Exact solutions for a quantum ring with a dipolar impurity

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Abstract We study analytically the Schrödinger equation for a system made up of a quantum ring with a dipolar impurity under the effect of an Aharonov–Bohm field, and we choose the pseudoharmonic oscillator as a confinement potential. We calculate the exact values of the energies and we also get the exact expressions of the wave functions. We study the effects of the dipole moment of the impurity on the energies of the levels as well as on those of the transitions and this for different materials.

Contents

1 Introduction ................................................
2 Exact solutions for 2D Schrödinger equation ............................... 2.1 Solution of the angular equation ...................................
2.2 Solution of the radial equation ....................................
3 Applications to 2D quantum rings ....................................
4 Conclusion ................................................
References ...................................................

1 Introduction

The interest for two-dimensional 2D materials comes from the great popularity of the graphene (and co. like silicene and manganene) and also from experimental achievements with the realization of quantum gases at low dimensions [1, 2] and before that from quasi-condensate experiments [3]. With the immense technological advancement in nano-processing, new beings appear in low-dimensional systems like quantum dots (QD) which can be regarded as low-dimensional hetero-structures whose carriers are confined in all spatial dimensions [4]. Their manufacturing techniques make it possible to control their properties and thus they are made in such a way that they acquire the same characteristics of atomic systems; this is why they are sometimes called artificial atoms [4, 5]. The confinement potential in QD may originate from various physical effects and possesses different symmetries in different nano-structures. The knowledge of the realistic profile of this confinement potential

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is necessary for a theoretical description of the electronic properties of QDs and, even more for fabrication of nano-devices [5]. For a long time, the pseudoharmonic oscillator (PHO) is used to study these compounds and recently it was found to be one of those that best correspond to QDs [6] (and the references therein).

For 2D disc-shaped quantum ring (QR) under the effect of an ionized donor atom, the conduction band electron is described by a PHO as a confinement potential and a donor impurity term [7–9]:

\[
V(r) = \frac{1}{2} m^* \omega_0^2 r^2 + \frac{\hbar^2}{2 m^*} \lambda^2 r^2 + \frac{e^2}{\varepsilon r - \varepsilon_{r, j}}
\]  
(1)

In the above expression, \(m^*\) is the effective mass of the electron, \(\varepsilon\) the static dielectric constant of the ring material, the dimensionless parameter \(\lambda\) characterizes the strength of the potential that describes the hollow region of the ring and \(\omega_0\) represents the confinement frequency of the harmonic potential [9,10]. The impurity is clustered around the origin and the \(\varepsilon_{r, j}\) are the position vectors that characterize its elements (whether the charge is discrete or continuous) while \(\varepsilon r\) is the position vector of the band electron and thus we consider the case \(||\varepsilon r|| > ||\varepsilon_{r, j}||\) for all values of \(j\).

These semiconductor (QR) can be made using many techniques. For instance, to get perfect circular QR, the most frequently used techniques are conventional molecular-beam epitaxy that creates a 2D electron gas in GaAs at the GaAs/GaAlAs interface, while asymmetric InGaAs QR can be made-up by solid-source beams [10].

The last term in 1 does not have a radial symmetry, and so, it adds a non-central term to the potential. This anisotropy in the charge distribution is present for most real systems in quantum chemistry and nuclear physics like those used to describe ring-shaped molecules such as benzene and also in the interactions between deformed pair of nuclei [11]. The study of non-central potentials is not easy because analytically solvable cases are rare [12–17], and this has led studies to use radial approximations of these potentials to find analytical solutions or to consider numerical methods for the computations of their properties.

In this work, we are interested in the analytical resolution of the 2D Schrödinger equation (SE) for a QR with a new non-central potential consisting of a PHO and a dipole term:

\[
V(r, \theta) = Ar^2 + \frac{B}{r^2} + C + D \frac{\cos \theta}{r^2}
\]  
(2)

We use this general form to write the potential because the first three terms represent the usual PHO with the following substitutions \(A = D \varepsilon_{r, e}^2\), \(B = D \varepsilon_{r, e}^2\) and \(C = -2D\varepsilon\) where \(D\varepsilon\) represents the dissociation energy and \(r_e\) is the equilibrium internuclear separation [18–20]:

\[
V_{\text{PHO}}(r) = D\varepsilon \left( \frac{r}{r_e} - 1 \right)^2
\]  
(3)

and also because it gives the first two terms of 1 when \(A = m^* \omega_0^2 / 2, B = h^2 \lambda^2 / 2m^*\) and \(C = 0\). Another advantage of the general form in 2 is that it corresponds to the Tan–Inkson model of QR if we put \(C = -2\sqrt{AB}\) [21].

As we mentioned above, the treatment of non-central potentials is difficult and that is why the previous studies of the donor impurity term (the last term in 1) either treat it numerically or consider it of radial symmetry by neglecting the anisotropies in the charge distribution of the donor. In this latter case, we must have an ionized impurity and we say that it is of the Coulomb type [5,7,22–27]. In our study, we treat the case of an electrically neutral impurity because it corresponds to most atomic and molecular systems. For this impurity, we use the
general form of an extended charge distribution whose effect on the band electron is given by the potential $e \int dq_a / | \vec{r} - \vec{a} |$ (where $dq_a$ is the charge element of the impurity with a position defined by the vector $\vec{a}$) and we treat it with the multipolar expansion in the same way as the last term in 1 given the similarity between the two. The Coulomb contribution of this potential disappears in our case, as it is proportional to the total charge of the impurity, which is zero. Here, we are left only with the dipole term $D \cos \theta / r^2$ where $D = ed$ and $\vec{d} = \int dq_a \vec{a}$ is the dipole moment of the impurity [28] (For simplicity, we will name $D$ the dipole moment while knowing that its unit is that of the product of a charge and a dipole moment). We neglect all the other multipolar terms starting from the quadrupole since their contributions start from the third power of the ratio $| \vec{r}_j | / | \vec{r} |$, which is less than one (For the same reasons that made $| \vec{r}_j | < | \vec{r} |$). This dipole term comes from the anisotropies in the charge distribution of the impurity, and it represents the last term in 2. We give as an example of this behavior the interaction with the permanent electric dipole moment in CdSe QD [29]. So in this work, we treat the system of 2D quantum ring with the potential defined in 2 and we do the study analytically.

We can find other examples of the presence of the dipole potential in 2D systems, and we quote here ultrathin semiconductor layers [30], spin-polarized atomic hydrogen absorbed on the surface of superfluid helium [31] and gapped graphene with two charged impurities [32,33]. This 2D dipole interaction corresponds also to the states of planar charged particles with perpendicular magnetic field [34] and to the electron pairing that stems from the spin-orbit interaction in 2D quantum well [35].

We add to the non-central PHO potential 2 a vector potential of the Aharonov–Bohm (AB) type as is done in several previous works [36–39], but we will keep here the analytical character of the solutions.

Our work is structured as follows: following this first section which represents the introduction, there will be a second one 2 dedicated to the analytical solutions of the SE for the new non-central PHO potential 2. Section 3 will be about applying our results to QRs. Finally, Sect. 4 contains the conclusion of the work.

2 Exact solutions for 2D Schrödinger equation

We are looking for the solutions of the stationary 2D SE when a charged particle $q$ is subject to the effects of the non-central scalar potential $V(r, \theta)$ defined by 2 and a vector potential of Aharonov–Bohm (AB) $\vec{A}_{AB}$:

$$\left[ \frac{1}{2\mu} \left( i\hbar \vec{\nabla} + e \vec{A}_{AB} \right)^2 + qV(r, \theta) \right] \psi(r, \theta) = E \psi(r, \theta) ; \vec{A}_{AB} = \frac{\phi_{AB}}{2\pi r} \vec{e}_\theta \quad (4)$$

Since the AB field satisfies the Coulomb gauge $\vec{\nabla} \cdot \vec{A}_{AB} = 0$, we have:

$$\left( i\hbar \vec{\nabla} + e \vec{A}_{AB} \right)^2 \psi(r, \theta) = \left( -\hbar^2 \Delta + e^2 A^2_{AB} + 2ie\hbar A_{AB} \cdot \vec{\nabla} \right) \psi(r, \theta) \quad (5)$$

It is more convenient to use the polar coordinates $(r,\theta)$ for Laplace operator because of the shape of the potential 2, so we write the SE of our system as:

$$\left[ -\frac{\hbar^2}{2\mu} \Delta + \frac{e^2 \phi^2_{AB}}{8\pi^2 \mu r^2} + i \frac{e\hbar \phi_{AB}}{2\mu r^2} \frac{\partial}{\partial \theta} + \left( A r^2 + B \frac{D \cos \theta}{r^2} \right) \right] \psi(r, \theta) = (E - C) \psi(r, \theta) \quad (6)$$
With the use of $E_r = 2\mu\hbar^{-2}(E - C)$ and $\beta = B + (\hbar^2/2\mu) (\phi_{AB}^2/\phi_0^2)$ ($\phi_0 = h/e$ is the magnetic flux quantum), we have:

$$
\left[ \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{2\mu A}{\hbar^2} r^2 - \frac{2\mu\beta}{\hbar^2} r^2 + \frac{1}{r^2} \left( \frac{\partial^2}{\partial \theta^2} - \frac{2i\phi_{AB}}{\phi_0} \frac{\partial}{\partial \theta} - \frac{2\mu D}{\hbar^2} \cos \theta \right) \right] \psi(r, \theta) = E_r \psi(r, \theta)
$$

(7)

We use the following form for the wave function $\psi(r, \theta) = r^{-1/2} R(r) \Theta(\theta)$ to split this equation into two parts:

$$
\left( \frac{d^2}{d\theta^2} - 2\frac{\phi_{AB}}{\phi_0} \frac{d}{d\theta} - E_\theta - \frac{2\mu D}{\hbar^2} \cos \theta \right) \Theta(\theta) = 0 \quad (8a)
\left[ \frac{d^2}{dr^2} + \left( E_\theta - \frac{2\mu\beta}{\hbar^2} + \frac{1}{4} \right) \frac{1}{r^2} - \frac{2\mu A}{\hbar^2} r^2 + E_r \right] R(r) = 0 \quad (8b)
$$

We have to find the angular eigenvalues $E_\theta$ and eigenfunctions $\Theta(\theta)$ from the angular equation and then use these expressions to resolve the radial part, and here, we get the $E_r$ with the $R(r)$; this give us the energies $E$ of the system from $E_r = 2\mu\hbar^{-2}(E - C)$ and also the eigenfunctions $\psi(r, \theta)$ from $\psi(r, \theta) = r^{-1/2} R(r) \Theta(\theta)$.

2.1 Solution of the angular equation

For the angular equation, we write the solutions $\Theta(\theta) = \exp(i\delta \theta) \Phi(\theta)$ with $\delta = \phi_{AB}/\phi_0$ to obtain a Mathieu type equation [40] through the use of the transformations $\theta = 2z$, $c = 4(\delta^2 - E_\theta)$ and $q = 4\mu\hbar^{-2}D$:

$$
\frac{\partial^2 \Phi(z)}{\partial z^2} + [c - 2q \cos(2z)] \Phi(z) = 0
$$

(9)

The period of $z$ in 9 is $\pi$ because $\theta$ is $2\pi$ periodic, so the solutions of this equation are the Mathieu functions cosine-elliptic $ce_{2m}$ or sine-elliptic $se_{2m+2}$, where $m$ is a nonnegative integer [41]. For a given value of the dimensionless parameter $q$ (or equivalently $D$ from $q = 4\mu\hbar^{-2}D$), the Mathieu solutions are periodic only for certain values of the other parameter $c$. These specific values of $c$ are called the characteristic values, and they are denoted $a_{2m}$ when we have $ce_{2m}$ solutions, while those related to $se_{2m+2}$ functions are denoted $b_{2m}$ [42,43]. So we have two types of solutions for the angular equation 8a, which are $ce_{2m}$ and $se_{2m+2}$, and also two types for the eigenvalues $E_\theta$ corresponding to the two different categories of the characteristic values, namely $a_{2m}$ (linked to the $ce$ solutions) and $b_{2m}$ (linked to the $se$ solutions) from the relation $c = 4(\delta^2 - E_\theta)$. This distinction between $ce$ and $se$ solutions is similar to the case of harmonic oscillator (HO) where we have two types of solutions denoted even and odd, but unlike the HO case, Mathieu’s eigenvalues do not have the same expressions for the two kinds of solutions and therefore we use two different names $a_{2m}$ and $b_{2m}$ to distinguish them.

These two expressions $a_{2m}$ and $b_{2m}$ of the characteristic values $c$ are different except for the case where $q = 0$ and we cannot express them using usual mathematical functions except for the limit cases of the $q$ parameter. For example for small values of $q$ ($q < 1$) and for $m > 3$, we have the following expressions ($v = 4m^2 - 1$) [41]:

$$
a_{2m}(q) \approx b_{2m}(q) = 4m^2 + P_m(q) = 4m^2 + \frac{1}{2v} q^2 + \frac{20m^2 + 7}{32v^3} (v^3 - 3) q^4 + \frac{36m^4 + 232m^2 + 29}{64v^5} (v^5 - 3) (v - 8) q^6 + O(q^8)
$$

(10)
Here, the coefficients are the same until the terms in $q^{2m-2}$. When $m \leq 3$, these polynomial coefficients are different for each value of $m$ and we find similar approximate polynomial forms for large $q$’s but with different coefficients too [41].

We see that at the limit $q \to 0$ (or $D \to 0$), the two values $a_{2m}$ and $b_{2m}$ are equal to $4m^2$ and so the corresponding solutions $ce_{2m}$ and $se_{2m+2}$ become degenerate. Since these $ce$ and $se$ solutions give the cos and sin functions, respectively, at this limit of zero dipole moment [41], we find the usual $\exp(i m \theta)$ solution corresponding to central potentials. So in our case, and because of the non-central term $r^{-2} \cos \theta$ in the potential, this degeneracy is removed when $D \neq 0$ as $a_{2m} \neq b_{2m}$ here [41]. Because we have $a_{2m}(q \to 0) = 4m^2$ and $b_{2m}(q \to 0) = 4m^2$ [10], we conclude that these two expressions of the Mathieu characteristic values generalize the quantum number $m$ in the same way as the $ce$ and $se$ Mathieu solutions generalize the trigonometric functions cos and sin found for central potentials. But as we mention before, the eigenfunctions $ce_{2m}$ and $se_{2m+2}$ are not degenerate like cos and sin since their corresponding eigenvalues $a_{2m}$ and $b_{2m}$ are equal only in the limiting case $q = 0$ (or $D = 0$).

The new phase factor $\exp(i \delta \theta)$ in $\Theta(\theta)$ coming from the AB field is added to the usual one $\exp(i m \theta)$ present in the Mathieu solutions $\Phi(\theta)$ from the Floquet theorem [42,43]. Through this new phase factor, the quantum numbers $m$ are shifted to $m' = m + \delta$ [36,38,44,45] and we write the formulas of the parameters $a_{2m}$ and $b_{2m}$ with this new number $m'$ instead of $m$ to get $a_{2(m+\delta)}$ and $b_{2(m+\delta)}$, respectively.

Using the relations of $c$ and $q$, we get the angular eigenvalues $E_\theta$ as a function of $D$:

$$E_\theta^{(m,\delta)} = \delta^2 - \frac{1}{4} c_{2(m+\delta)} (\frac{4\mu}{\hbar^2} D) \approx \left( \frac{\phi_{AB}}{\phi_0} \right)^2 - \left( m + \frac{\phi_{AB}}{\phi_0} \right)^2 + P(m+\phi_{AB}/\phi_0)(D)$$  \hspace{1cm} (11)

We use the same symbol $c_{2m}$ for both $a_{2m}$ and $b_{2m}$ in the $E_\theta$ formulas to simplify the notations without forgetting that they represent two different expressions of the eigenvalues. From now on, this will be the case in all the relations.

The last relation in 11 is an approximate expression of $E_\theta$ for small values of $D$ where $P(D)$ is a polynomial of even powers of $D$ starting from the power 2; we get this polynomial by using the relation $q = 4\mu h^{-2} D$ and replacing $m$ by $m + \delta$ in the expressions represented by 10. It is used to connect the solutions to the quantum number $m$ and to show that our angular solutions give the right ones within the limit $D \to 0$ and when the AB field is zero ($\delta = 0$).

It is interesting to note that the same angular Eq. 8a appears when we consider the motion of charged particles on a 1D circular ring in a double-well potential and a AB flux [46]. The phase factor $\exp(i \delta \theta)$ in the solution $\Theta(\theta)$ is typical of the AB phenomenon, and it is similar to that appearing when studying the electronic states near the Fermi level of a nanotube with sufficiently large diameter [47]. We find also a similar $\phi_{AB}/\phi_0$ phase factor in the solutions for the case of an AB ring described with Dirac equation [38,45].

### 2.2 Solution of the radial equation

Now having in mind the values of $E_\theta^{(m,\delta)}$, we start the resolution of the radial Eq. 8b. To do so, we put $r = a \sqrt{\rho}$, $a^2 = h/\sqrt{2\mu A}$ and $\eta = (E_\theta - 2\mu \beta h^{-2} + 1/4)$, so we get:

$$\left[ 4\rho \frac{d^2}{d\rho^2} + 2 \frac{d}{d\rho} - \rho + \frac{\eta}{\rho} + E_r a^2 \right] R(\rho) = 0$$  \hspace{1cm} (12)
To solve this equation, we use the following transformation:

\[ R(\rho) = \rho^{\alpha} e^{-\rho/2} \omega(\rho) \] (13)

and we get a new differential equation for \( \omega(\rho) \):

\[
\left[ \rho \frac{d^2}{d\rho^2} + \left( 2 \left( \alpha + \frac{1}{4} \right) - \rho \right) \frac{d}{d\rho} + \frac{1}{\rho} \left( \left( \alpha - \frac{1}{4} \right)^2 - \frac{1}{4} \right) + \frac{E_r a^2}{4} - \left( \alpha + \frac{1}{4} \right) \right] \omega(\rho) = 0
\] (14)

We use the fact that \( \alpha \) is a free parameter to cancel the term in \( 1/\rho \), so we put:

\[
\left( \alpha - \frac{1}{4} \right)^2 - \frac{1}{4} = 0
\]

Since we require \( \omega(\rho) \) to be nonsingular at \( \rho \to 0 \), we choose the positive solution for \( \alpha \):

\[
\alpha = \frac{1}{2} \left( \frac{1}{2} + \sqrt{1 - 4\eta} \right)
\] (15)

Finally, we put:

\[ 4n_r = E_r a^2 - 4\alpha - 1 \] (16)

to simplify the Eq. 14 to the form:

\[ \left( \rho \frac{d^2}{d\rho^2} + \left( 2\alpha + \frac{1}{2} - \rho \right) \frac{d}{d\rho} + n_r \right) \omega(\rho) = 0 \] (17)

The solutions of this equation are the hypergeometric functions \( _1F_1 \) (\( N \) is the normalized constant):

\[ \omega(\rho) = N_1 F_1 \left( -n_r, 2\alpha + 1/2, \rho \right) ; n_r \in \mathbb{N} \] (18)

In terms of the variables \( r \) and \( \theta \), the general form of the wave function \( \psi(r, \theta) \) is:

\[ \psi(r, \theta) = N e^{i\beta \theta} \Phi(\theta) \left( \frac{r}{a} \right)^{2\alpha} e^{-r^2/2a^2} _1F_1 \left( \left( \alpha + \frac{1}{4} \right) - \frac{E_r a^2}{4}, 2\alpha + \frac{1}{2}, \frac{r^2}{a^2} \right) \] (19)

To determine the normalization constant \( N \), we substitute this expression into the condition \( \int |\psi(r, \theta)|^2 r dr d\theta = 1 \) and we recall that Mathieu functions \( \Phi(\theta) \) are normalized to \( \pi \) by definition as we have \( \int_0^{2\pi} ce_{2n}(\theta) ce_{2m}(\theta) d\theta = \delta_{nm}\pi \) and \( \int_0^{2\pi} ce_{2n+2}(\theta) ce_{2m+2}(\theta) d\theta = \delta_{nm}\pi \) for all nonnegative integers \( n \) and \( m \) [41]. We use Laguerre polynomials of degree \( n \) from the relation [48]:

\[ L_n^{(2\alpha - 1/2)} \left( \frac{r^2}{a^2} \right) = \frac{(n+2\alpha-1/2)!}{n!(2\alpha-1/2)!} _1F_1 \left( -n, 2\alpha + \frac{1}{2}, \frac{r^2}{a^2} \right) \] (20)

and the identity [49]:

\[ \int_0^\infty q^{k+1/2} e^{-q} L_n^k(q) L_m^k(q) dq = \frac{\Gamma(n+k+1)^2 \Gamma(m+k+1) \Gamma(k+3/2) \Gamma(m-1/2)}{n!m!\Gamma(k+1)\Gamma(-1/2)} \times _3F_2 \left( -n, k+3/2, 3/2; k+1, -m+3/2; 1 \right) \] (21)
to get the formula:

\[
N = \frac{(n + 2\alpha - 1/2)!}{(2\alpha - 1/2)!\alpha^n (n + 2\alpha + 1/2)} \times \left[ \frac{2\Gamma (2\alpha + 1/2) \Gamma (-1/2)}{\Gamma (n + 2\alpha + 1/2) \Gamma (2\alpha + 1) \Gamma (n - 1/2)} \right]^{1/2} F_2 (-n, 2\alpha + 1, 3/2; 2\alpha + 1/2, -n + 3/2; 1)
\]

(22)

One can also use the general result of the PHO in \(N\) dimensions [19] by setting \(N = 2\) and replacing \(m\) by \(\sqrt{c_{2m}/2}\) 10 and thus obtain a more compact version of this constant.

For the energies, we use the Eqs. 15 and 16 and the relations \(\eta = E_\theta - 2\mu B \hbar^2 + 1/4\), \(\beta = B + (\hbar^2/2\mu) \delta^2\), \(E_\theta = \delta^2 - (1/4)c_{2(m+\delta)}\) and \(E_r = 2\mu \hbar^{-2}(E - C)\) to get the eigenvalues of a 2D quantum ring confined with a PHO potential and subject to the effects of both a dipolar impurity and an AB field:

\[
E = \sqrt{\frac{2\hbar^2 A}{\mu} \left( 2n_r + 1 + \sqrt{\frac{2\mu \beta}{\hbar^2} - E_\theta} \right) + C} = \sqrt{\frac{2\hbar^2 A}{\mu} \left( 2n_r + 1 + \sqrt{\frac{c_{2m+\delta}}{4} + \frac{2\mu B}{\hbar^2}} \right) + C}
\]

(23)

We can check the validity of this expression by studying its limits when canceling the different parameters. Starting with the case where the AB field is absent, which corresponds to \(\delta = 0\), we find the energies for the non-central dipolar PHO 2 (to our knowledge, this potential has not yet been studied):

\[
E = \sqrt{\frac{2\hbar^2 A}{\mu} \left( 2n_r + 1 + \frac{c_{2m+\delta}}{4} \right) + C}
\]

(24)

Similarly, if we cancel the dipole term of the potential 2 by setting \(D = 0\) in 23 (or equivalently \(q = 0\) in \(c_{2(m+\delta)}\) (q)), we obtain the case of the Tan–Inkson model [21] with an AB field:

\[
E = \sqrt{\frac{2\hbar^2 A}{\mu} \left( 2n_r + 1 + \sqrt{(m + \phi_{AB} / \phi_0)^2 + \frac{2\mu B}{\hbar^2}} \right) + C}
\]

(25)

We can also write the energies 23 according to the parameters \(D_e\) and \(r_e\) of the PHO expression 3:

\[
E_{n_r,m} = \sqrt{\frac{2\hbar^2 D_e}{\mu r_e^2} \left( 2n_r + 1 + \frac{2\mu}{\hbar^2} D_e r_e^2 + \frac{1}{4} c_{2(m+\delta)} \left( \frac{4\mu}{\hbar^2} D_e \right) \right)} - 2D_e
\]

(26)

These general relations give the usual PHO energies [19] when \(D = 0\) because \(c_{2m} = 4m^2\) in this case from 10 (\(\delta = 0\) as we consider that there is no AB field here). They also give the usual harmonic oscillator solutions if we add the assumptions \(A = \mu \omega^2/2\) and \(B = C = 0\) to a null dipole moment:

\[
E = \hbar \omega (2n_r + |m| + 1)
\]

(27)

3 Applications to 2D quantum rings

To apply these results to the two-dimensional QR, we use the notations of the potential 1, so we have \(A = m^* \omega_0^2/2\), \(B = \lambda^2 \hbar^2/2m^*\) \((m^* = \mu)\) and \(C = 0\) in 23 to write the energies as follows:
Corrections of the energies in ħω₀ units versus the dipole moment in atomic units for the ce states and for \( m = 0, 1, 2 \)

\[
E_{n_r, m} = \hbar \omega_0 \left( 2n_r + 1 + \sqrt{\lambda^2 + \frac{1}{4} c^2_{2(m+\delta)} \left( \frac{4m^*}{\varepsilon_r \hbar^2 D_\theta} \right)} \right)
\]

We have also written \( D_\theta = D_\theta / \varepsilon_r \) to introduce the same parameters of the QR potential 1.

Focusing on the effects of the dipole moment on the energies, we see in their expression 28 that the main modification is due to the parameter \( c^2 \) which replaces \( m \); So we will study the effects on these energies through the root term:

\[
\lambda_{ce, se} = \sqrt{\lambda^2 + \frac{1}{4} c^2_{2(m+\delta)} \left( \frac{4m^*}{\varepsilon_r \hbar^2 D_\theta} \right)}
\]

and especially through the correction that \( D_\theta \) adds to this value. Therefore, we will focus on the dimensionless difference \( \lambda_{ce, se} - \lambda_0 \) where \( \lambda_0 = \sqrt{\lambda^2 + m^2} \) since it will give us also the energy corrections \( \Delta E = E_{n_r, m} - E_{n_r, m} (D_\theta = 0) \) in ħω₀ units. The energies 28, as well as the corrections \( \lambda_{ce, se} - \lambda_0 \), depend on the type of angular solutions that one chooses (which Mathieu solution \( \Phi (\theta) \) in the wave function \( \psi (r, \theta) \) in 23) and this through the parameter \( c^2_{2(m+\delta)} \) which represents either \( a^2_{2(m+\delta)} \) when we have ce solutions or \( b^2_{2(m+\delta)} \) when we get se ones. We call ce states the eigen-functions associated with the ce solutions and se states the ones related to the se solutions. We also use the ce and se indices to indicate the dependence of the eigenvalues on these two types of angular solutions; we associate these indices with the energies as well as with the \( \lambda \) parameters.

Parameter values used in our computations correspond to GaAs devices where \( \lambda = 2, m^* = 0.067 m_e, \varepsilon_r = 12.65 [9,10,50–52] \), and we use the Hartree atomic units defined by \( \hbar = e = m_e = 4\pi \varepsilon_0 = 1 \). For the energy numerical values, we have \( \hbar \omega_0 \approx 0.1 \sim 1 \text{ eV} [9,10,51,53] \) and this means that the energies of the levels considered in our work \((n = 1&2 \text{ and } m = 0&1)\) are in the intervals 0.5 to 0.8 eV or 5 to 8 eV depending on the value of \( \hbar \omega_0 \). For \( D_\theta \), we choose them in the range 1 to 10 a.u. because it corresponds to the experimental values of most molecular systems [54].

Because of the behavior of the Mathieu characteristic values \( a_{2m} \) and \( b_{2m} \), the corrections for the ce states \( m = 0 \) and the se states \( m = 1 \) are negative, while they are positive for all the other states for both ce and se solutions \((m = 0 \text{ states exist only for ce solutions [41,48])}\). We see in Figs. 1 and 2 that the corrections decrease with increasing \( m \) and also that their values...
corresponding to $ce$ solutions are larger than those related to $se$ ones for the same quantum numbers $n_r$ and $m$. These figures also show that we can neglect the modifications for $m \geq 2$ as they are $10^2$ smaller than those corresponding to the $s$-states ($m = 0$) and so they give corrections of the order of $10^{-5}$ eV or less. Depending on the values of $\hbar \omega_0$ mentioned above ($\hbar \omega_0 \approx 0.1 \sim 1$ eV), the energy corrections for $m = 0$ are around $10^{-3}$ eV while those corresponding to $m = 1$ are just a little bit smaller for $ce$ states and approximatively equal to $10^{-4}$ eV for $se$ states.

Since these corrections are not the same for the different values of $m$, the dipolar term modifies the transition energies between the levels; in Figs. 3 and 4, we give as an example the effects on the transitions $(n, 1) \rightarrow (n, 0)$ and $(n, 2) \rightarrow (n, 1)$. Note that the presence of the dipole term increases the transition energies by more than 1% in the case of $(n, 1) \rightarrow (n, 0)$ while it decreases that of $(n, 2) \rightarrow (n, 1)$ by about 0.1%; this concerns $ce$ states. Regarding the $se$ states, the presence of the dipole increases the energy of the $(n, 2) \rightarrow (n, 1)$ transition by less than 0.04%.

Fig. 2  Corrections of the energies in $\hbar \omega_0$ units versus the dipole moment in atomic units for the $se$ states and for $m = 1, 2, 3$

Fig. 3  Correction of the energy of the transition $(n, 1) \rightarrow (n, 0)$ in $\hbar \omega_0$ units versus the dipole moment in atomic units for $ce$ solutions
Fig. 4 Correction of the energy of the transition $(n, 2) \rightarrow (n, 1)$ in $\hbar \omega_0$ units versus the dipole moment in atomic units for both $ce$ and $se$ solutions.

Fig. 5 Corrections of the energies of the $ce$ s-states ($m=0$) in $\hbar \omega_0$ units versus the dipole moment in atomic units for some materials.

From 29, we see also that the corrections increase with the ratio $m^*/\varepsilon_r$ and thus they are more pronounced for the compounds $Ga_{1-x}Al_xAs$, since the effective mass for these materials is given by the formula $m^* = (0.067 + 0.085x)m_e$ with $x$ real [55]. We show in Figs. 5, 6 and 7, these modifications in the energy corrections for $x = 0.3$ used in [51,55] and also for the parameters of $CdSe$ $m^*/\varepsilon_r = 0.13/9.3$ studied in [29]. We observe that the dipole-induced corrections are 2 times greater for the $Ga_{1-x}Al_xAs$ than for the $GaAs$ and they are 7 times more pronounced than the latter in the case of $CdSe$.

Concerning the effects of the AB field, they are very large compared to those due to the dipole potential since they appear directly in the Mathieu exponent while the dipole moment appears in the Mathieu parameter (This is why we choose $\delta = 0$ in the precedent Figs. 1, 2, 3, 4, 5, 6, 7 that represent the effects of $D$ on the energies); the AB corrections are of the order of $10^{-1}\hbar \omega$. We notice that they increase the energies of the system and they are equal for both $ce$ and $se$ solutions. These corrections also increase with increasing $m$ (Fig. 8).
Fig. 6  Corrections of the energies of the ce p-states \((m = 1)\) in \(\hbar\omega_0\) units versus the dipole moment in atomic units for some materials

Fig. 7  Corrections of the energies of the se p-states \((m = 1)\) in \(\hbar\omega_0\) units versus the dipole moment in atomic units for some materials

4 Conclusion

In this work, we have analytically solved the Schrödinger equation for a quantum ring confined by a pseudoharmonic potential and under the effect of a dipolar impurity and an Aharonov–Bohm field. We have obtained the exact expressions of the energies for this new non-central potential as well as those of the wave functions by using the Mathieu functions ce and se in the angular part of the solutions. Our calculations show that the AB field is present through a phase in the wave functions and so it shifts the quantum number \(m\) of the system. The corrections corresponding to this AB field increase the energies and they are much larger than those due to the dipole potential.

The first characteristic of the dipole term is that it removes the degeneracy present for central potentials; thus, the energies depend on the orientation of the solutions compared to the dipole direction, which broke the central symmetry by becoming a privileged one. Corrections are more pronounced for ce states and therefore, states whose orientations are
in the same direction as the dipole; this is similar to the dependence of $3D$ energies on the azimuth number $m$ as soon as we have a Hamiltonian term depending on the direction such as the one representing the effect of a constant magnetic field.

Our solutions generalize the azimuthal quantum number $m$ through the Mathieu characteristic values. The corrections are larger for $m = 0$, and they decrease as $m$ increases. This dependence on $m$ generates a correction on the transition energies between the levels, and it is more apparent for those between the lowest ones such as $(n, 1) \rightarrow (n, 0)$ and $(n, 2) \rightarrow (n, 1)$. All these corrections depend on the chosen material, and we show that they are proportional to the ratio of the effective mass on the static dielectric constant $m^* / \varepsilon_r$.

Finally, we mention that if we add another vector potential $B_r/2$ to the AB one, we will no longer have the possibility to treat the system analytically and we will then have to use perturbative methods, which is beyond the scope of this work as we are looking for analytical solutions.

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