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Energy states of the Hulthen plus Coulomb-like potential with position-dependent mass function in external magnetic fields

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We need to solve a suitable exponential form of the position-dependent mass (PDM) Schrödinger equation with a charged particle placed in the Hulthen plus Coulomb-like potential field and under the actions of the external magnetic and Aharonov–Bohm (AB) flux fields. The bound state energies and their corresponding wave functions are calculated for the spatially-dependent mass distribution function of interest in physics. A few plots of some numerical results with respect to the energy are shown.

Keywords: Schrödinger equation, Hulthen plus Coulomb-like potential, position-dependent mass distribution functions, perpendicular magnetic and Aharonov–Bohm flux fields

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1. Introduction

The exact solutions of quantum wave equations, expressed in analytical form, describing one-electron atoms and few-body systems are essential in studying the atomic structure theory and more areas. In fact, the exact analytical solutions are essentially used in quantum-chemical, quantum electrodynamics and theory of molecular vibrations. They are also used to examine the correctness of models, approximations in computational physics, nuclear physics, nanostructures and computational chemistry.[1–16]

On the other hand, the position-dependent mass (PDM) idea arises after the effect of the periodic field on the non-relativistic motion of electrons in periodic lattices. In fact, it happens in typical semiconductors by the effects of impurities in perturbed periodic lattices.[17] Recently, a considerable interest in the mass dependence on the internuclear distance has been revived in solving different equations with various physical potential models.[18–29] Furthermore, a number of studies take the effect of an electric field or a magnetic field into account in studying different systems.[30–34] For further study we cite Refs. [35] and [36]. In addition, it is found to be more interesting that nearly all desired analytic solutions of the non-relativistic equation have been expressed in terms of hypergeometric functions.[38–40]

However, in all these areas, the studies of the non-relativistic and relativistic quantum dynamics of charged particles in the presence of magnetic fields and Aharonov–Bohm (AB) flux fields, which are perpendicular to the plane where the particles are confined, have been carried out over the past few years.[41] In fact, the investigation of systems consisting of non-relativistic as well as relativistic charged particles, that are confined by the magnetic fields, has attracted a great deal of attention due to their applications (such as in graphene,[15,16,42] semiconductor structures,[43] chemical physics,[44] molecular vibrational and rotational spectroscopy of molecular physics,[45] biology,[46] environmental sciences,[47] and cosmic string[48]). Recently, Eshghi *et al.*[49] solved the Schrödinger equation with the superposition of Morse-plus-Coulomb potentials with two different physically PDM distribution functions of the exponential and inverse-square forms in the external perpendicular magnetic and AB flux fields. Also, these authors have investigated the Schrödinger equation with a position-dependent mass charged particle interacted via the superposition of the Morse-plus-Coulomb potentials under the actions of external magnetic and Aharonov–Bohm flux fields.[49] Also, Jiang *et al.* have investigated the solutions of the Schrödinger equation with a position-dependent mass.[50] However, in the present work, we intend to extend the work in Ref. [51] and solve the Schrödinger equation with a charged particle under the actions of Hulthen plus Coulomb-like potential field having the general form:

$$V(\rho) = -\frac{V_0\,\mathrm{e}^{-\lambda\rho}}{1-q\,\mathrm{e}^{-\lambda\rho}} + \frac{V_1}{\rho}, \tag{1}$$

where λ is a mass constant, V_0 and V_1 are the positive potential parameters and q is the real parameter in the physically presumed PDM distribution function of the exponential form:

$$M(\rho) = \frac{M_0}{1-q\,\mathrm{e}^{-\lambda\rho}}, \tag{2}$$

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with λ being a mass constant in the external perpendicular magnetic and AB flux fields.

Figures 1–4 show the plots for the potential form $V(\rho)$ in Eq. (1) and mass distribution function $M(\rho)$ in Eq. (2) versus ρ for various parameter values.

For example, figure 1 shows the behavior of the potential model $V(\rho)$ changing with ρ for $q=3$ and $q=4$, namely for the case of $q>0$. Further, figure 2 shows the behavior of $V(\rho)$ changing with ρ for $q=-1$, -2 and -3, namely for the case of $q<0$, for $M_0=0.4$, 0.5, 0.6.

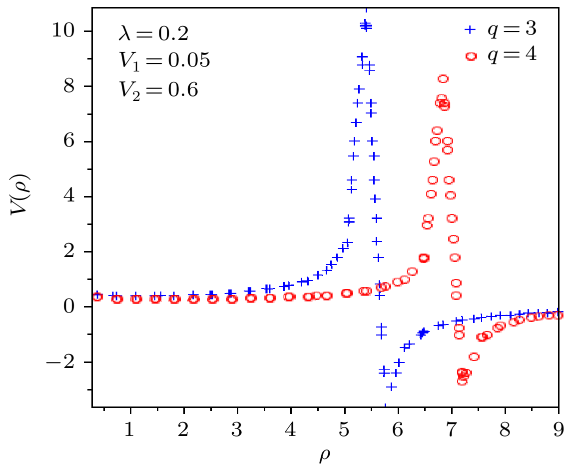

Fig. 1. (color online) The potential model (1) versus ρ for two selected values of $q>0$.

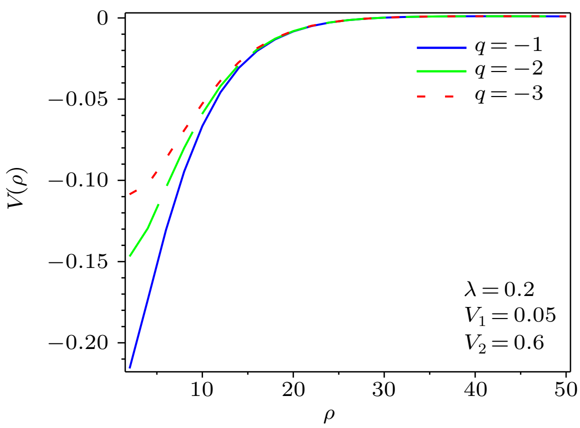

Fig. 2. (color online) The potential model (1) versus ρ for three selected values of $q<0$.

For $q>0$, figure 3 shows the plots of mass function versus ρ for $q=3$ and $q=4$. For the case of $q<0$, figure 4 shows the plots of mass function versus ρ for $M_0=0.4$, 0.5, 0.6.

The rest of this paper is organized as follows. In Section 2, we solve the Schrödinger equation for a charged particle under the actions of Hulthen plus Coulomb-like potential with a suitable choice of spatially dependent mass function and subjected to the external magnetic fields. The series method is used to determine the energy states and their corresponding wave functions. Further, we use the energy levels to obtain the thermodynamic quantities of the system in a systematic manner. Section 3 is devoted to our discussion and conclusions.

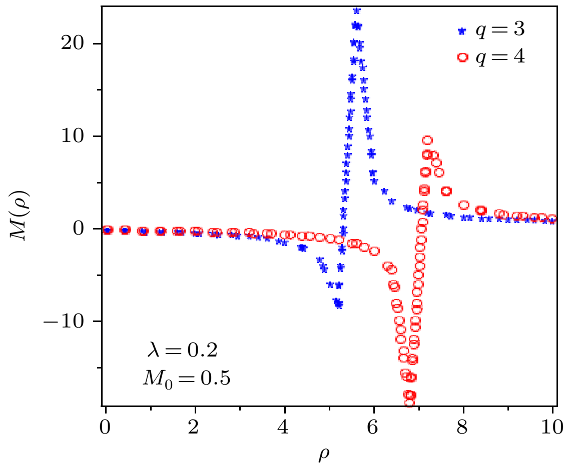

Fig. 3. (color online) The mass function (2) versus ρ for $q>0$ with $M_0=0.4, 0.5, 0.6$.

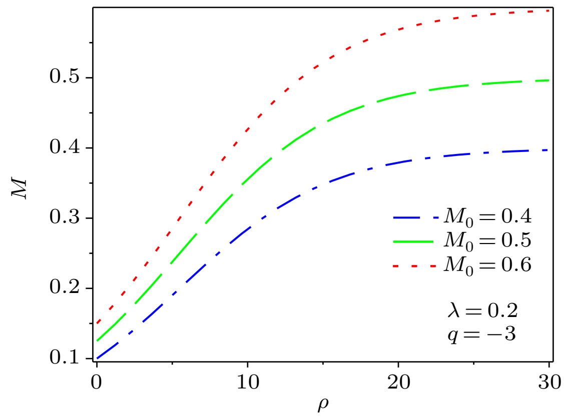

Fig. 4. (color online) The mass function (2) versus ρ for $q<0$ with $M_0=0.4, 0.5, 0.6$.

2. Schrödinger equation with q-deformed PDM function

In this section, we are to solve the Schrödinger equation for a charged particle with a physically position-dependent mass (PDM) distribution function interacted via the Hulthen plus Coulomb-like potential field and exposed to external perpendicular magnetic and AB flux fields treated in two-dimensional space cylindrical coordinates. We are to calculate the bound state energies and their corresponding wave functions. The general form of the Schrödinger equation for a charged particle with the PDM system under the action of a certain potential field and in the presence of the vector potential is given by

$$\left(\hat{p}+\frac{e}{c}\boldsymbol{A}\right)\cdot\frac{1}{2M(\rho)}\left(\hat{p}+\frac{e}{c}\boldsymbol{A}\right)\Psi(\rho,\varphi,z)$$
$$=[E_{nm}-V(\rho)]\Psi(\rho,\varphi,z), \tag{3}$$

where $M(\rho)$ and $\boldsymbol{A}$ are the spatially dependent mass and mass constant, respectively.

We assume that the vector potential has the simple form:

$$\boldsymbol{A} = \left(0,\ \frac{B_0\,\mathrm{e}^{-\lambda\rho}}{1-q\,\mathrm{e}^{-\lambda\rho}} + \frac{\Phi_{\mathrm{AB}}}{2\pi\rho},\ 0\right),$$

where B_0 and Φ_{AB} are the magnetic and AB flux fields.

Substituting the vector potential (1) and the spatially dependent mass (2) into Eq. (3) and using the approximation of Aldrich[52] with some lengthy but straightforward calculations, we arrive at the following radial second-order differential equation:

$$\begin{aligned}
&\frac{\mathrm{d}^2R(\rho)}{\mathrm{d}\rho^2} + \frac{(1+q)\lambda\,\mathrm{e}^{-\lambda\rho}}{1-q\,\mathrm{e}^{-\lambda\rho}}\frac{\mathrm{d}R(\rho)}{\mathrm{d}\rho} \\
&+\Bigg[\vartheta(m,\lambda,\Phi_{\mathrm{AB}},B_0)\frac{\mathrm{e}^{-2\lambda\rho}}{\left(1-q\,\mathrm{e}^{-\lambda\rho}\right)^2} \\
&+\delta(\lambda,V_0,V_1,M_0)\frac{\mathrm{e}^{-\lambda\rho}}{\left(1-q\,\mathrm{e}^{-\lambda\rho}\right)^2} \\
&-\omega(m,\Phi_{\mathrm{AB}})\frac{\mathrm{e}^{-\lambda\rho}}{1-q\,\mathrm{e}^{-\lambda\rho}} \\
&+\varepsilon(M_0,E_{nm})\frac{1}{1-q\,\mathrm{e}^{-\lambda\rho}}\Bigg]R(\rho)=0, \qquad (4)
\end{aligned}$$

and

$$\begin{aligned}
\vartheta(m,\lambda,\Phi_{\mathrm{AB}},B_0) &= -m^2\lambda^2 - \frac{2meB_0\lambda}{\hbar c} - \left(\frac{eB_0}{\hbar c}\right)^2 \\
&\quad - \left(\frac{e}{\hbar c}\right)^2\frac{B_0\lambda\Phi_{\mathrm{AB}}}{\pi} - \left(\frac{e\lambda\Phi_{\mathrm{AB}}}{2\pi\hbar c}\right)^2, \\
\delta(\lambda,V_0,V_1,M_0) &= \frac{2M_0}{\hbar^2}(V_0 - V_1\lambda), \\
\omega(m,\Phi_{\mathrm{AB}}) &= \frac{em\Phi_{\mathrm{AB}}}{\pi\hbar c}, \quad \varepsilon(M_0,E_{nm}) = \frac{2M_0}{\hbar^2}E_{nm},
\end{aligned}$$

where m is the magnetic quantum number.

Now using the parameterized Nikoforov–Uvarov method[53] with the following substitution $z = 1/(1-q\,\mathrm{e}^{-\lambda\rho})$ into Eq. (4), we can simply write Eq. (4) as the following expression

$$\begin{aligned}
&\frac{\mathrm{d}^2F(z)}{\mathrm{d}z^2} + \frac{(1-q)z}{qz(1-z)}\frac{\mathrm{d}F(z)}{\mathrm{d}z} \\
&+\frac{1}{z^2(1-z)^2}\left[-\xi_2z^2+\xi_1z-\xi_0\right]F(z)=0, \qquad (5)
\end{aligned}$$

with the following identifications:

$$\begin{aligned}
-\xi_2 &= \frac{1}{q\lambda^2}\left(\vartheta(m,\lambda,\Phi_{\mathrm{AB}},B_0) - \delta(\lambda,V_0,V_1,M_0)\right), \\
\xi_1 &= \frac{1}{q\lambda^2}\big(-2\vartheta(m,\lambda,\Phi_{\mathrm{AB}},B_0) - \delta(\lambda,V_0,V_1,M_0) \\
&\quad -\omega(m,\Phi_{\mathrm{AB}}) + \varepsilon(M_0,E_{nm})\big), \\
-\xi_0 &= \frac{1}{q\lambda^2}\left(\vartheta(m,\lambda,\Phi_{\mathrm{AB}},B_0) + \omega(m,\Phi_{\mathrm{AB}})\right), \\
c_1 &= 1,\ c_2 = 2-\frac{1}{q},\ c_3 = 1,\ c_4 = 0,\ c_5 = -\frac{1}{2q}, \\
c_6 &= \frac{1}{4q^2}+\xi_2,\ c_7 = -\xi_1,\ c_8 = \xi_0, \\
c_9 &= \frac{1}{4q^2}+\xi_2-\xi_1+\xi_0,\ c_{10} = 1-2\sqrt{\xi_0}, \\
c_{11} &= 2+2\sqrt{\frac{1}{4q^2}+\xi_2-\xi_1+\xi_0}-2\sqrt{\xi_0}, \\
c_{12} &= -\sqrt{\xi_0},\ c_{13} = -\frac{1}{2q}-\sqrt{\frac{1}{4q^2}+\xi_2-\xi_1+\xi_0}+\sqrt{\xi_0}. \qquad (6)
\end{aligned}$$

We can write the energy eigenvalues in a rather simpler form as

$$E_{nm} = \frac{1}{2W_3}\left[-(W_1+2n)^2+2\left(n^2+W_1n+W_4\right)\right] \pm \sqrt{\frac{(W_1+2n)^2-2\left(n^2+W_1n+W_4\right)}{4W_3} - \frac{\left(n^2+W_1n+W_4\right)^2-W_2(W_1+2n)^2}{W_3^2}}, \quad (7)$$

where we have defined

$$\begin{aligned}
W_1 &= 1-2\sqrt{\frac{1}{q\lambda^2}\left(-\vartheta(m,\lambda,\Phi_{\mathrm{AB}},B_0)-\omega(m,\Phi_{\mathrm{AB}})\right)}, \\
W_2 &= \frac{2}{q\lambda^2}\delta(\lambda,V_0,V_1,M_0)+\frac{1}{4q^2}, \\
W_3 &= \frac{2M_0}{q\lambda^2\hbar^2}, \\
W_4 &= -\sqrt{\frac{1}{q\lambda^2}\left(-\vartheta(m,\lambda,\Phi_{\mathrm{AB}},B_0)-\omega(m,\Phi_{\mathrm{AB}})\right)} \\
&\quad +\frac{1}{2q}+\frac{1}{q\lambda^2}\left[\delta(\lambda,V_0,V_1,M_0)-\omega(m,\Phi_{\mathrm{AB}})\right]. \qquad (8)
\end{aligned}$$

Here we need to examine the behaviors of the energy states in Eq. (7), so we plot the energy states as a function of the magnetic field and AB flux field for various mass parameters with considering the case of positive sign in Eq. (7) as shown in Figs. 5 and 6.

Therefore, it is obvious from Fig. 5 that the energy state is sensitive to the variation of magnetic field and it becomes strongly bound with a stronger field as the mass parameter M_0 changes. The energy state is overlapping for different values of mass parameter. Therefore, there is a limit to taking the mass of a charged particle for different field strengths. Clearly, the taken mass value must be small enough to avoid any overlapping of the energy state. In Fig. 6, the energy state decreases with increasing the AB flux field, Φ. However, the energy states is higher for larger mass value.

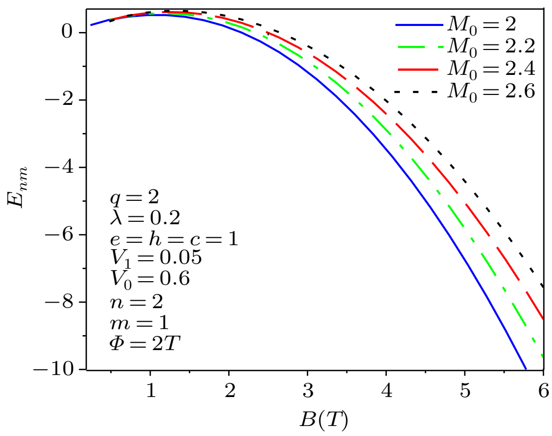

Fig. 5. (color online) The energy state versus magnetic field B for various values of M_0.

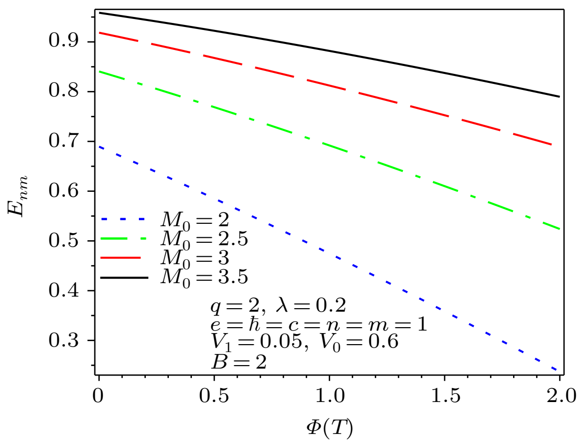

Fig. 6. (color online) The energy state versus the AB flux field Φ for various values of M_0.

In Figs. 7 and 8, we also plot the energy state as a function of the magnetic and AB flux field (curve and linear, respectively) for the negative sign case in Eq. (7). Clearly, there is no limit to the mass parameter value in this case. The energy state curve becomes strongly negative or bound with increasing magnetic field for a chosen mass parameter value. However, the energy state curve is linear and becomes strongly bound with increasing AB flux field.

To proceed in our discussion, we can use energy spectrum formula (7) to study the thermodynamics properties of a charged particle in the presence and absence of scalar and vector fields. Having calculated the energy states, we can immediately obtain the thermodynamic quantities of the system in a systematic manner. In order to obtain all thermodynamic quantities of the nonrelativistic particle system, we should concentrate, at first, on the calculation of the partition function Z. In this case, the partition function Z at temperature T, is obtained and throughout the calculation the Boltzmann factor is taken as

$$Z=\sum_{n=0}^{\infty}\exp\left(-\beta E_{n,m}\right),$$

where $\beta = 1/k_{\rm B}T$ and $k_{\rm B}$ is the Boltzmann constant.[54] In this area, some of the authors have calculated the partition functions of real physical systems, see Refs. [55]–[58]. Recently, some progress has been made of calculations of classical vibration partition functions of weakly bounded diatomic molecules.[59]

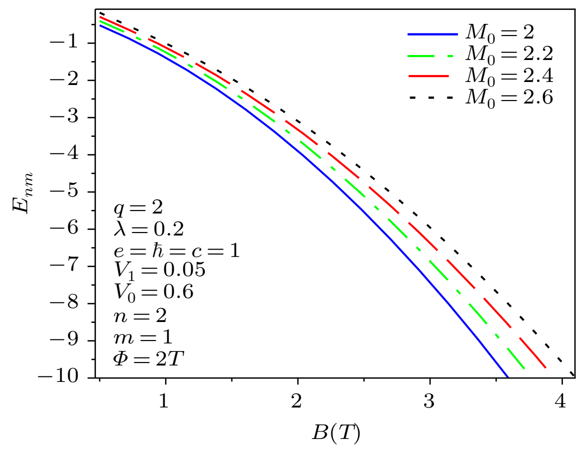

Fig. 7. (color online) The energy states versus of the magnetic field B for different values of M_0.

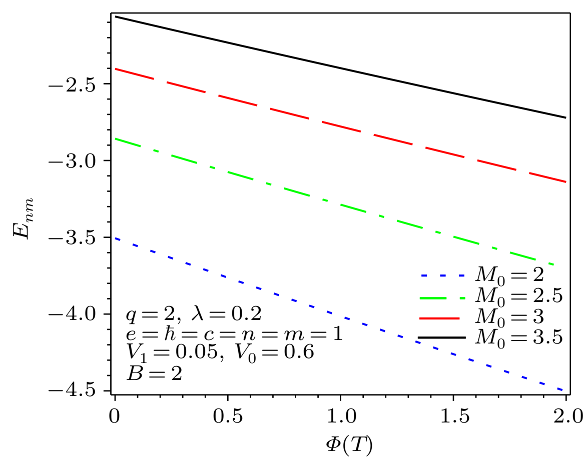

Fig. 8. (color online) The energy states versus of the AB flux field Φ for different values of M_0.

On the other hand, after using Eq. (6) and the parameterized NU method,[53] we can simply obtain the wave function as

$$F(z) = Nz^{-\sqrt{\frac{1}{q\lambda^2}\left(-\vartheta\left(m,\lambda,\Phi_{\rm AB},B_0\right)-\omega\left(m,\Phi_{\rm AB}\right)\right)}}\times(1-z)^{\frac{1}{2q}+\sqrt{\frac{1}{4q^2}+\frac{1}{q\lambda^2}\left(3\delta\left(\lambda,V_0,V_1,M_0\right)-\varepsilon\left(M_0,E_{nm}\right)\right)}}$$

$$\times P_n\left(-2\sqrt{\frac{1}{q\lambda^2}\left(-\vartheta\left(m,\lambda,\Phi_{\mathrm{AB}},B_0\right)-\omega\left(m,\Phi_{\mathrm{AB}}\right)\right)},2\sqrt{\frac{1}{4q^2}+\frac{1}{q\lambda^2}\left(3\delta\left(\lambda,V_0,V_1,M_0\right)-\varepsilon\left(M_0,E_{nm}\right)\right)}\right)(1-2z). \quad (9)$$

where N is the normalized constant.

3. Concluding remarks

We solved the Schrödinger equation for a charged particle with an exponential form position-dependent mass (PDM) placed in the field of the general superposition of Húlthen plus Coulomb-like potential fields under the actions of external magnetic and AB flux fields. We calculated the bound state energies and the corresponding wave functions with a suitable change with respect to the spatially dependent mass variable as functions of the magnetic and AB flux fields by using the parameterized NU method. Finally, some results of the energy values are shown in Figs. 5–8.

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