

A Procedure to Solve the Eigen Solution to Dirac Equation

Ying-Qiu Gu *

School of Mathematical Science, Fudan University, Shanghai 200433, China

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Abstract: In this paper, we provide a procedure to solve the eigen solutions of Dirac equation with complicated potential approximately. At first, we solve the eigen solutions of a linear Dirac equation with complete eigen system, which approximately equals to the original equation. Take the eigen functions as base of Hilbert space, and expand the spinor on the bases, we convert the original problem into solution of extremum of an algebraic function on the unit sphere of the coefficients. Then the problem can be easily solved. This is a standard finite element method with strict theory for convergence and effectiveness.

Keywords: Dirac equation, spinor field, algorithm, finite element method

1 Introduction

To study the properties of the elementary particles we solve the eigen solutions of Dirac equations. In some cases with symmetrical potential, the eigen solutions of Dirac can be solved exactly [1]- [6]. However, in the usual cases, the rigorous solution is absent, and we have to solve the approximate solutions with required accuracy. Quantum field theory provides a method to solve the approximate solutions. However it is inconvenient for some cases due to the complicated procedure, infinity problem.

In this paper, we provide a standard finite element method to solve the eigen solutions approximately, which is efficient for most cases and can be easily realized by computer. The solving procedure is that, at first, we solve the eigen solutions ψ_n of a linear Dirac equation with complete eigen functions, which approximately equals to the original equation. The normalized eigensolutions ψ_n form the bases of Hilbert space, and we can represent the solutions of the original Dirac equation by $\phi = \sum X_n \psi_n$, where X_n are coefficients. Substituting it into the action of the original equation, we convert the problem into solving the extremum of an algebraic equation on the unit sphere $\sum X_n^2 = 1$, which is much simpler than the original one. The calculation shows that this procedure is effective and convenient and suitable for the nonlinear Dirac equations. This process is similar to second quantization, but here

only normal mathematics is involved and the calculation can be easily performed by computer. In what follows, we take an electron in Coulomb potential and magnetic field as an example to show the solving procedure.

2 Equations and Simplification

At first, we introduce some notations. Denote the Minkowski metric by $\eta_{\mu\nu} = \text{diag}(1, -1, -1, -1)$, Pauli matrices by

$$\sigma = (\sigma^j) = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}. \quad (2.1)$$

Define 4×4 Hermitian matrices as follows

$$\alpha^\mu = \left\{ \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}, \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \right\}, \quad \gamma = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad (2.2)$$

where $\mu \in \{0, 1, 2, 3\}$, $x^0 = ct$. The Dirac equation for an electron in potential A^μ is given by

$$\alpha^\mu (\hbar i \partial_\mu - e A_\mu) \phi = \mu c \gamma \phi, \quad (2.3)$$

in which the potential reads

$$A_0 = -\frac{Ze}{r}, \quad \mathbf{A} = \frac{1}{2} B(-y, x, 0) = \frac{1}{2} B r \sin \theta (-\sin \varphi, \cos \varphi, 0). \quad (2.4)$$

The corresponding Lagrangian is given by

$$\mathcal{L} = \phi^\dagger \alpha^\mu (i \partial_\mu - e A_\mu) \phi - \mu c \phi^\dagger \gamma \phi. \quad (2.5)$$

* Corresponding author e-mail: yqgu@fudan.edu.cn

If the magnetic field $B \neq 0$, the rigorous solution is absent.

In this case, the magnetic quantum number m_z and the spin s are still conserved, which also hold for most cases. So the eigen solution takes the following form[6]

$$\phi = (u_1, u_2 e^{\theta i}, -iv_1, -iv_2 e^{\theta i})^T \exp(m_z \phi i - \frac{mc^2}{\hbar} it), \quad (2.6)$$

where the index ‘T’ stands for transpose, $m_z \in \{0, \pm 1, \pm 2, \dots\}$, and $u_k, v_k (k = 1, 2)$ are real functions of r and θ .

In the case $B = 0$, we have $u_1 = u_2, v_1 = \pm v_2$ and the solution can be solved in the form of spin spherical harmonics[1]. However this solution has complicated coefficients, which is inconvenient for expansion as bases of Hilbert space.

In order to simplify (2.5) for approximate computation, we make transformation

$$g = u_1 + u_2 i \quad f = v_1 - v_2 i. \quad (2.7)$$

Substituting it into (2.5) we get

$$\mathcal{L} = (\mathcal{L}_0 + \mathcal{L}_B + \mathcal{L}_f) \mu c, \quad (2.8)$$

$$\mathcal{L}_0 \equiv \left(\text{Re} \left[e^{\theta i} \left(-\bar{g}(\partial_r + \frac{1}{r}\partial_\theta) f + f(\partial_r + \frac{1}{r}\partial_\theta) \bar{g} \right) \right] - \frac{1}{r \sin \theta} (m_z + \frac{1}{2})(\bar{g} \bar{f} - g f) \right) \rho + \frac{Z\alpha\rho}{\epsilon(|g|^2 + |f|^2) - \frac{Z\alpha\rho}{2\pi} |g|^2 - (2 + \kappa)|f|^2}, \quad (2.9)$$

$$\mathcal{L}_f \equiv \left(\kappa - \frac{Z\alpha\rho}{r} \right) |f|^2, \quad (2.10)$$

$$\mathcal{L}_B \equiv \mu_B B \cdot \frac{i(gf - \bar{g}\bar{f})r \sin \theta}{\rho}, \quad (2.11)$$

in which $\epsilon \ll 1$ is dimensionless energy defined by $m = (1 - \epsilon)\mu$, $\rho = \frac{\hbar}{\mu c}$ is the Compton wave length used as length unit, κ is a constant to improve convergent rate. In the case (2.4) we set $\kappa = 0$ due to the small value of α or weakness of electromagnetic interaction. For the strong interaction we can set κ equal to the average potential[7]. $\mu_B = \frac{\hbar e}{2m}$ is the Bohr magneton of electron.

In (2.8), \mathcal{L}_0 almost keeps all invariance of relativity and has simple and complete eigensolutions, which can be used as the bases of Hilbert space, we call it the representation space of spinor. \mathcal{L}_f and \mathcal{L}_B are the trouble terms with small energy, which act as perturbation in the calculation.

In what follows we take $\mu c = 1$ as energy unit, then (2.8) becomes dimensionless. For (2.9), we can solve the rigorous eigensolutions by making transformation

$$g = U(r)M(\theta), \quad f = V(r)N(\theta), \quad M = P(\theta) + Q(\theta)i. \quad (2.12)$$

By variation of (2.9) we find $N = M e^{-i\theta}$ and

$$\partial_\theta P = \cot \theta m_z P + (m_z + K)Q, \quad (2.13)$$

$$\partial_\theta Q = -\cot \theta (m_z + 1)Q + (m_z + 1 - K)P, \quad (2.14)$$

in which $K = \pm 1, \pm 2, \dots$ corresponding to orbital angular momentum, P, Q are associated Legendre functions. The radial functions satisfy

$$\partial_r^2 U + \frac{2}{r} \partial_r U - \left(\frac{K(K-1)}{r^2} + \frac{\epsilon(2-\epsilon)}{\rho^2} + \frac{Z\alpha(2-\epsilon)}{r\rho} \right) U = 0, \quad (2.15)$$

and

$$V = \frac{(r\partial_r U - (K-1)U)\rho}{(2-\epsilon)r}. \quad (2.16)$$

The above equations can be easily solved, and the solutions are all elementary functions. The normalizing conditions are as follows

$$\int_0^\pi (P^2 + Q^2) 2\pi \sin \theta d\theta = 1, \quad \int_0^\infty (U^2 + V^2) r^2 dr = 1. \quad (2.17)$$

3 Eigen Solutions to the equation

Due to the parity invariance of the eigensolutions, if g takes the form $\sum U_n \exp(2n\theta i)$, then f will be $\sum V_n \exp((2n-1)\theta i)$, or vice versa. Considering the case $m_z = 0$, by solving (2.13) and (2.14), we have normalized functions M_K . Some simple ones are displayed as follows

$$M_{-2} = \frac{\sqrt{3}}{8\sqrt{\pi}} (3e^{2\theta i} + 1), \quad M_1 = \frac{1}{2\sqrt{\pi}}, \quad M_3 = \frac{\sqrt{3}}{16\sqrt{\pi}} (e^{2\theta i} + 2 + 5e^{-2\theta i}). \quad (3.1)$$

In usual cases, taking $|K| \leq 3$ is enough for approximate solution. By (2.15), we get

$$U = \left[C_1 r^{K-1} L_{n-K}^{2K-1} \left(\frac{2r}{r_n} \right) + C_2 r^{-K} L_{n+K-1}^{1-2K} \left(\frac{2r}{r_n} \right) \right] \exp \left(-\frac{r}{r_n} \right) \beta, \quad (3.2)$$

where L is Laguerre polynomials, $n \geq |K|$ is positive integer, $C_1 = 0$ corresponding to $K < 0$ and $C_2 = 0$ corresponding to $K > 0$, and

$$\epsilon_n = \frac{2Z^2 \alpha^2}{Z^2 \alpha^2 + 4n^2}, \quad r_n = \frac{(Z^2 \alpha^2 + 4n^2) \rho}{4Z\alpha n}. \quad (3.3)$$

Substituting (3.2) and (3.3) into (2.16), we can get function V . For all eigensolutions we have

$$\int_0^\infty U_{K,n}^2 r^2 dr = 1 - \frac{1}{2} \epsilon_n, \quad \int_0^\infty V_{K,n}^2 r^2 dr = \frac{1}{2} \epsilon_n. \quad (3.4)$$

Since the solution $U_{K,n}$ can be easily generated by computer, here we only display the simplest one

$$U_{1,1} = \frac{\sqrt{2(2-\epsilon_1)}}{\sqrt{r_1^3}} e^{-\frac{r}{r_1}}, \quad V_{1,1} = \frac{-\sqrt{2}\rho}{\sqrt{(2-\epsilon_1)r_1^5}} e^{-\frac{r}{r_1}}. \quad (3.5)$$

Due to the normalization of the eigenfunctions, the calculation of expansion of (g, f) is convenient. For example, we take

$$g = \sum_{k=0}^3 X_k U_{1,k+1} M_1 + (X_4 U_{-2,3} + X_5 U_{-2,4}) M_{-2} + (X_6 U_{3,3} + X_7 U_{3,4}) M_3, \quad (3.6)$$

$$f = \left[\sum_{k=0}^3 X_k V_{1,k+1} M_1 + (X_4 V_{-2,3} + X_5 V_{-2,4}) M_{-2} + (X_6 V_{3,3} + X_7 V_{3,4}) M_3 \right] e^{-\theta i}. \quad (3.7)$$

Substituting them into (2.9) we have the action

$$I_0 \equiv 2\pi \int_0^\pi dr \int_0^\pi \mathcal{L}_0 r^2 \sin \theta d\theta = \sum_{k=0}^7 (\epsilon - \epsilon_k) X_k^2, \quad (3.8)$$

which is diagonal due to eigenfunctions of \mathcal{L}_0 . This can be used to check the correctness of computing program. Usually, (g, f) is mainly related with the eigenfunctions whose quantum numbers near that of (g, f) .

Substituting (3.6, 3.7) into (2.10), we can get action $I_e = -\sum a_{k,l} X_k X_l$, and then we have

$$I_0 + I_e = \sum_{k=0}^7 (\varepsilon - \varepsilon_k) X_k^2 - \sum_{k,l=0}^7 a_{k,l} X_k X_l, \quad (3.9)$$

which becomes the approximate action of an electron in Coulomb potential. Solving the eigenvalues of (3.9) we get the numerical energy spectrums. Comparing them with rigorous one

$$\begin{aligned} \varepsilon_{K,n} &= 1 - \left(1 + \frac{\alpha^2}{(n - |K| + \sqrt{K^2 - \alpha^2})^2} \right)^{-\frac{1}{2}} \\ &= \frac{\alpha^2}{2n^2} + \left(\frac{1}{2n^3|K|} - \frac{3}{8n^4} \right) \alpha^4 + O(\alpha^6), \end{aligned} \quad (3.10)$$

we have the accuracy $O(\alpha^6)$ for (3.6, 3.7).

Now we compute the magnetic energy of (2.11). Substituting (3.2, 3.3, 3.4) and (2.16) into \mathcal{L}_B , we get the energy of magneton

$$\delta E = g_s \mu_B B, \quad g_s = -\frac{K(2m_z + 1)}{2K - 1}, \quad (3.11)$$

g_s is similar to the Lande factor, which is independent of n . From the above equations we find that, for the eigenfunctions of \mathcal{L}_0 the relations become simple and neat. So these eigenfunctions form a good coordinate system for expansion of the original functions (g, f).

Substituting (3.6) and (3.7) into \mathcal{L}_B we get action

$$I_B = -\mu_B B \sum_{k,l=0}^7 b_{k,l}(Z) X_k X_l. \quad (3.12)$$

We solve the eigen values of the coefficient matrix, and then we can compute the anomalous magnetic moment of a free electron. In this case, the eigenfunctions just act as the bases of representation space, rather than the electron is really in Coulomb potential. By adjusting parameter Z , when $Z=12$ and $\bar{r}=45\rho$ we get the magnetic moment $g_s = -1.001159652$, which means the wave function of a free electron is a concentrated package. However the magnetic moment of an electron is not a constant, which depends on its state.

The total approximation action corresponding to the original equation (2.3) is given by

$$I = I_0 + I_e + I_B = \sum_{k=0}^7 (\varepsilon - \varepsilon_k) X_k^2 - \sum_{k,l=0}^7 (a_{k,l} + \mu_B B b_{k,l}) X_k X_l. \quad (3.13)$$

Solving the eigenvalues and eigenvectors of the coefficient matrix, and substituting them into approximation (3.6, 3.7), we get the approximation solutions to the original problem (2.3). This process is equivalent to solving the extremum of (3.13) on the sphere $\sum X_k^2 = 1$, which is also suitable for the case with nonlinear potentials.

4 Discussion and Conclusion

In this paper we provide a convenient procedure to approximately solve the eigen solutions to the Dirac equation with complicated potentials. (2.9) has complete eigen functions and (2.15) is similar to the Schrödinger equation. The approximate equation (2.9) keeps all main properties of the original equation (2.8), such as energy spectrums, invariance etc. Expressing the physical variables and relations of spinor by the eigen functions of the representation space, we have simple and neat formalism, such as (3.2, 3.3, 3.4) and (3.11).

This procedure is a standard finite element method which has strict mathematical theory for its convergence and effectiveness. Practical simulation shows the procedure is also suitable for computing nonlinear potentials. The procedure can be easily realized by computer. For the total action of the original problem similar to (3.13), we can design high convergent speed numerical program.

It should be mentioned the base functions as an ensemble have orthogonality for different (n, K) , but the radial base functions corresponding to different K are not definitely orthogonal. Besides, under what conditions the bases of the representation space have completeness is still a problem.

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Ying-Qiu Gu

Senior Engineer, received the PhD degree in Institute of Mathematics at Fudan University. His research interests are in the areas of fundamental physics including the mathematical methods and models for elementary systems, general relativity and foundation of physics.