ONE-DIMENSIONAL DIRAC EQUATION FOR THE RELATIVISTIC HYDROGEN ATOM

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ABSTRACT

In this article one-dimensional relativistic atoms is studied for confined (in a one-dimensional box) and unconfined cases using the Dirac equation. We obtain the exact solution for the energy spectrum of the hydrogen-like atom which must be determined via solutions to transcendental equations via shifted Coulomb potential and the wave functions expressed in terms of Whittaker functions.

Key words: *Single-particle Dirac Hamiltonian, one-dimensional box, shifted Coulomb potential, Whittaker equation, Dirac matrices, eigenvalues, boundary condition, unitary transform, continuity condition, energy spectra.*

1D relativistic unconfined Coulomb problem for Dirac equation (Z < 137)

Single-particle 1D Dirac matrix Hamiltonian can be expressed by the following equation,

$$\hat{H}_1 = v_F \begin{pmatrix} 0 & \hat{p}_x - i\hbar m \\ \hat{p}_x + i\hbar m & 0 \end{pmatrix} + U(x) \qquad (1)$$

where, v_F - Fermi velocity;

For carbon nanotubes or graphene nanoribbons: $v_F \approx c/300$;

$2\hbar v_F|m|$ - band gap;

$\hat{p}_x$ - momentum operator acts along the axis of the effectively 1D system.

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

As a result of the unitary transform above with Eq. (1) can be obtained the following system of equations

$$\begin{pmatrix} \frac{d}{dx} & -m \\ m & -\frac{d}{dx} \end{pmatrix} \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} = i(\varepsilon - V(x)) \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} \qquad (2)$$

where,

$\varepsilon = E/\hbar v_F$ – the eigenvalue;

$V(x) = U(x)/\hbar v_F$ – potential energy.

Shifted 1D Coulomb potential expressed by this following equation,

$$V(x) = -\frac{U_0}{a + |x|} \qquad (3)$$

where, a – shift length;

$U_0 = \frac{e^2}{4\pi\epsilon}\frac{1}{\hbar c}\frac{c}{v_F}$ - effective fine-structure constant;

In the case of carbon nanotubes or graphene nanoribbons: $U_0 \approx \frac{300}{137}$.

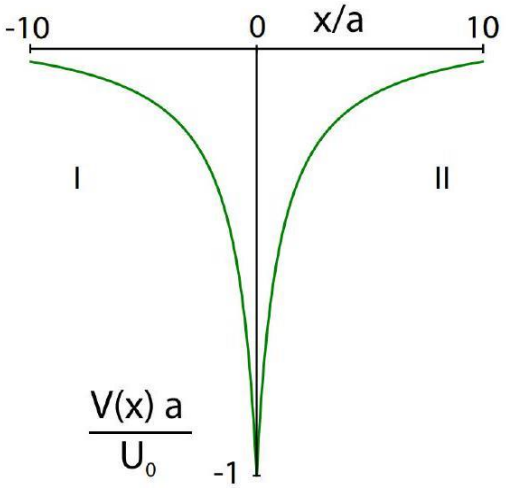

Figure 1. A plot of the shifted Coulomb potential, defined by Eq.(3).

Upon substitution of Eq.(3) into Eq.(2), the wave-function component $\psi_1(x)$ for $x > 0$ satisfies a modified form of the confluent hypergeometric equation, called the Whittaker differential equation, in the variable $\xi = 2\kappa(a + x)$.

$$\frac{d^2}{d\xi^2}\psi_1(\xi) + \left(-\frac{1}{4} + \frac{\mu}{\xi} + \frac{\frac{1}{4} - \nu^2}{\xi^2}\right)\psi_1(\xi) = 0 \qquad (4)$$

where,

$$\mu = \frac{\varepsilon U_0}{\kappa}, \nu = iU_0 - \frac{1}{2} \qquad (5)$$

$\xi = 2\kappa(a + x), \kappa = \sqrt{m^2 - \varepsilon^2} > 0, (|\varepsilon| < |m|).$

Full solution to the system of equations (2) for $x < 0$ we get,

$$\Psi_{\mathrm{I}}(x) = \frac{c_I}{\sqrt{a}}\begin{pmatrix} \frac{\kappa + i\varepsilon}{m} W_{\mu,\nu+1}(\xi_{\mathrm{I}}) \\ W_{\mu,\nu}(\xi_{\mathrm{I}}) \end{pmatrix} \qquad (6)$$

similarly, for $x > 0$

$$\Psi_{\mathrm{II}}(x) = \frac{c_{\mathrm{II}}}{\sqrt{a}}\begin{pmatrix} W_{\mu,\nu}(\xi_{\mathrm{II}}) \\ -\frac{\kappa + i\varepsilon}{m} W_{\mu,\nu+1}(\xi_{\mathrm{II}}) \end{pmatrix} \qquad (7)$$

where, $\xi_{\mathrm{I,II}} = 2\kappa(a \mp x)$.

Using the continuity condition for both wave-function components

$\psi_{1,2}^{\mathrm{I}}\big|_{x=0-} = \psi_{1,2}^{\mathrm{II}}\big|_{x=0+}$

with Eqs. (6) and (7) yields the ratio of constants

$c_{\mathrm{II}}/c_{\mathrm{I}} = \pm i$

where c_I can be found via the normalization condition for a spinor wave function:

$$\int_{-\infty}^{\infty} (|\psi_1|^2 + |\psi_2|^2)dx = 1 \qquad (8)$$

In this section our purpose is to define energy spectrum of free one-dimensional hydrogen-like atom for different nuclear charge, α. Bound-state eigenvalues must be determined from the transcendental equation,

$$\frac{\Delta}{\kappa + iE}\frac{W_{\mu,\nu}(2\kappa a)}{W_{\mu,\nu+1}(2\kappa a)} = \pm i \qquad (9)$$

Solving Eq.(9) numerically gives us energy spectrum as shown following table:

Table 1. The energy spectra of a 1D relativistic hydrogen-like atom with the nuclear charge $\alpha(m = 1, a = 1)$.

n	$\alpha = \frac{300}{137}$	$\alpha = \frac{600}{137}$	$\alpha = \frac{900}{137}$
1	-0.24829187032284	-0.26021641213585	-0.47373645162354
2	0.350155527939304	0.052206645405011	-0.21586792183446
3	0.570467329052877	0.256234815560192	-0.02080151997428
4	0.702830692763858	0.406058399301097	0.135004167667563
5	0.778301610553801	0.513552654757854	0.257842483926782
6	0.831386314948085	0.597117022979481	0.358857435824922
7	0.865918685626946	0.660261761839575	0.440706677830491
8	0.892277155652545	0.711214996076439	0.509455061553548
9	0.910742384774136	0.751099432648736	0.566306606345639
10	0.925611524242110	0.784186682365787	0.614864312166522

1D relativistic confined Coulomb problem for Dirac equation (Z < 137)

Consider first the case of quantum particle confined in a impenetrable relativistic box of size L. Such system can be described by stationary one dimensional Dirac equation which is given by (natural units, $\hbar = m = c = 1$)

$$H_0\psi = (-i\alpha\nabla + \beta)\psi = \varepsilon\psi \qquad (10)$$

where α, β are the well known Dirac matrices.

In the Dirac representation, the four-component Dirac spinor ψ, can be expressed 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.

That is,

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

Equation (10) is equivalent to the following coupled equations:

$$-i\sigma\cdot\nabla\chi + \phi = \varepsilon\phi \quad -i\sigma\cdot\nabla\phi - \chi = \varepsilon\chi$$

where, σ - Pauli matrices.

Using one can find energy levels with $k = \sqrt{\varepsilon^2 - 1}$

Solution of Eq.(10) for the boundary condition, $\phi_1(0) = \phi_1(L) = 0$ can be written as following

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

$$\Rightarrow \phi_n(x) = A_n\begin{pmatrix} i\sin(k_n x)\\ 0\\ 0\\ \dfrac{k_n}{\varepsilon_n+1}\cos(k_n x)\end{pmatrix} \qquad (11)$$

where,

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

In Eq.(11), we determine the coefficient A_n by introducing the notation

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

Based on the normalization condition,

$$\int_0^L |\phi_n(x)|^2 dx = 1 \Rightarrow$$

$$\Rightarrow A_n = \sqrt{\frac{2}{L(B_n^2 - 1)}} \qquad (12)$$

Substituting Eq.(12) into Eq.(11), we get the following

$$\phi_n(x) = \sqrt{\frac{2}{L(B_n^2 - 1)}} \begin{pmatrix} i\sin(k_n x) \\ 0 \\ 0 \\ B_n \cos(k_n x) \end{pmatrix} \qquad (13)$$

$$H\psi = E\psi \qquad (14)$$

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.(14).

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

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

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

We multiply both sides of the above equation by ϕ_m^* and integrate. After that, we have the following equation.

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

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

or

$$\varepsilon_n C_n + \sum V_{mn}C_n = EC_n \qquad (15)$$

In the Eq.(15),

$$V_{mn} = \int \phi_m^* V\phi_n dx$$

The Coulomb potential was generally expressed as follows

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

We assume that the particle moves along the x axis in a bounded interval.

That is,

$0 \le x \le L \Rightarrow x > 0 \Rightarrow$

$$\Rightarrow V(x) = -\frac{Z}{x + a}$$

Finally, we can find energy levels of relativistic 1D hydrogen atom in box with the help of determining eigenvalues, i.e. diagonalizing of following matrix.

$$\begin{pmatrix} \varepsilon_1 - V_{11} & -V_{12} & \cdots & -V_{1N} \\ -V_{21} & \varepsilon_2 - V_{22} & \cdots & -V_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ -V_{N1} & -V_{N2} & \cdots & \varepsilon_N - V_{NN} \end{pmatrix} \qquad (16)$$

Table 2. The energy spectra of a 1D relativistic hydrogen-like atom in box with the nuclear charge $\alpha = 300/137$ and box's size $L(m = 1, a = 1)$.

n	$L = 100$	$L = 250$	$L = 500$
1	0.931151040261464	0.967625066439388	0.982045113843811
2	0.932042822356621	0.967698648406548	0.982064867701628
3	0.932523381516482	0.967879546581070	0.982107320955538
4	0.934690887592249	0.968165614679432	0.982176906393252
5	0.937281069840522	0.968419787472559	0.982243856381033
6	0.938817990577198	0.969135023480703	0.982395688516130
7	0.944252087567858	0.969216740350925	0.982448913789835
8	0.948881003915669	0.970249509767593	0.982717969261936
9	0.950875387242086	0.970810327663230	0.982742365997686
10	0.958600554037474	0.971502479761593	0.983047425296241

Table 3. The energy spectra of a 1D relativistic hydrogen-like atom in box with the nuclear charge α and box's size $L = 100(m = 1, a = 1)$.

n	$\alpha = \frac{300}{137}$	$\alpha = \frac{600}{137}$	$\alpha = \frac{900}{137}$
1	0.931151040261464	0.851771547325166	0.768663883304231
2	0.932042822356621	0.851823815440437	0.768852207058082
3	0.932523381516482	0.853740936940714	0.770557952000192
4	0.934690887592249	0.854437324198081	0.771604808524253
5	0.937281069840522	0.857405019784025	0.774219276009389
6	0.938817990577198	0.860615260161324	0.777723608134698

7	0.944252087567858	0.862547331625738	0.779427607692845
8	0.948881003915669	0.869014080865159	0.786020363837518
9	0.950875387242086	0.872590163146551	0.788707138806166
10	0.958600554037474	0.876689412768860	0.793871855975820

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