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## ONE-DIMENSIONAL RELATIVISTIC CONFINED ATOM

***Annotation.*** *In this work we consider the model of one-dimensional atom. One-dimensional relativistic atom is studied for the confined case using the Dirac equation. We also consider the confined Dirac particle in a constant uniform electric field. Furthermore, a calculation method of the energy eigenvalues and critical charge are given for the nucleus of one-dimensional relativistic atom.*

***Key words:*** *Dirac equation, unitary transformation, one-dimensional box, boundary condition, confined Dirac particle, critical charge, Coulomb potential.*

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## BIR O'LCHOVLI RELYATIVISTIK CHEGARALANGAN ATOM

***Annotatsiya.*** *Ushbu ishda biz bir o'lchovli atom modelini ko'rib chiqamiz. Bir o'lchovli relyativistik atom Dirak tenglamasi yordamida chegaralangan holat uchun o'rganildi. Bir jinsli elektrik maydondagi chegaralangan Dirak zarrachasini ham ko'rib chiqildi. Shuningdek, bir o'lchovli relativistik atom yadrosi uchun kritik zaryad va sathlarga mos energiya qiymatlarini hisoblash usuli keltirilgan.*

***Kalit so'zlar:*** *Dirak tenglamasi, unitar almashtirish, bir o'lchovli quti, chegaraviy shart, chegaralangan Dirak zarrachasi, kritik zaryad, Kulon potensiali.*

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## ОДНОМЕРНЫЙ РЕЛЯТИВИСТСКИЙ ОГРАНИЧЕННЫЙ АТОМ

***Аннотация.*** *В данной работе рассматривается модель одномерного атома. Одномерный релятивистский атом изучается для ограниченного случая с использованием уравнения Дирака. Мы также рассматриваем ограниченную Дираковскую частицу в постоянном однородном электрическом поле. Кроме того, для ядра одномерного релятивистского атома дается метод расчета собственных значений энергии и критического заряда.*

***Ключевые слова:*** *уравнение Дирака, унитарное преобразование, одномерный ящик, граничное условие, ограниченная Дираковская частица, критический заряд, Кулоновский потенциал.*

**Introduction.** In relativistic quantum mechanics, the motion of particles is described by equations that incorporate the principles of special relativity. The most common equation for spin ½ particles is the Dirac equation. The electron's motion is governed by relativistic equations like the Dirac equation (in one spatial dimension), which accounts for spin and relativistic energy-momentum relations. The relativistic energy levels are quantized, but they differ significantly from the non-relativistic Schrödinger equation solutions. For a confined relativistic atom, the energy spectrum is computed by solving the Dirac equation with the chosen potential and boundary conditions. The quantized energy levels differ from the non-relativistic case. A one-dimensional relativistic confined atom in quantum mechanics extends the concept of the one-dimensional relativistic atom by introducing confinement to the system. This confinement typically restricts the motion of the particle (e.g., an electron) within a finite spatial region, modeling scenarios where the atom or particle is trapped inside a bounded region, such as a quantum well, potential box, or finite domain. This model is particularly useful for studying relativistic quantum effects in finite systems and has applications in condensed matter physics, quantum optics, and the study of low-dimensional materials.

**Literature review.** The low-energy spectrum of a typical one-dimensional (1D) Dirac material is described by a single-particle matrix Hamiltonian,

$$\widehat{H} = v_F \begin{pmatrix} 0 & \hat{p}_x - i\hbar m \\ \hat{p}_x + i\hbar m & 0 \end{pmatrix} + U(x) \qquad (1)$$

where $v_F$ is the Fermi velocity, $2\hbar v_F|m|$ represents the band gap, and the momentum operator $\hat{p}_x$ acts along the axis of the effectively 1D system [1].

Applying the following unitary transformation to Eq. (1),

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{2}$$

we obtain the system of equations represented by Eq.(3)

$$\begin{pmatrix} \frac{d}{dx} & -m \\ m & -\frac{d}{dx} \end{pmatrix}\begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} = i\big(\varepsilon - V(x)\big)\begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} \tag{3}$$

Here, the eigenvalue and potential energy are scaled as $\varepsilon = E/\hbar v_F$ and $V(x) = U(x)/\hbar v_F$, respectively.

The potential $V(x)$ is modeled as a 1D Coulomb potential, given explicitly by

$$V(x) = -\frac{U_0}{a + |x|} \tag{4}$$

where $a$ is the shift length, and $U_0 = \frac{e^2}{4\pi\epsilon}\frac{1}{\hbar c}\frac{c}{v_F}$ is an effective fine-structure constant [1].

**Research methodology.** We analyze a quantum particle confined within a one-dimensional relativistic box of size $L$. This system is governed by the stationary one-dimensional Dirac equation, expressed in natural units where $\hbar = m = c = 1$.

$$H_0\psi = (-i\alpha\nabla + \beta)\psi = \varepsilon\psi \tag{5}$$

where $\alpha, \beta$ are Dirac matrices [2].

In the Dirac representation, the four-component Dirac spinor $\psi$ can be written in terms of the large and small two-component semi-spinors, $\phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$ and $\chi = \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix}$ respectively. Thus, $\psi$ is expressed as

$$\psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \tag{6}$$

Equation (5) can be rewritten as the following set of coupled equations:

$$\begin{aligned} -i\sigma \cdot \nabla\chi + \phi &= \varepsilon\phi, \\ -i\sigma \cdot \nabla\phi - \chi &= \varepsilon\chi. \end{aligned} \tag{7}$$

where, $\sigma$ - Pauli matrices. The energy levels can be determined with $k = \sqrt{\varepsilon^2 - 1}$ [2].

The solution of Eq.(5) under the boundary conditions $\phi_1(0) = \phi_1(L) = 0$ can be expressed as follows

$$\psi(x) = A\begin{pmatrix} i\sin(kx) \\ 0 \\ 0 \\ \frac{k}{\varepsilon + 1}\cos(kx) \end{pmatrix} \Rightarrow$$

$$\Rightarrow \phi_n(x) = A_n\begin{pmatrix} isin(k_n x) \\ 0 \\ 0 \\ \frac{k_n}{\varepsilon_n + 1}cos(k_n x) \end{pmatrix} \tag{8}$$

where, $k_n = \frac{n\pi}{L}$, $n = 1,2,\ldots$, $\varepsilon_n = \sqrt{k_n^2 + 1}$.

In Eq.(8), we determine the coefficient $A_n$ by normalization condition introducing the following notation

$$B_n = \frac{k_n}{\varepsilon_n + 1} \tag{9}$$

Then,

$$H\psi = E\psi \tag{10}$$

Given that,

$H = H_0 + V(x)$, $H_0\phi_n = \varepsilon_n\phi_n$, $\psi = \sum C_n\phi_n$, $\delta_{mn} = \int \phi_m^*\phi_n dx$

the following can be obtained from Eq.(10).

$$[H_0 + V(x)]\psi = E\psi \Rightarrow$$

$$\Rightarrow \sum C_n H_0\phi_n + \sum C_n V\phi_n = E\sum C_n\phi_n \Rightarrow$$

$$\Rightarrow \sum C_n \varepsilon_n \phi_n + \sum C_n V \phi_n = E \sum C_n \phi_n$$

By multiplying both sides of the above equation $\phi_m^*$ and integrate, we obtain the following

$$\sum C_n \varepsilon_n \delta_{mn} + \sum C_n \int \phi_m^* V \phi_n dx = E \sum C_n \delta_{mn} \Rightarrow$$

$$\Rightarrow C_n \varepsilon_n + \sum C_n V_{mn} = C_n E$$

or

$$\varepsilon_n C_n + \sum V_{mn} C_n = E C_n \tag{11}$$

In the Eq.(11),

$$V_{mn} = \int_0^L \phi_m^* V \phi_n dx \tag{12}$$

In this case, the Coulomb potential is generally expressed as follows

$$V(x) = -\frac{Z}{a + |x|} \tag{13}$$

We assume that the particle moves along the $x$ axis in a bounded interval. That is,

$$0 \le x \le L \quad \Rightarrow \quad x > 0 \quad \Rightarrow \quad V(x) = -\frac{Z}{x + a}$$

**Analysis and results.** The energy levels of relativistic 1D hydrogen-like atom in box with the help of determining eigenvalues from the Eq.(11). The value of charge $Z$ is the equal to the critical charge for a given energy state of the atom when $E = -1$. There is a direct relationship between energy levels and the critical charge of nucleus. If the energy levels of a nucleus are shifted upward (less negative), the critical charge will also increase. Conversely, if the energy levels shift downward (more negative), the critical charge will decrease. The relationship between energy and charge of the unconfined atom $\varepsilon = \varepsilon(\xi)$ is given by Table 1 and Fig.1.

**Table 1. Dependence values of charge and energy.**

| $\xi$ | $\varepsilon$ |
|---|---|
| 300/137 | -0.270537 |
| 310/137 | -0.35209 |
| 320/137 | -0.435331 |
| 330/137 | -0.520175 |
| 340/137 | -0.606539 |
| 350/137 | -0.694343 |
| 360/137 | -0.783509 |
| 370/137 | -0.873961 |
| 380/137 | -0.965624 |
| 390/137 | -1.05842 |

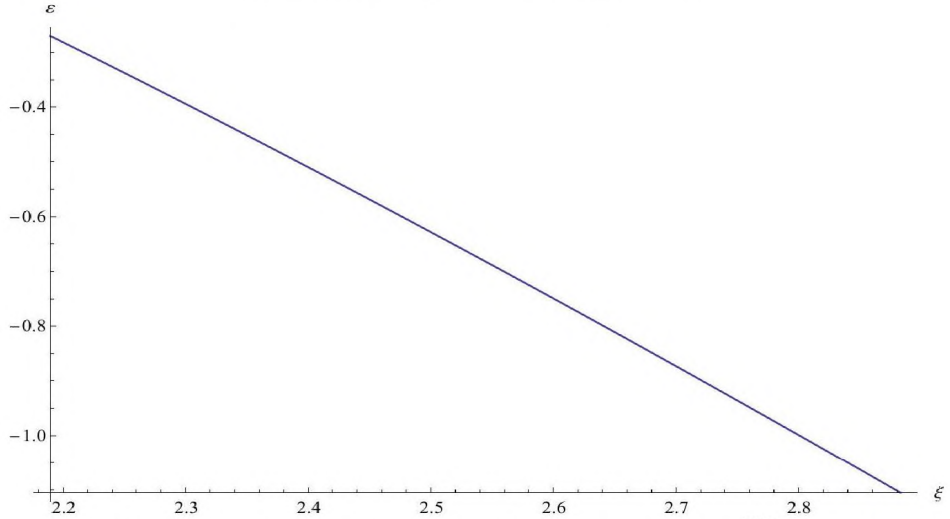



**Figure 1. The relationship of energy and charge ($\xi_{cr} \approx \frac{383.71}{137}$ =2.801).**

Confined Dirac particle also appear in different topics of modern condensed matter physics and related topics. In many cases such system interacts with external electromagnetic fields. Thus, we also consider the case of confined Dirac particle interacting with external constant uniform electric field.

The wave function of the Dirac particle can be written in two-component form as

$$\Psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \tag{14}$$

And satisfies a Dirac equation

$$H\Psi = \varepsilon\Psi \tag{15}$$

$$H = \gamma a_0 \begin{pmatrix} 0 & -k_x + ik_y & 0 & 0 \\ -k_x - ik_y & 0 & 0 & 0 \\ 0 & 0 & 0 & k_x + ik_y \\ 0 & 0 & k_x - ik_y & 0 \end{pmatrix} + V(x) \tag{16}$$

If the particle in confined in graphene nanoribbon with zigzag edges, the wave function meets the boundary condition for each type of wave function separately [3]

$$\phi_A(x = 0) = \phi_B(x = L) = 0 \tag{17}$$

For constant uniform electric field the potential is given as

$$V(x) = \omega x \tag{18}$$

Therefore the Dirac equation is reduced to

$$H\Psi = E\Psi \tag{19}$$

The wave function can be expanded using the complete set of eigenfunctions of the unperturbed system, specifically the graphene nanoribbon, as shown

$$\Psi = \sum C_n \psi_n(x) \tag{20}$$

where

$$\psi_n(x) = \begin{Bmatrix} \sin(k_n x) \\ \pm \frac{i}{\tilde{\varepsilon}} \left[ -k_n \cos(k_n x) + k_y \sin(k_n x) \right] \end{Bmatrix} \tag{21}$$

with $\tilde{\varepsilon} = \pm\sqrt{k_n^2 + k_y^2}$ $\left(\tilde{\varepsilon} = \frac{\varepsilon}{\gamma a_0}\right)$ [3].

Inserting the expansion in Eq. (20), in to Eq. (19), we obtain the system of algebraic equations which is given in Eq. (11). In this case, the matrix elements can be calculated by

$$V_{mn} = \int_0^L \psi_m^* V \psi_n dx \tag{22}$$

**Conclusion/Recommendations.** In conclusion, the study of one-dimensional relativistic confined atoms reveals fascinating physics with profound implications for both fundamental research and technological applications. By advancing theoretical models, enhancing experimental techniques, and promoting interdisciplinary collaboration, this field can significantly contribute to the understanding of relativistic quantum systems and their practical relevance. Therefore, we introduced a method for calculating the energy spectrum of a one-dimensional relativistic confined atom. This method also enables the determination of the critical charge. Using this approach, we computed the atom's energy spectra and estimated the critical charge.

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