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Nonrelativistic molecular models under external magnetic and AB flux fields

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ABSTRACT

By using the wave function ansatz method, we study the energy eigenvalues and wave function for any arbitrary m-state in two-dimensional Schrödinger wave equation with various power interaction potentials in constant magnetic and Aharonov–Bohm (AB) flux fields perpendicular to the plane where the interacting particles are confined. We calculate the energy levels of some diatomic molecules in the presence and absence of external magnetic and AB flux fields using different potential models. We found that the effect of the Aharonov–Bohm field is much as it creates a wider shift for $m \neq 0$ and its influence on $m = 0$ states is found to be greater than that of the magnetic field. To show the accuracy of the present model, a comparison is made with those ones obtained in the absence of external fields. An extension to 3-dimensional quantum system have also been presented.

1. Introduction

It is commonly known that the anharmonic and harmonic oscillator potentials play an important role in the history of molecular and quantum chemistry and have also been used to describe the

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molecular structure and molecules [1,2]. Also, the Kratzer-type potential describing the molecular vibrations is important in studying the dynamical variables of diatomic molecules [3]. This potential have a wide applications in various fields of physics and chemistry such as molecular physics, solid-state physics, chemical physics, quantum chemistry, the molecular dynamics study of linear diatomic molecules and the theoretical works on the spectral properties of a diatomic molecule system [4]. Therefore, we found that it is necessary to study the exact bound state solutions of the two-dimensional (2D) solution of the Schrödinger equation for these potentials under the influence of external magnetic and Aharonov–Bohm fields.

The 2D hydrogen model was treated as an atomic spectroscopy and used as a simplified model of the ionization process of the highly excited 3D hydrogen atom by circular-polarized microwaves [5]. The field-free relativistic Coulomb interaction has been studied by many authors by using various techniques [6–8]. The nonrelativistic H-like atom under the influence of magnetic field has been the subject of study over the past years [9–11]. In the presence of a low magnetic field, the quasi-classical solution of the Dirac equation has been obtained by factorization method [12]. In the framework of the variational method, the ground-state Dirac energies and relativistic spinless lowest few states have been calculated for arbitrary strength values of magnetic field [13,14]. The Klein–Gordon wave equation was solved exactly for particular values of magnetic field in which the wave function can be expressed in closed analytical form [15]. The polynomial solutions of the Schrödinger equation was obtained for the ground-state and a few first excited states of 2D hydrogenic atoms for particular values of the magnetic field strength perpendicular to the plane of transversal motion of the electron using a relativistic wave function [16]. Recently, within the framework of power-series solutions, the Klein–Gordon and Dirac equations have been solved for the 2D hydrogen-like systems when an arbitrary external magnetic field is applied [17]. For particular values of magnetic field B, it is found that the exact polynomial solutions can be found using the well-known methods in literature [15,18–22].

Recently, the spectral properties in a 2D charged particle (electron or hole) confined by a PHO potential in the presence of external strong uniform magnetic field $\overrightarrow{B}$ along the z direction and Aharonov–Bohm (AB) flux field created by a solenoid have been studied. The Schrödinger equation is solved exactly for its bound states (energy spectrum and wave functions) [23,24]. So, it is natural that the relativistic effects for a charged particle under the action of this potential could become important, especially for a strong coupling. Within this annals, we have also studied the exact analytical bound state energy eigenvalues and normalized wave functions of the spinless relativistic equation with equal scalar and vector pseudo-harmonic interaction under the effect of external uniform magnetic field and AB flux field in the framework of the NU method [25]. Robnik and Romanovsky [26] studied the Schrödinger equation of the hydrogen atom in a strong magnetic field in 2D. Setare and Hatami [27] considered the exact solutions of the Dirac equation for an electron in a magnetic field with shape invariant method. Villalba [28] analyzed the relativistic Dirac electron in the presence of a combination of a Coulomb field, a $1/r$ scalar potential as well as the Dirac magnetic monopole and an Aharonov–Bohm potential using the algebraic method of separation of variables. Schmid-Burrgh and Gail [29] solved the stationary Dirac equation for an electron embedded in a uniform magnetic field and in an electrostatic potential periodic along the field lines. The eigenvalues and width of the lowest band gap are calculated. Kościk and Okopińska have studied quasi exact solutions for two interacting electrons via Coulombic force and confined in an anisotropic harmonic oscillator in 2D anisotropic dot [30]. An ansatz for wave function has been applied to obtain the D-dimensional solutions of radial Schrödinger equation with some anharmonic potentials [31].

Recently, the 2D solution of the Schrödinger equation for the Kratzer potential with and without the presence of a constant magnetic field has been studied for the first time within the framework of the asymptotic iteration method (AIM) [32]. Effect of constant magnetic field on the energy eigenvalues of a particle moving under the Kratzer potential was precisely presented by Aygun et al. [32]. Furthermore, we have studied the spectral properties of the quantum dots by solving the Schrödinger equation for the anharmonic oscillator potential and superposition of pseudoharmonic-linear-Coulomb potential in presence/absence of external uniform magnetic and AB flux fields in the framework of the Nikiforov–Uvarov (NU) method and analytical exact iteration method (AEIM) [33]. Also, we have studied the effect of these external fields on the energy states and wave functions of a