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An approximate analytical solution of the Klein–Gordon equation for the finite electric dipole potential

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Abstract

The Klein–Gordon equation for the finite electric-dipole potential is solved approximately by the method of matching of asymptotic solutions. Near-continuum state energies are found analytically.

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The two-centre Coulomb problem is a classical problem in quantum mechanics that arose at its early stages [1–7]. It has found application in many realistic problems of atomic physics [1], molecular physics [2] and slow heavy ion collision physics [11]. The non-relativistic two-centre Coulomb problem admits separation of variables and can be solved exactly [7]. The corresponding relativistic extension of this problem is a complicated mathematical problem. Unlike the Schrödinger equation for the two-centre Coulomb potential, the variables in the Dirac equation and Klein–Gordon equation cannot be separated in any system of coordinates. This fact makes impossible the solution of the relativistic two-centre Coulomb problem in closed form. Therefore various asymptotic or variational methods have to be used for the solution of the relativistic two-centre Coulomb problem. One such asymptotic method has been introduced by Popov and co-workers for the solution of the two-centre Dirac equation for the Coulomb potential [8, 9]. Matching logarithmic derivatives of the asymptotic solution of the Dirac equation they obtained an algebraic equation for finding the energy eigenvalues.

The basic idea of the asymptotic matching method is the following: firstly, by solving the wave equation asymptotically one obtains a wave function $\psi_0(r)$ which is valid for small distances from the centres in a region $0 < r < r_1$ and $\psi_\infty(r)$ which is an asymptotic solution of the wave equation in a region $r_2 < r < \infty$. If these regions overlap with each other, i.e.

$$r_2 < r_1$$

one can equate logarithmic derivatives of $\psi_\infty(r)$ and $\psi_0(r)$ in the region $r_2 < r < r_1$ to obtain the spectral equation for finding energy eigenvalues.

In this paper we apply the same method to solve approximately the Klein–Gordon equation for the finite electric-dipole potential. Besides being an interesting mathematical problem,

the two-centre Coulomb problem for the Klein–Gordon equation has also several practical applications in nuclear and particle physics. The motion of a meson in the field of two nuclei or the motion of a gluon in the field of a quark–antiquark pair in hybrid mesons can be described by the two-centre Klein–Gordon equation. The non-relativistic counterpart of this problem, i.e. the Schrödinger equation for a finite electric-dipole potential has been treated by many authors [7, 10, 12–15]. It is well known that there exists a critical distance $r_{\rm cr}$ below which no bound states of the electron in a finite electric-dipole field can be supported [12, 13]. This distance is known also as the Fermi–Teller radius. At this distance the electronic eigenenergies of ns states merge with the quasimolecular continuum edge.

The potential of the finite electric dipole is given as

$$V = \frac{Z\alpha}{r_1} - \frac{Z\alpha}{r_2} \tag{1}$$

where r_i is the distance from the ith charge, $\alpha^{-1} = 137$ (the system of units $\hbar = m_e = c = 1$ is used) and Z is the charge of the centres. The motion of a relativistic spinless particle in a field of two Coulomb centres is described by the following Klein–Gordon equation:

$$[(E - V)^2 + (\Delta - 1)]\psi = 0 \tag{2}$$

where V is given by (1). The variables in this equation cannot be separated for any system of coordinates. It can be written as

$$(E^2 - 2EV + V^2 + \Delta - 1)\psi = 0. \tag{3}$$

This is the Schrödinger equation with an effective potential

$$V_{\rm eff} = 2EV - V^2$$

and effective energy

$$E_{\rm eff} = E^2 - 1.$$

At large distances from the dipole one can neglect the term V^2 and write

$$\left(-\tfrac{1}{2}\Delta + EV\right)\psi = \tfrac{1}{2}(E^2 - 1)\psi \tag{4}$$

i.e. we have the Schrödinger equation for a finite electric-dipole potential, the variables of which can be separated in prolate spheroidal coordinates by the following substitution:

$$\psi = \frac{U(\xi)}{(\xi^2 - 1)^{\frac{1}{2}}}\frac{V(\eta)}{(1 - \eta^2)^{\frac{1}{2}}}\,{\rm e}^{{\rm i}m\phi} \tag{5}$$

where $\xi = (r_1 + r_2)R^{-1}$, $\eta = (r_1 - r_2)R^{-1}$, $\phi = \operatorname{arccot}(y/x)$ and R is the distance between charges.

This leads to the differential equations

$$U''(\xi) + \left[-\lambda^2 + \frac{A}{\xi^2 - 1} + \frac{1 - m^2}{(\xi^2 - 1)^2}\right]U(\xi) = 0 \tag{6}$$

$$V''(\eta) + \left[-\lambda^2 + \frac{D\eta - A}{1 - \eta^2} + \frac{1 - m^2}{(1 - \eta^2)^2}\right]V(\eta) = 0 \tag{7}$$

where

$$\lambda^2 = -\frac{R^2}{4}(E^2 - 1) \tag{8}$$

$D = 2|E|RZ\alpha$, A is the constant of separation and m is the azimuthal quantum number. The boundary conditions are given as

$$U(1) = 0 \qquad U(\xi)_{\xi \mapsto \infty} = 0 \qquad V(\pm 1) = 0.$$

Formally the last equations coincide with those for the non-relativistic electron–finite electric-dipole system, which was treated and solved asymptotically [10]. Here we use the results of that treatment.

The asymptotic solution of equation (6) for $\xi \gg 1$ can be written as [10]

$$U(\xi) \approx (p\xi)^{\frac{1}{2}} K_{i\nu}(p\xi) \tag{9}$$

where $K_{i\nu}$ is the McDonald function and $\nu^2 = A - \frac{1}{4}$. The solution of (7) for small η is also found in [10]

$$V(\eta) \approx [S'(\eta)]^{-\frac{1}{2}} \operatorname{Ai}(-D^{\frac{1}{3}} S) \tag{10}$$

where Ai is the Airy function,

$$S(\eta) = \left(\frac{3}{2} \int_0^{\eta} \eta^{\frac{1}{2}} (1 - \eta^2)^{-\frac{1}{2}} \, \mathrm{d}\eta \right)^{\frac{2}{3}}$$
$$S'(\eta) = \frac{\mathrm{d}S}{\mathrm{d}\eta}.$$

So for large $\lambda\xi$ and small η the asymptotic solution of the given equation can be written as ($m = 0$)

$$\varphi \sim \left[\frac{\pi}{\nu \sin(h\pi\nu)} \right]^{\frac{1}{2}} (p\xi)^{\frac{1}{2}} (\xi^2 - 1)^{-\frac{1}{2}} \sin\left(\nu \ln \frac{2}{p\xi} + \arg \Gamma(1 + \mathrm{i}\nu) \right) \tag{11}$$

where the following asymptotic formula for the McDonald function (for $x \mapsto 0$) and the Airy function (for $\eta \to 0$) are used:

$$K_{i\nu}(x) \sim \left[\frac{\pi}{\nu \sin(h\pi\nu)} \right]^{\frac{1}{2}} (x)^{\frac{1}{2}} \sin\left(\nu \ln \frac{2}{x} + \arg \Gamma(1 + \mathrm{i}\nu) \right)$$
$$\operatorname{Ai}(S) \sim c_1 - c_2 S$$

with $c_1 = 0.355$, $c_2 = 0.259$

Now we find the asymptotic behaviour of the wave function at large distances from the dipole. In this case we consider two regions for charges of centres: $Z < 137$ and $Z > 137$. As is shown in [8, 9] for $Z < 137$ the relativistic two-centre Coulomb wave function near the centres can be written as

$$\varphi \sim (\xi^2 - \eta^2)^{\gamma - 1}$$

where

$$\gamma = (1 - Z^2\alpha^2)^{\frac{1}{2}}.$$

For supercritical charges, i.e. for

$$Z > 137$$

the regularization of the Coulomb potential is needed [8, 9]. In this work we choose the following cutoff:

$$V(r) = \begin{cases} \frac{Z\alpha}{r} & \text{for } r > b \\ \frac{Z\alpha f(r)}{b} & \text{for } 0 < r < b \end{cases}$$

with

$$f(r) = 1$$

i.e. the spherical distribution of the nuclear charge. Then for the asymptotics of the wave function one can write [8]

$$\varphi \sim \xi^2 - \eta^2. \tag{12}$$

Thus in the general case the small-distance asymptotics of the wave function (assuming that $R \ll 1$) can be written as

$$\varphi_1 \sim (\xi^2 - \eta^2)^\beta$$

where β is defined as

$$\beta = \begin{cases} \nu - 1 & \text{for } Z < 137 \\ 1 & \text{for } Z > 137. \end{cases}$$

For small η we can write this as

$$\varphi \sim \xi^{2\beta}. \tag{13}$$

Due to the fact that $|E| \sim 1$ (near-continuum states) the wave functions ψ and ψ_1 overlap with each other giving us an algebraic equation for finding the energy

$$\frac{1}{2} + \nu \cot\left[\nu \ln\frac{2}{\lambda} + \arg\Gamma(1 + \mathrm{i}\nu)\right] = -2\beta$$

here we took into account the relation $\ln\frac{2}{p\xi} \approx \ln\frac{2}{p}$. This gives us the following equation:

$$\lambda = \exp\left[\frac{1}{\nu}\arg\Gamma(1 + \mathrm{i}\nu) - \frac{1}{\nu}\operatorname{arccot}\left[-\frac{1 + 4\beta}{2\nu}\right] - \ln 2\right]. \tag{14}$$

To find $E(R)$ from this we should express ν via $E(R)$ using the following relation [10]:

$$\nu = \left[\frac{8\pi^2}{\Gamma^4\left(\frac{1}{4}\right)}(D - D_{\mathrm{cr}}) - \frac{R^2}{6}(E^2 - 1)\right]^{\frac{1}{2}} \tag{15}$$

where [10]

$$D_{\mathrm{cr}} = \frac{\Gamma^4\left(\frac{1}{4}\right)}{32\pi}\left(1 - \frac{2}{3\pi}\right)$$

is the critical dipole moment at which $E(R)$ reaches the boundary of the continuum. Inserting equation (14) into equation (8) and expressing E from the obtained equation we get

$$E_\pm \approx \pm\left[1 - \frac{2}{R^2}\exp(\omega(\nu, Z))\right] \tag{16}$$

where

$$\omega(\nu, Z) = \frac{2}{\nu}\arg\Gamma(1 + \mathrm{i}\nu) - \frac{2}{\nu}\operatorname{arccot}\left[-\frac{1 + 4\beta}{2\nu}\right] - 2\ln 2. \tag{17}$$

For $Z < 137$ we have a transcendental equation for $E(R)$

$$E_\pm \approx \pm 1 \mp \frac{2}{R^2}\exp\left[\frac{2}{\nu}\arg\Gamma(1 + \mathrm{i}\nu) - \frac{2}{\nu}\operatorname{arccot}\frac{3 - 4\gamma}{2\nu} - 2\ln 2\right] \tag{18}$$

where ν is given by equation (15). This equation can be solved by iteration only for $Z < 137\sqrt{7/4}$ (because the iteration procedure converges only for $3 - 4\gamma < 0$). The first iteration gives

$$E_\pm \approx \pm 1 \mp \frac{2}{R^2}\exp\left[-\frac{\Gamma^2\left(\frac{1}{4}\right)}{\pi(4Z\alpha R - 2D_{\mathrm{cr}})^{\frac{1}{2}}}\operatorname{arccot}\frac{\Gamma^2\left(\frac{1}{4}\right)(3 - 4\gamma)}{4\pi(4Z\alpha R - 2D_{\mathrm{cr}})^{\frac{1}{2}}}\right]. \tag{19}$$

It is easy to see that this formula has the correct non-relativistic limit which can be obtained by assuming $\gamma \to 1$ and

$$\operatorname{arccot}\left(\frac{\Gamma^2\left(\frac{1}{4}\right)(3-4\gamma)}{4\pi(4Z\alpha R-2D_{\mathrm{cr}})^{\frac{1}{2}}}\right)\to\pi$$

that follows from the fact that for the near-continuum state $4Z\alpha R - 2D_{\mathrm{cr}} \to 0$. Subtracting the rest energy (which is equal to 1 in these units) from the expression obtained in this way we have

$$E_{\pm}\approx\mp\frac{2}{R^2}\exp\left[-\frac{\Gamma^2\left(\frac{1}{4}\right)}{(4Z\alpha R-2D_{\mathrm{cr}})^{\frac{1}{2}}}\right]. \tag{20}$$

This is the formula for the non-relativistic electron-finite electric-dipole system which was obtained in [10].

For $Z > 137$ we have the spectral equation

$$E_{\pm}\approx\pm1\mp\frac{2}{R^2}\exp\left[\frac{2}{\nu}\arg\Gamma(1+\mathrm{i}\nu)-\frac{2}{\nu}\operatorname{arccot}\frac{5}{2\nu}-2\ln 2-\frac{2\pi}{\nu}\right]. \tag{21}$$

The approximate solution of this equation gives the near-continuum state energy term for the supercritical case:

$$E_{\pm}\approx\pm1\mp\frac{2}{R^2}\exp\left[-\frac{\Gamma^2\left(\frac{1}{4}\right)}{\pi(4Z\alpha R-2D_{\mathrm{cr}})^{\frac{1}{2}}}\left(\operatorname{arccot}\frac{5\Gamma^2\left(\frac{1}{4}\right)}{4\pi(4Z\alpha R-2D_{\mathrm{cr}})^{\frac{1}{2}}}-\pi\right)\right]. \tag{22}$$

Thus we have solved approximately and analytically the Klein–Gordon equation for the finite-electric dipole potential. The solution is obtained for both undercritical ($Z < 137$) as well as supercritical ($Z > 137$) cases. The solution obtained is valid for near-continuum states, i.e. for energies with absolute values close to 1. The above results could be useful for various problems of few-body systems physics coming from atomic, molecular, nuclear and particle physics.

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