Rayleigh-Ritz Variational Method for Spin-Less Relativistic Particles

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Abstract: ***In relativistic quantum theory, for many problems of physical interest, exact solutions are not available even in one dimension. Therefore it is highly desirable to investigate and apply the methods of approximation which work in non-relativistic cases to relativistic conditions. In this article we extend the well-known Rayleigh-Ritz variational method used in non-relativistic quantum mechanics to relativistic case. To test the validity of the approach we apply the method to relativistic spin-less quantum particles under different potential conditions, such as free particle in an infinite well, charged particle in a coulomb potential and particle in an infinite range linear potential. The results are then compared with those of exact methods, comparison validates the method to a very good extent.***

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1. Introduction

In relativistic quantum theory, for many problems of physical interest, exact solutions are not available even in one dimension. Therefore it is highly desirable to investigate and apply the methods of approximation which work in non-relativistic cases to relativistic conditions [1]. It is found that the extension of well-known non-relativistic approximations might be possible if the relativistic wave equations are reduced to Schrödinger like form. Several researchers have extended Rayleigh-Ritz Variational method for relativistic spin-half particles [2], [3], [4], [5], [6]. But Rayleigh-Ritz Variational method for relativistic spin-zero particles has not been done. In this article we discus relativistic approach to Variational method and apply the same to obtain approximate ground state eigenenergies of relativistic spin-less particles in certain well-known potentials.

2. Review of Non Relativistic Rayleigh-Ritz Variational Method

Variational principles are widely used in quantum mechanical problems [7]. We come across variational methods such as Hulthen, Schwinger, Rayleigh-Ritz principle etc,. Rayleigh-Ritz principle for estimation of ground state energy is one of the best known and widely used of all variational principles [8], the other variational principles mentioned above are used in scattering theory and also applicable elsewhere. Here in this section, we review Rayleigh-Ritz Principle to find ground state energy.

Let $|\psi\rangle$ be any stationary state of a system and E be the corresponding expectation value of the Hamiltonian H. Therefore

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = E \qquad (1)$$

Let E_0 be the ground state of H.

Expanding $|\psi\rangle$ in a complete set of eigenfunctions of H as

$$|\psi\rangle = \sum_n C_n|\phi_n\rangle$$

where $|\phi_n\rangle$ obeys the equation

$$H|\phi_n\rangle = E_n|\phi_n\rangle$$

Therefore we could write

$$E = \frac{\left\langle \sum_n C_n\phi_n \middle| H \middle| \sum_n C_n\phi_n \right\rangle}{\left\langle \sum_n C_n\phi_n \mid \sum_n C_n\phi_n \right\rangle} = \frac{\sum_n C_n^* C_n E_n}{\sum_n C_n^* C_n} \qquad (2)$$

Since the ground state energy E_0 is less than all the higher energy values, we have

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geq \frac{\sum_n C_n^* C_n E_0}{\sum_n C_n^* C_n} \qquad (3)$$

or

$$E \geq E_0$$

Thus the expectation value of H gives an upper limit to the ground state energy eigenvalue, this is known as Rayleigh-Ritz principle. Generally, in order to obtain a good estimate of E, one chooses a trial wave function $|\psi(\alpha)\rangle$ parametrized in terms of α, and evaluates the expectation value of H for a family of states as

$$E(\alpha) = \frac{\langle\psi(\alpha)|H|\psi(\alpha)\rangle}{\langle\psi(\alpha)|\psi(\alpha)\rangle} \qquad (4)$$

Then minimizing $E(\alpha)$ with respect to α one can get an approximate value for ground state energy.
Further, the improvement in the trial function could be done by numerical iterations to reduce the error between the approximate and exact value of ground state energy.

3. Extension of Rayleigh-Ritz Variational Method to find ground state eigenvalues of Relativistic spin-zero particles

In relativistic quantum mechanics, for a free particle with rest mass energy we can write

$$E^2 = P^2c^2 + m^2c^4$$

The general potential $V(x)$ is introduced as fourth component of vector potential using minimal coupling scheme as [9]

$$[E - V(x)]^2 = P^2c^2 + m^2c^4$$

The corresponding wave equation in one dimension is

$$[E - V(x)]^2 \psi(x) = \left(-\hbar^2c^2 \frac{d^2}{dx^2} + m^2c^4\right)\psi(x) \quad (5)$$

The above equation could be reduced to Schrödinger form as

$$E_{eff}\, \psi(x) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_{eff}(x)\right]\psi(x) \quad (6)$$

Where

$$E_{eff} = \frac{E^2 - m^2c^4}{2mc^2}$$

$$V_{eff}(x) = \frac{2EV(x) - V^2(x)}{2mc^2}$$

The Hamiltonian

$$H_{eff} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_{eff}(x)$$

is hermitian as both the terms on right hand side of the above equation are hermitian.

For weak potentials V_{eff} will have the same sign as V.

In order to get bound states one has to have condition [10]

$$\int V_{eff}(x)\, dx \le 0.$$

Thus we write

$$H_{eff}\, \psi_n(x) = E_n\, \psi_n(x)$$

As $\psi_n(x)$ are orthogonal, thus E_n are real.

We follow the formal method of Rayleigh-Ritz principle as done in non relativistic case[11].

Let ψ_α be a trial function with variational parameter α describing the system, that could be expanded in terms of complete orthonormal set as

$$\psi_\alpha = \sum a_n \psi_n$$

Thus the expectation value of the Hamiltonian

$$E_{eff}(\alpha) = \frac{\langle \psi_\alpha | H_{eff} | \psi_\alpha \rangle}{\langle \psi_\alpha | \psi_\alpha \rangle} = \frac{\sum E_n |a_n|^2}{\sum |a_n|^2} \ge E_0 \quad (7)$$

Hence

$$E_{eff}(\alpha) \ge E_0$$

Therefore ground state eigenenergy could be approximately obtained by minimizing $E_{eff}(\alpha)$ with respect to variational parameter α.

4. Relativistic free particle in an infinite square well potential

Let us consider a non-relativistic particle of mass m moving in the one dimensional infinite square well defined by

$$V_x = 0 \text{ for } -a < x < a$$

$$V_x = \infty \text{ for } |x| > a.$$

This problem could be solved exactly [11] to get the exact ground-state energy

$$E_0 = \frac{\hbar^2\pi^2}{8ma^2} = 1.23370\frac{\hbar^2}{ma^2}$$

In relativistic approach, we take trial function as

$$\phi(x) = (a^2 - x^2)(1 + \alpha x^2) \quad (8)$$

Since the particle is free within the box, we can write $V_{eff} = 0$ for $-a < x < a$

Therefore

$$H_{eff} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

Thus

$$E_{eff}(\alpha) = \frac{\langle \phi | H_{eff} | \phi \rangle}{\langle \phi | \phi \rangle} \quad (9)$$

Substituting for H_{eff} equation 9 becomes,

$$E_{eff}(\alpha) = \frac{-\frac{\hbar^2}{2m}\int_{-a}^{+a}(a^2 - x^2)(1+\alpha x^2)\frac{d^2}{dx^2}\left[(a^2 - x^2)(1+\alpha x^2)\right]dx}{\int_{-a}^{+a}(a^2 - x^2)^2(1+\alpha x^2)^2\, dx} \quad (10)$$

On evaluating the above integral we get,

$$E_{eff}(\alpha) = \frac{3\hbar^2}{4ma^2}\left[\frac{11a^4\alpha^2 + 14a^2\alpha + 35}{a^4\alpha^2 + 6a^2\alpha + 21}\right] \quad (11)$$

Minimizing $E_{eff}(\alpha)$ with respect to variational parameter α, we write

$$\frac{d}{d\alpha}\left[E_{eff}(\alpha)\right] = 0$$

This gives a quadratic equation in α as,

$$26a^4\alpha^2 + 196a^2\alpha + 42 = 0$$

On solving the above equation, we get two different roots as

$$\alpha = -\frac{0.22075}{a^2}, \quad \alpha = -\frac{7.31771}{a^2} \quad (12)$$

Taking $\alpha = -\frac{0.22075}{a^2}$, the equation 11 becomes

$$E_{eff}(\alpha_0) = 1.23372\frac{\hbar^2}{ma^2}$$

Substituting for E_{eff}, we get

$$E=\sqrt{\left[m^2c^4+2.46744\frac{\hbar^2c^2}{a^2}\right]} \quad (13)$$

Using binomial expansion [12]

$$E=\left[mc^2+1.23372\frac{\hbar^2}{ma^2}-0.7610\frac{\hbar^8}{m^3c^2a^4}+.....\right] \quad (14)$$

Thus it is clear that the first term is rest energy, the second term represents the approximate non relativistic upper bound for ground state energy, which is in very good agreement with exact value of ground state energy [11], and the third term represents the first order relativistic corrections to it neglecting contributions from higher order terms.

5. Relativistic-spin less charged particle in a Coulomb potential

In this section we consider a relativistic spin-less charged particle in a coulomb potential, we work out eigenenergy values for s state, we compare our results with that of results obtained by formal method of solving Klein Gordon equation.

For a non relativistic charged particle in a Coulomb potential $V(r)=-\frac{e^2}{r}$, we expect that the ground state wave function to have no angular momentum, no nodes, behave like r^0 as $r\to 0$ and vanish as $r\to\infty$.

So we choose the trial function

$$\psi(r,\theta,\phi,\alpha)=e^{-\alpha r} \quad (15)$$

Where α is the variational parameter

We find (upon ignoring angular variables),

$$E(\alpha)=\frac{\int_0^\infty\left[e^{-\alpha r}\left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}-\frac{e^2}{r}\right)e^{-\alpha r}\right]r^2dr}{\int_0^\infty e^{-2\alpha r}r^2dr} \quad (16)$$

On evaluation of the above integral we get

$$E(\alpha)=\frac{\hbar^2\alpha^2}{2m}-e^2\alpha \quad (17)$$

Minimizing $E(\alpha)$ with respect α,

We get

$$\alpha_0=\frac{me^2}{\hbar^2}$$

Thus

$$E(\alpha)=-\frac{me^4}{2\hbar^2}=-\frac{mc^2\gamma^2}{2} \quad (18)$$

Where

$$\gamma=\frac{e^2}{\hbar c}=\frac{1}{137}$$

is called fine structure constant.

Similarly for a relativistic charged particle in a Coulomb potential $V(r)=-\frac{e^2}{r}$, once again we expect that the ground state wave function to have no angular momentum, no nodes, behave like r^0 as $r\to 0$ and vanish as $r\to\infty$.

Hence we choose the trial function

$$\psi(r,\theta,\phi,\alpha)=e^{-\alpha r}$$

Where α is the variational parameter

The effective potential thus takes the form

$$V_{eff}=\frac{-\frac{2Ee^2}{r}-\frac{e^4}{r^2}}{2mc^2}$$

Thus, we find (upon ignoring angular variables)

$$\langle E_{eff}(\alpha)\rangle=\frac{\int_0^\infty\left[e^{-\alpha r}\left(-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+\left\{\frac{-\frac{2Ee^2}{r}-\frac{e^4}{r^2}}{2mc^2}\right\}\right)e^{-\alpha r}\right]r^2dr}{\int_0^\infty e^{-2\alpha r}r^2dr} \quad (19)$$

On evaluating the above integral we get,

$$\langle E_{eff}(\alpha)\rangle=\frac{\hbar^2\alpha^2}{2m}-\left[\frac{e^2E\alpha+e^4\alpha^2}{mc^2}\right] \quad (20)$$

Minimizing $\langle E_{eff}(\alpha)\rangle$ with respect to variational parameter α,

We write

$$\frac{d}{d\alpha}\left[\langle E_{eff}(\alpha)\rangle\right]=0$$

We get

$$\alpha_0=\frac{e^2E}{\hbar^2c^2-2e^4}$$

Thus we obtain

$$\langle E_{eff}(\alpha_0)\rangle=-\frac{E^2e^4}{2mc^2\left(\hbar^2c^2-2e^4\right)} \quad (21)$$

Upon substituting

$$E_{eff}=\frac{E^2-m^2c^4}{2mc^2}$$

we get

$$E=\frac{mc^2}{\sqrt{1+\frac{e^4}{\hbar^2c^2-2e^4}}}$$

Neglecting $2e^4$ in comparison with $\hbar^2c^2$, We get

$$E=mc^2\left[1+\gamma^2\right]^{-\frac{1}{2}} \quad (22)$$

Where

$$\gamma=\frac{e^2}{\hbar c}=\frac{1}{137}$$

is the fine structure constant.

The formal method of solving Klein Gordon equation for

Coulomb potential yield energy eigenvalues as [13], [14]

$$E = mc^2\left[1+\frac{\gamma^2}{\lambda^2}\right]^{-\frac{1}{2}} \tag{23}$$

Where bound states exists only if $\lambda = n' + s + 1$, in which n' is zero or positive integer and s is a non negative solution of the radial equation. Since we have applied the relativistic variational approach to $l = 0$ state, we find an excellent agreement between equation 22 and equation 23. Expanding the expression 22 for the energy levels, we get the results to terms of γ^4 as,

$$E = mc^2\left[1-\frac{\gamma^2}{2}+\frac{3}{8}\gamma^4\right] \tag{24}$$

The first term on right hand side of equation 24 is the rest energy, the second term is non relativistic ground state energy and the third term is the first order relativistic correction.

6. Relativistic Spin-Less Particle in an Infinite Range Linear Potential

In this section we consider a relativistic spin less particle in an infinite range linear potential which could be written as $V(x)=\infty$ for $x<0$ and $V(x)=kx$ for $x\geq 0$. The formal solution of Schrödinger equation gives complicated Airy functions. But we use variational approach to find ground state energy with a trial wave function of the form

$$\psi_\alpha(x) = Nxe^{-\frac{\alpha x^2}{2}} \tag{25}$$

Where α is variational parameter and N is normalization constant.

Non relativistically, we write the Hamiltonian of the particle in such a linear potential as

$$H = -\frac{1}{2}\frac{d^2}{dx^2}+kx$$

Here we have set atomic units $\hbar = m = 1$ to seek the solutions. Then the expectation value of the Hamiltonian for the trial wave function is:

$$E(\alpha) = \langle\psi(\alpha)|H|\psi(\alpha)\rangle \tag{26}$$

Substituting for $\psi(\alpha)$, we get

$$E(\alpha) = \int_0^\infty Nxe^{-\frac{\alpha x^2}{2}}\left(-\frac{1}{2}\frac{d^2}{dx^2}+kx\right)Nxe^{-\frac{\alpha x^2}{2}}dx \tag{27}$$

Where N is normalization constant.

On evaluating the above integrals we get,

$$E(\alpha) = \frac{3\alpha}{4}+\frac{2k}{\sqrt{\pi\alpha}} \tag{28}$$

Then we minimize with respect to α, to get the lowest value of $E(\alpha)$. Thus we put

$$\frac{d}{d\alpha}(E(\alpha)) = 0$$

Setting $k = 1$ for simplicity, we get,

$$\alpha_0 = \frac{2^{\frac{4}{3}}}{3^{\frac{2}{3}}\pi^{\frac{1}{3}}} \tag{29}$$

Substituting this in 28 we get the following value for the lowest energy:

$$E(\alpha_0) = 1.86105 \tag{30}$$

This can be compared with $E_{exact} = 1.85575$ [7], we find an excellent agreement.

Now we shall extend the same analysis for relativistic spin less particle.

The effective Hamiltonian for a relativistic spin less particle in an infinite range linear potential could be written as, $(\text{with} k = \hbar = m = 1)$

$$H_{eff} = -\frac{1}{2}\frac{d^2}{dx^2}+\frac{2Ex-x^2}{2} \tag{31}$$

Where again we have set, $k = 1$,

$$E_{eff}(\alpha) = \int_0^\infty Nxe^{-\frac{\alpha x^2}{2}}\left(-\frac{1}{2}\frac{d^2}{dx^2}+\frac{2Ex-x^2}{2}\right)Nxe^{-\frac{\alpha x^2}{2}}dx \tag{32}$$

On evaluating the above integrals, we get,

$$E_{eff}(\alpha) = \frac{3\alpha}{4}+\frac{2E}{\sqrt{\pi\alpha}}-\frac{3}{2\alpha} \tag{33}$$

Minimizing $E_{eff}(\alpha)$ with respect to variational parameter α, we get the following equation:

$$\frac{3}{4}-\frac{E}{\sqrt{\pi\alpha_0^{\frac{3}{2}}}}+\frac{3}{2\alpha_0^2} = 0$$

In order to obtain the root of the above equation to evaluate the bound state energy, we ignore the contribution from the quadratic term as its contribution is small for higher values of α. Thus we get,

$$\alpha_0 = \frac{2^{\frac{4}{3}}E^{\frac{2}{3}}}{3^{\frac{2}{3}}\pi^{\frac{1}{3}}} \tag{34}$$

Therefore

$$E_{eff}(\alpha_0) = 3E^{\frac{2}{3}}\left(\frac{6}{\pi}\right)^{\frac{1}{3}}$$

Substituting for $E_{eff}(\alpha_0)$, we get $E = 2.93882$. This contains the rest energy $(mc^2 = 1)$, Thus the ground state energy of a particle in an infinite range linear potential with relativistic correction is

$$E = 1.93882 \tag{35}$$

7. Results and Discussions

The variational method seems to be a powerful approximate method to obtain eigenenergies of quantum mechanical systems. It is extensively used in non relativistic quantum mechanics. In this article we have extended the Rayleigh-Ritz

Variational method for spin-less relativistic particles. To test the validity of the method extended for relativistic particles, we applied the same for free particle in an infinite square well potential by using an approximate trial function, we applied the method for a charged particle in a Coulomb potential by taking the exact wave function as trial function and the next section we applied the method for a relativistic spin less particle in an infinite range linear potential by assuming a model trial function instead of complicated airy functions. In all the three cases we found that the Variational method extended for relativistic case works effectively and the results are in good agreement with the results obtained by solving Klein Gordon equation and Schödinger equation. Thus the method becomes a very important tool to find eigenenergies of relativistic particles for which exact solutions are not available by formal methods. One could use iterative technique to improve trial function. It would be better if one could bracket the relativistic eigenenergies with lower and upper bounds. Further it would be interesting and important to extend this method to find excited energy states of relativistic particles.

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