+\delta_0), \quad E > M \\ f &= \sqrt{|E|-M}\,\sin(kr+\delta_0), \quad g = \sqrt{|E|+M}\,\cos(kr+\delta_0), \quad E < -M \end{aligned} \tag{14}$$

Because f and g tend to constants at the origin, ψ is divergent and not single-valued at the origin, but the probability in a small volume near the origin is finite and definite. The hermitian condition of the Hamiltonian is

$$\begin{aligned} &\int \psi_1^+ H\psi_2(d^3x) - \int (H\psi_1)^+\psi_2(d^3x) \\ &= (f_1^* g_2 - g_1^* f_2)\big|_0^\infty = \left[g_1 g_2\left(\frac{f_1}{g_1} - \frac{f_2}{g_2}\right)\right]_{r=0} \end{aligned} \tag{15}$$

Just like the case in the Schrödinger equation, the right-handside of (15) in infinity is vanishing in average. Therefore, in the present case the hermitian condition of the Hamiltonian becomes

$$\left.\frac{f}{g}\right|_{r=0} = \text{const.} \tag{16}$$

The physical meaning of this condition is that the radial probability current of wavefunctions at the origin must be vanishing, because for the complex combination of wavefunctions $\psi = c_1\psi_1 + c_2\psi_2$, the radial probability current at the origin is proportional to

$$-i(f^*g - g^*f)\big|_{r=0} = Im(c_1^* c_2)\left[g_1 g_2\left(\frac{f_1}{g_1} - \frac{f_2}{g_2}\right)\right]_{r=0} \tag{17}$$

Besides, if condition (16) holds, the energy eigenfunctions are orthogonal to each other. The different choice of the constant C in (16) corresponds to the different phase shifts for scattering states and the different energy levels for bound states.

In the terminology of Weyl and von Neumann this kind of Hamiltonian is of limit circle type at the origin and of limit point type in infinity. For the Hamiltonian of this kind, there are eigenfunctions with the eigenvalues E = ±iM, that are finite at the origin

$$f_{\pm} = M e^{\pm i\pi/8} e^{-\sqrt{2}Mr}, \quad g_{\pm} = M e^{\mp i\pi/8} e^{-\sqrt{2}Mr}, \quad E = \pm iM \tag{18}$$

The numbers of independent solutions with E = ± iM are called deficiency indices (m_+,m_-). For the present case, $m_+ = m_- = 1$. According to the general mathematical method[2], the ratio of radial functions at the origin satisfies a condition with a real parameter θ :

$$\left.\frac{f}{g}\right|_{r=0} = \left.\frac{e^{i\theta}f_+ + e^{-i\theta}f_-}{e^{i\theta}g_+ + e^{-i\theta}g_-}\right|_{r=0} \tag{19}$$

Substituting (18) into (19), we obtain the constant C in (16) as follows:

$$C = \frac{\cos(\theta + \pi/8)}{\cos(\theta - \pi/8)} = \frac{1}{\sqrt{2}}[1 - \tan(\theta - \pi/8)] \tag{20}$$

where $-\infty < C < +\infty$.

For a definite C, from (14) we have the scattering phase shift

$$\tan\delta_0 = \begin{cases} -C\sqrt{\dfrac{E-M}{E+M}} & E > M \\ C\sqrt{\dfrac{|E|+M}{|E|-M}} & E < -M \end{cases} \tag{21}$$

where $|E| < M$, the solutions to (13) are

$$f = \sqrt{M+E}\, e^{-\sqrt{M^2-E^2}\, r}; \quad g = \sqrt{M-E}\, e^{-\sqrt{M^2-E^2}\, r} \tag{22}$$

The energy levels for the bound states satisfy

$$\sqrt{\frac{M+E}{M-E}} = C \tag{23}$$

Kazama-Yang-Goldhaber introduced an infinitesimal extra magnetic moment[4]

$$\frac{Ze}{2M}(1+\kappa), \quad |\kappa| \ll 1 \tag{24}$$

that is, introduced an additional term in Hamiltonian

$$H_{\text{add}} = -\kappa q \beta \boldsymbol{\sigma} \cdot \boldsymbol{r}(2Mr^3)^{-1} \tag{25}$$

H_{add} is of no effect for the finite r, but important near the origin, and it determines the constant C as[4]

$$\left.\frac{f}{g}\right|_{r\to 0+} = -\frac{\kappa q}{|\kappa q|} = C \tag{26}$$

From (23) there is a zero energy solution for C = 1, but no bound state for C = -1.

Dai and Ni[6] introduced a principle, called "principle of orthogonality and variation". The orthogonal condition of eigenfunctions is the same as (16), but according to the variation principle, "real physical ground state is the state with the lowest energy among all the possible states", the extreme value for (23) occurs at E = M or -M, obviously. However, the solutions with E = ± M are not the bound states for (13). Ref.[6] assumed that the lowest energy is zero, then C = 1. This result coincides with that of Ref.[4]. This assumption is put by hand and seems to be artificial.

Yamagishi[7] discovered that the constant C in (16) is related to the vacuum fractional electric charge, so C is related to the parameter of θ vacuum by the Witten formula[8]. This condition for determining C seems to be a physically admissible one, even though the result from it is different from those from Ref.[4] and [6].

It is possible to follow the physical model in the Schrödinger equation discussed in Sec.2, that is, to introduce an infinitesimal pseudoscalar potential[12]

$$H_{add} = i\,\frac{\varepsilon}{r}\gamma_5 \tag{27}$$

It takes effect only near the origin. The radial equation (13) becomes

$$f' - \frac{\varepsilon}{r} f = -(E+M)g, \quad g' + \frac{\varepsilon}{r} g = (E-M)f \tag{28}$$

H_{add} is equivalent to a centrifugal potential with a small angular momentum

$$\kappa = -\varepsilon \tag{29}$$

In the usual Dirac equation $\kappa = \mp(j + 1/2)$. H_{add} determines the constant C as

$$C = \begin{cases} 0 & \varepsilon < 0 \\ \infty & \varepsilon > 0 \end{cases} \tag{30}$$

From (23), there is no bound state.

Now, There are four methods and three results for determining the constant parameter. It will be judged by further experiments that which one is correct.

4. FERMIONS MOVING IN THE NONABELIAN MAGNETIC MONOPOLE FIELD

In 1974 't Hooft and Polyakov[13] found out an analytic magnetic monopole solution with a finite energy in SU(2) gauge theory. Embedding it into SU(5) grand unified model one obtains an SU(5) fundamental magnetic monopole solution. The Dirac equation for fermions moving in this monopole field can be solved exactly[14]. Outside the core of monopole, the fundamental monopole solution is the same as the Wu-Yang solution[9], and in the abelian gauge, the Dirac equation becomes that equation discussed by Kazama-Yang-Goldhaber. It is a common viewpoint that the U(1) monopole solution is an approximate form of the nonabelian monopole solution outside its core. Under this viewpoint it is possible to study the meaning of that constant parameter in terms of the exact solution of a fermion moving in the nonabelian magnetic monopole field.

The Dirac equation for a fermion moving in the SU(5) fundamental magnetic monopole field is as follows:

$$[\boldsymbol{\alpha}\cdot(-i\nabla - e\boldsymbol{W}) + \beta M]\psi = E\psi \tag{31}$$

In the Prasad-Sommerfield limit[15], the magnetic monopole solution is

$$\boldsymbol{W} = \frac{\hat{r}\wedge\boldsymbol{\tau}}{2er}[1 - v(r)], \quad v(r) = \frac{M_m r}{\sinh M_m r} \tag{32}$$

where M_m is the mass of magnetic monopole, $M_m \gg M$, and $\boldsymbol{\tau}$ are the isotopic Pauli matrices. For the lowest angular momentum, $j = 0$[15], we have

$$\begin{aligned} \psi(x)_a &= \sum_{a'=\pm\frac{1}{2}} \mathscr{D}^{1/2}_{aa'}(R_\delta^{-1}) \frac{1}{r} \begin{pmatrix} i\, f^{(2)}_{a'} \phi^{(2)}_{a'}(R_\delta) \\ g^{(2)}_{a'} \phi^{(2)}_{a'}(R_\delta) \end{pmatrix} \\ \phi^{(2)}_a(R_\delta) &= \frac{1}{\sqrt{4\pi}} \begin{pmatrix} -\mathscr{D}^{1/2}_{a,-1/2}(R_\delta) \\ \mathscr{D}^{1/2}_{a,1/2}(R_\delta) \end{pmatrix}, \quad R_\delta = R(\varphi, \theta, \delta) \end{aligned} \tag{33}$$

In fact, $\psi(x)$ is independent of δ. Transforming $\psi(x)$ into the abelian gauge, we can express $f^{(2)}_a$ and $g^{(2)}_a$ by the Kazama-Yang-Goldhaber solutions f_a and g_a

$$f^{(2)}_a = f_a, \quad g^{(2)}_a = \pm g_a, \quad a = \pm\frac{1}{2} \tag{34}$$

where the subscript a denotes the isotopic index.

The combinations of $f^{(2)}_a$ and $g^{(2)}_a$

$$\begin{aligned} F_1 &= f^{(2)}_{1/2} + f^{(2)}_{-1/2}, \quad G_1 = g^{(2)}_{1/2} - g^{(2)}_{-1/2} \\ F_2 &= f^{(2)}_{1/2} - f^{(2)}_{-1/2}, \quad G_2 = g^{(2)}_{1/2} + g^{(2)}_{-1/2} \end{aligned} \tag{35}$$

satisfy two separated sets of equations and their exact solutions[14] are as follows:

$$\begin{aligned} F_1 &= \sqrt{E+M}\left[\frac{2k}{M_m}\sin kr + \tanh\frac{M_m r}{2}\cos kr\right] \\ G_1 &= \sqrt{E-M}\left[-\frac{2k}{M_m}\cos kr + \coth\frac{M_m r}{2}\sin kr\right] \\ F_2 &= \sqrt{E+M}\left[-\frac{2k}{M_m}\cos kr + \coth\frac{M_m r}{2}\sin kr\right] \\ G_2 &= -\sqrt{E-M}\left[\frac{2k}{M_m}\sin kr + \tanh\frac{M_m r}{2}\cos kr\right] \end{aligned} \quad E > M \tag{36}$$

In the region where r is small but outside the core

$$\frac{1}{M_m} \ll r \ll \frac{1}{M}, \frac{1}{k} \tag{37}$$

we take the arbitrary combination of these two solutions

$$\begin{aligned} F_1 &\sim \sin\delta_0\sqrt{E+M}\cos kr, \quad G_1 \sim \sin\delta_0\sqrt{E-M}\sin kr \\ F_2 &\sim \cos\delta_0\sqrt{E+M}\sin kr, \quad G_2 \sim -\cos\delta_0\sqrt{E-M}\cos kr \end{aligned} \tag{38}$$

then, from (34) and (35) we obtain

$$\left.\begin{aligned} f_{\frac{1}{2}} &= \sqrt{E+M}\sin(kr+\delta_0), \quad g_{\frac{1}{2}} = -\sqrt{E-M}\cos(kr+\delta_0) \\ f_{-\frac{1}{2}} &= -\sqrt{E+M}\sin(kr-\delta_0), \quad g_{-\frac{1}{2}} = \sqrt{E-M}\cos(kr-\delta_0) \end{aligned}\right\} \quad E > M \tag{39}$$

It is nothing but the type of solutions (14). However, the two isotopic states are correlated. This correlation guarantees the hermitian of the Hamiltonian. Now, (15) becomes

$$[f^*_{(1)\frac{1}{2}}g_{(2)\frac{1}{2}} - g^*_{(1)\frac{1}{2}}f_{(2)\frac{1}{2}} + f^*_{(1)-\frac{1}{2}}g_{(2)-\frac{1}{2}} - g^*_{(1)-\frac{1}{2}}f_{(2)-\frac{1}{2}}]_{r=0} = 0 \tag{40}$$

where subscripts (1) and (2) denote two solutions with the different energies. Obviously, equation (40) holds if one substitutes (39) into it. Therefore, the Hamiltonian is hermitian for any δ_0. Note that there is no bound state for fermions moving in the SU(5) fundamental magnetic monopole field.[14,16]

In sum, the hermitian of an operator, for example, a Hamiltonian defined in a half-line is related to the boundary condition of wavefunctions. The Hamiltonian has a one-parameter family of self-adjoint extensions if its eigenfunctions are neither vanishing nor divergent at the origin. Taking a constant parameter guarantees the hermitian of the Hamiltonian, orthogonality of its eigenfunctions, and the vanishing radial probability current of the eigenfunctions at the origin. However, choice of different constant parameters causes different scattering phase shifts and different energy levels of bound states. Of course, it is not admissible in physics. The physical reason for the arbitrariness may be that an unknown physical condition must have been missed. Perhaps, this condition is related to the assumption of the point source. In the problem of the monopole the difficulty will be overcome by adding a new degree of freedom (for example, introducing the isotopic spin). There also exists the difficulty in the problem of fermions moving in a strong Coulomb field.

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