A variational approach to ground state energy estimation in relativistic quantum systems

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Received 22 September 2023; accepted 31 January 2024

The variational method in quantum mechanics plays a crucial role in estimating upper bound values of eigenenergies, particularly in the efficient determination of ground state energies.This study applies the variational method to analyze ground state energies in quantum systems featuring certain relativistic elements within their Hamiltonians allowing to assess its efficacy. Furthermore, we compare the results obtained through this method with existing literature, shedding light on its accuracy and applicability in the context of relativistic quantum systems.

Keywords: Variational method; bound states; relativistic systems.

DOI: https://doi.org/10.31349/RevMexFisE.21.020212

1. Introduction

In quantum mechanics, exact solutions of the Schrödinger equation exist only for a few idealized systems. To address general problems, researchers must rely on approximation methods [1]. Various approximation techniques have been developed, each with its own domain of applicability. To study stationary states in quantum mechanics, researchers often turn to approximation methods, including the perturbation method, the WKB approximation, and the variational principle.

Among these methods, the variational method stands out for its effectiveness in estimating ground state energies and providing qualitative insights into the behavior of wave functions [5]. This method proves particularly valuable when dealing with systems for which the Hamiltonian is known, but the eigenvalues and eigenstates remain elusive. According to the variational principle, for any given trial function $|\psi\rangle$ parameterized by a variational parameter, the energy E always exceeds the exact energy E_0:

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0. \tag{1}$$

Equality in the above condition is achieved only when the trial function $|\psi\rangle$ is proportional to the true ground state $|\psi_0\rangle$. While the variational method can also approximate the energies of the first few excited states, its application becomes increasingly intricate with higher excited states. Consequently, the method primarily finds utility in determining ground state energies.

This paper leverages the variational method to compute the ground state energy of various relativistic systems. Specifically, we focus on three distinct systems: the hydrogen atom, the quantum harmonic oscillator, and quantum anharmonic oscillators. Our aim is to determine the ground state energies for these systems while considering the influence of relativistic effects. By doing so, we seek to understand the interplay between relativistic and non-relativistic effects and to provide valuable insights into the behavior of these systems within the framework of relativistic quantum mechanics.

2. Formalism

Guided by physical intuition and informed guesswork, we begin by selecting a trial wavefunction that is designed to encapsulate all the relevant physical properties associated with the ground state of the quantum system under investigation. However, in cases where certain properties remain unknown or uncertain, we introduce adjustable parameters represented as $\alpha_1, \alpha_2, \ldots$ into the trial wavefunction. These parameters allow us to account for the variability or imprecision in our knowledge of the system. With the trial wavefunction in place, we proceed to compute the ground state energy. This calculation involves employing the variational principle, as expressed in Eq. (1), and utilizing the relativistic Hamiltonian, which represents the total energy of the system.

The outcome of this calculation is an expression for the ground state energy, denoted as $E_0(\alpha_1, \alpha_2, \ldots)$, and it explicitly depends on the adjustable parameters $\alpha_1, \alpha_2, \ldots$:

$$E_0(\alpha_1, \alpha_2, \ldots) = \frac{\langle\psi_0(\alpha_1, \alpha_2, \ldots)|H|\psi_0(\alpha_1, \alpha_2, \ldots)\rangle}{\langle\psi_0(\alpha_1, \alpha_2, \ldots)|\psi_0(\alpha_1, \alpha_2, \ldots)\rangle}. \tag{2}$$

To identify the values of these adjustable parameters that minimize the expectation value of the energy, we differentiate $E_0(\alpha_1, \alpha_2, \ldots)$ with respect to each parameter, setting

the resulting derivatives equal to zero:

$$\frac{\partial E_0(\alpha_1,\alpha_2,\ldots)}{\partial \alpha_i} = \frac{\partial}{\partial \alpha_i}\frac{\langle\psi_0(\alpha_1,\alpha_2,\ldots)|H|\psi_0(\alpha_1,\alpha_2,\ldots)\rangle}{\langle\psi_0(\alpha_1,\alpha_2,\ldots)|\psi_0(\alpha_1,\alpha_2,\ldots)\rangle} = 0. \quad (3)$$

Here, i ranges over the parameters, such as $i = 1, 2, \ldots$. Once we've determined these parameter values, we can substitute them back into Eq. (2), yielding an approximate value for the ground state energy, denoted as $E_0(\alpha_1, \alpha_2, \ldots)$. Importantly, this approximate energy value serves as an upper bound for the true ground state energy, denoted as $E_{\min}$.

Moreover, by employing the trial wavefunction $|\psi_0(\alpha_1, \alpha_2, \ldots)\rangle$, we are able to approximate the exact ground state eigenstate, offering valuable insights into the characteristics of the ground state of the relativistic quantum system under investigation.

3. Hydrogen-like systems

The hydrogen atom, as the simplest atomic system, provides an ideal setting for a rigorous quantum mechanical analysis. In our approach, we adopt a trial wavefunction described by Eq. (4), which takes the form:

$$\psi(x) = Ae^{-\alpha r}. \quad (4)$$

Here, α represents a variational parameter, and A is the normalization constant, calculated as $A = \sqrt{\alpha^3/\pi}$. This choice of wavefunction is made with the aim of encompassing all the essential physical properties of the ground state. The total relativistic Hamiltonian for a hydrogen-like atom is defined by Eq. (5), where k is a parameter associated with the atomic nucleus and z represents the atomic number.

$$H = mc^2 + \frac{1}{2}\frac{p^2}{m} - \frac{k}{r}. \quad (5)$$

With this expression we proceed to evaluate its expectation value, denoted as $\langle H\rangle$ which is nothing but E_0:

$$\langle H\rangle = E_0 = \left\langle mc^2 + \frac{1}{2}\frac{p^2}{m} - \frac{k}{r}\right\rangle. \quad (6)$$

Breaking down each component: $\langle mc^2\rangle$ represents the average rest energy of the particle, which remains constant and is equal to mc^2.

$\langle(1/2)(p^2/m)\rangle$ quantifies the expectation value of the kinetic energy of the particle. To evaluate this term, we integrate the kinetic energy operator over the trial wavefunction, resulting in $(\hbar^2/2m)\alpha^2$.

$\langle(k/r)\rangle$ signifies the potential energy due to the interaction with the atomic nucleus. Similarly, integrating this term over the wavefunction results in $k\alpha$.

As a result, the value of energy can be expressed as:

$$E_0 = mc^2 + \frac{\hbar^2}{2m}\alpha^2 - k\alpha. \quad (7)$$

To determine the optimal value of α that minimizes the expectation value $\langle E\rangle$, we take its derivative with respect to α:

$$\frac{dE_0}{d\alpha} = \frac{\hbar^2}{m}\alpha - k = 0. \quad (8)$$

Solving this equation for α yields:

$$\alpha = \frac{km}{\hbar^2}. \quad (9)$$

Substituting this optimal value of α back into the expectation value of energy:

$$E_{\min} = mc^2 + \frac{\hbar^2}{2m}\left(\frac{km}{\hbar^2}\right)^2 - k\left(\frac{km}{\hbar^2}\right). \quad (10)$$

Simplifying further:

$$E_{\min} = mc^2 - \frac{k^2 m}{2\hbar^2}. \quad (11)$$

In this expression, the first term corresponds to the rest energy of the particle, while the second term represents a Rydberg-like expression for the energy levels of the hydrogen atom. It's essential to note that this equation accurately describes the exact relativistic ground state energy of the system, as confirmed by prior studies [6, 7].

4. The quantum harmonic oscillator

In this section, we explore the ground state energy of a relativistic quantum harmonic oscillator using the variational method. We begin by selecting a trial wavefunction of the form:

$$\Psi(x) = Ae^{-\alpha x^2}. \quad (12)$$

Here, α is a variational parameter, and A serves as the normalization constant, defined as:

$$A = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}}. \quad (13)$$

To account for relativistic effects, we modify the Hamiltonian expression, originally given as:

$$H^2 = p_x^2c^2 + m^2c^4. \quad (14)$$

We introduce an interaction term coupling momentum with the position, as defined in [8]:

$$p_x \longrightarrow p_x - im\omega x, \quad p_x^\dagger \longrightarrow p_x + im\omega x. \quad (15)$$

Under this coupling, the square of momentum becomes:

$$p_x^2 = \frac{1}{2}\left[p_x p_x^\dagger + p_x^\dagger p_x\right]. \quad (16)$$

As a result, the expression takes the form:

$$H = \sqrt{p_x^2c^2 + m^2\omega^2x^2c^2 + m^2c^4}. \tag{17}$$

Utilizing the variational method, we proceed to evaluate the expectation value of E:

$$\langle H^2\rangle = \left\langle -\hbar^2c^2\frac{d^2}{dx^2} + m^2x^2\omega^2c^2 + m^2c^4 \right\rangle. \tag{18}$$

Solving for this expectation value, we find:

$$\langle H^2\rangle = \hbar^2c^2|A|^2\sqrt{\frac{\pi\alpha}{2}} + |A|^2\frac{m^2\omega^2c^2}{2}\frac{\sqrt{\pi}}{(2\alpha)^{\frac{3}{2}}} + m^2c^4. \tag{19}$$

Applying the uncertainty principle,

$$\Delta H = \sqrt{\langle H^2\rangle - \langle H\rangle^2}. \tag{20}$$

In the case of a sharply defined energy, we have $\Delta H = 0$, implying $\langle H^2\rangle = \langle H\rangle^2$. Consequently, we obtain:

$$\langle H\rangle = \sqrt{\hbar^2c^2|A|^2\sqrt{\frac{\pi\alpha}{2}} + |A|^2\frac{m^2\omega^2c^2}{2}\frac{\sqrt{\pi}}{(2\alpha)^{\frac{3}{2}}} + m^2c^4}. \tag{21}$$

Upon substituting the expression for A, we derive:

$$E_0 = \sqrt{\hbar^2c^2\alpha + \frac{m^2\omega^2c^2}{4\alpha} + m^2c^4}. \tag{22}$$

To minimize $\langle E\rangle$ with respect to α, we differentiate with respect to α, leading to:

$$\alpha = \frac{m\omega}{2\hbar}. \tag{23}$$

Substituting this optimal α value back into (22), we arrive at the minimum expectation value of E:

$$E_{min} = \sqrt{\hbar m\omega c^2 + m^2c^4}. \tag{24}$$

Expanding (24) binomially, we can express the total relativistic energy as:

$$E_{min} = mc^2 + \frac{1}{2}\omega\hbar + \frac{1}{8}\frac{\omega^2\hbar^2}{mc^2} + \dots \tag{25}$$

Remarkably, this decomposition reveals the various components of the total relativistic energy, including the rest energy, non-relativistic energy, and relativistic corrections. Importantly, our result aligns with the findings presented in Refs. [9, 10].

5. Anharmonic oscillator

Quantum mechanical anharmonic oscillators (AHO) have garnered significant attention over the years due to their relevance in various branches of physics, including field theories, molecular physics, and solid-state physics, among others [11]. These systems have been thoroughly investigated using both analytical and numerical approaches. To estimate the relativistic energy of such a system, we select the following trial wavefunction:

$$\psi(x) = Ae^{-\frac{\lambda^2x^2}{2}}. \tag{26}$$

Here, λ represents a variational parameter, and A serves as the normalization constant:

$$A^2 = \frac{\lambda}{\sqrt{\pi}}. \tag{27}$$

The relativistic Hamiltonian expression for this system is given as:

$$H = \sqrt{p^2c^2 + m^2c^4} + Bx^4. \tag{28}$$

Expanding the relativistic kinetic term $(p^2c^2 + m^2c^4)^{1/2}$ binomially and retaining significant terms, we find:

$$H = mc^2 + \frac{1}{2}\frac{p^2c^2}{mc^2} + Bx^4. \tag{29}$$

To calculate $\langle H\rangle$, we break it down into its constituent parts and get:

$$E_0 = mc^2 + \frac{1}{4}\frac{\hbar^2\lambda^2}{m} + \frac{3B}{4}\frac{1}{\lambda^4}. \tag{30}$$

To find the minimum expectation value E_0 with respect to the variational parameter λ, we differentiate with respect to λ, yielding:

$$\lambda = \left(\frac{6Bm}{\hbar^2}\right)^{\frac{1}{6}}. \tag{31}$$

Substituting this optimal λ value back into the expression for $\langle E\rangle$, we obtain:

$$E_{min} = mc^2 + \frac{1}{4}\frac{\hbar^2}{m}\left(\frac{6Bm}{\hbar^2}\right)^{2/6} + \frac{3B}{4}\left(\frac{\hbar^2}{6mB}\right)^{4/6} = mc^2 + 1.082\left(\frac{\hbar^2}{2m}\right)^{2/3}B^{1/3}. \tag{32}$$

Clearly, for any general anharmonic system, the relativistic ground state energy comprises the rest energy and the kinetic energy of the system. This result provides valuable insights into the behavior of anharmonic oscillators within the framework of relativistic quantum mechanics.

6. Conclusions

In this study, we applied the variational principle to estimate ground state energies within various relativistic quantum systems. Our investigation encompassed systems ranging from the hydrogen atom to quantum harmonic and anharmonic oscillators. While our method efficiently captures and represents both non-relativistic and relativistic features, affirming its adaptability in handling systems exhibiting a blend of these behaviours, the comprehensive understanding and precise dissection of these components warrant further theoretical exploration and analysis.

The potential implications encompass advancements in understanding quantum systems with mixed relativistic attributes, facilitating future theoretical and experimental investigations. It demonstrates the robustness of the variational principle in estimating ground state energies, even in the presence of relativistic effects. Furthermore, our method's versatility allows for the determination of ground state energies in any relativistic system for which the potential is known. These findings contribute to the advancement of relativistic quantum mechanics and its applications in various areas of physics.

Conflict of Interest

The authors have no conflicts to disclose.

1. W. Nolting, *Theoretical Physics 7: Quantum Mechanics - Methods And Applications*. (Springer Cham, 2017), https://doi.org/10.1007/978-3-319-63324-4.
2. A. Messaiah, *Quantum Mechanics*, **Vol. 1.** (Holland Publishing Co., Amsterdam, 1961).
3. E. C. Kemble, A Contribution to the Theory of the B. W. K. Method, *Phys. Rev.*, **48** (1935) 549 https://doi.org/10.1103/PhysRev.48.549
4. M. N. Sergeenko, *Semiclassical wave equation and exactness of the WKB method, Phys. Rev. A.* **53** (1996) 3798, urlhttps://doi.org/10.1103/PhysRevA.53.3798.
5. D. Griffiths and D. Schroeter, *Introduction to Quantum Mechanics*. (Cambridge University Press, 2018).
6. A. F. Terzis, A simple relativistic Bohr atom, *Eur. J. Phys*. **29** (2008) 735, https://dx.doi.org/10.1088/0143-0807/29/4/008.
7. P. Strange, *Relativistic Quantum Mechanics*, With Applications in Condensed Matter and Atomic Physics (Cambridge University Press, 1998), https://doi.org/10.1017/CBO9780511622755.
8. B. Mirza and M. Mohadesi, The Klein-Gordon and the Dirac Oscillators in a Noncommutative Space, *Commun. Theor. Phys*. **42** (2004) 664, https://dx.doi.org/10.1088/0253-6102/42/5/664.
9. N. Rao and B. Kagali, Energy profile of the one-dimensional Klein- Gordon oscillator. *Physica Scripta* **77** (2007) 015003, https://dx.doi.org/10.1088/0031-8949/77/01/015003
10. F. Amal, S. T, and B. A. Kagali, A modified Bohr's quantization rule to estimate the energy levels of relativistic systems, *Phys. Scr.* **98** (2023) 095024, https://dx.doi.org/10.1088/1402-4896/acef76.
11. G. M. Gayathri *et.al.*, Ground State Energies of a Sextic Anharmonic Oscillator Including Quartic Anharmonicity, *Int. Jr. Sc. Res.*, **5** (2016) 2395.