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Nonlinear optical properties of modified Möbius squared potential well: influence of electric and magnetic fields

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ABSTRACT

This work presents a numerical study on the electronic and optical properties of modified Möbius squared potential well in the presence of static electric and magnetic fields. The potential well is formed within GaAs/AlGaAs hetero structures. Schrödinger's equation is solved within the framework of effective mass and envelope wave function approximations to get the wave functions and their corresponding energies of states. The optical absorption coefficients and relative refractive index changes are calculated via the expressions derived from the compact density matrix approach. The numerical results present strong blue shifts on the optical responses of modified Möbius squared potential well when the external electromagnetic fields are strengthening.

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Möbius quantum well; optical absorption; refractive index changes; electric and magnetic fields

1. Introduction

The studies on getting the energy eigenvalues and wave function distributions of wave equations have always been of interest. Knowing them is essential in quantum mechanics, fluid mechanics, optics as well as in molecular physics, and chemistry [1–8]. For instance, the electronic and optical properties of semiconductor hetero structure can be achieved by examining them [9–16]. Furthermore, the potential energy functions imply much important information about the molecular structure of materials [17–19]. Therefore, a wide range of studies from nonrelativistic solutions of the Schrödinger equation to the relativistic solutions of Klein-Gordon and Dirac equations with various potential functions have been searched by many researchers for years. Nevertheless, the exact solution of the Schrödinger equation is only obtainable for limited

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cases, such as hydrogen atom and the harmonic oscillator. Hence, some methods such as Nikiforov–Uvarov (NU) [20–25], supersymmetric quantum mechanics [26,27], factorisation technique [28–30], asymptotic iteration method [31,32], series expansion [33], and algebraic approach [34] are developed to get approximate solutions of quantum mechanical equations with many complex potential functions.

Modified Möbius squared (MMS) potential is one of the special potentials which has an exponential form [35,36]. Exponential-type potentials are very successful in the explanation of diatomic molecules in molecular physics [37]. Möbius square potential is assumed as the general form of Hulthen, Morse, and also Hua potential [37,38] and consulted in the molecular, chemical, and high-energy physics studies to understand the internuclear interaction curves and electronic states of diatomic molecules [21,22,39–41]. The studies on the wave equation solutions with Möbius squared potential can be summarised as follows: Yazarloo and coworkers have solved the Schrödinger equation in D-dimensions with the Möbius square potential by employing the NU method within some approximations and obtained the energy eigenvalues and eigen functions as well as the oscillator strength parameter while the structure parameter of the system is changing [37]. Okorie et al. obtained the bound state solutions of the Schrödinger equation with the factorisation method for MMS potential and investigated the thermodynamic properties [30]. In another study, Okorie and coworkers calculated the energy spectra of generalised Möbius square potential for different diatomic molecules [40]. Yabwa and coworkers have solved the time-independent Schrödinger equation with MMS potential plus Hulthen potential by employing some methods and calculating the bound state energies and radial wave functions of each potential [42]. Onyenegecha et al. have found the approximate solutions of the Schrödinger equation for MMS plus Kratzer potential in the framework of NU method [43]. Antia et al. obtained the approximate solution of the Schrödinger equation for inversely quadratic Yukawa plus Möbius square potential employing the parametric NU method [24]. Okon and coworkers studied the Möbius square plus screened-Kratzer potential using the NU method to present the bound state energies of two diatomic molecules [25]. Njoku et al. solved the Schrödinger equation for the combination of MMS and Eckart potentials with the parametric NU method to get the quantum information [44].

Solutions of Klein-Gordon and Dirac equation with MMS confinement are examined by different researchers as given in the followings: Onyenegecha et al. have obtained the non-relativistic and relativistic energy eigenvalues and related wave functions by solving the Klein-Gordon equation in D-dimension with MMS potential using NU method [35]. They also obtained non-relativistic eigenvalues for some selected diatomic molecules. D-dimensional Klein-Gordon equation with generalised Möbius square potential is examined by Okorie [45]. Antia et al. evaluated the approximate solution of the D-dimensional Klein–Gordon equation with equal scalar and vector Möbius square plus Yukawa potentials with the parametric NU method [21]. Ikot et al. calculated the energy eigenvalues and corresponding wave functions of Möbius square potential by solving D + 1 dimensional Dirac equation within symmetry limits [22]. Maghsoodi and coworkers have obtained the bound state solution of the Dirac equation by considering spin symmetries for Möbius square potential with the NU method [23]. Ikot and coworkers obtained the approximate solution of the Dirac equation for a Möbius square plus Mie type potentials with Coulomb-like interaction term employing the NU method [39]. They also solved the Dirac equation for the combination of Möbius square and inversely quadratic Yukowa potentials in the presence of coulomb-like interaction and obtained the energy eigenvalues and related eigen functions with the NU method [46].

Optical properties of MMS potential have been studied for the first time by Onyenegecha for a spherical quantum dot [36]. Onyenegecha, first calculated the electronic properties of the system by solving the Schrödinger equation with the NU method and then displayed the shifts in the optical absorption and linear refractive indexes while the structural parameters are changing. In relation to the MMS potential, the optical properties of Hulthen [47,48] and Morse [49–51] potentials are studied by some researchers. In the present paper, the electronic and optical properties of MMS potential are examined in a single well. To the best of our knowledge, it is the first study for the optical absorption coefficients (OACs) and relative refractive index changes (RRICs) of a quantum well confined with MMS potential. We believe that the present study has importance in the explanation of the optical properties of diatomic molecules.

2. Theory

This paper considers the confinement of one electron within a MMS potential through one dimension (z) and investigates the electronic and optical properties of charge carrier. The MMS potential is given as follows:

$$V_M(z) = -V_0\left(\frac{A + Be^{-2\eta z}}{1 - e^{-2\eta z}}\right)^2, \tag{1}$$

where V_0 represents the depth of potential, η determines the screening of the potential, A and B are the parameters related with the range of the potential and molecular bond length, respectively. Hence, the limits of the Möbius potential are as follows: $V_M(z) \to -\infty$ for $z \to 0$ and $V_M(z) \to -A^2V_0$ for $z \to \infty$. The MMS potential well is subjected to the external electric and magnetic fields. Electric field with strength F is applied along the growth direction as, $\boldsymbol{F} = (0,\ 0,\ F)$ and magnetic field with strength B is implemented perpendicular to the growth direction as, $\boldsymbol{B} = (B,\ 0,\ 0)$. If the system is exposed to a magnetic field parallel to the growth direction, Zeeman splitting effect should be taken into account. However, this effect is quite small compared to the transition energies. Under these conditions, the time-independent Schrödinger equation can be written as below:

$$\left[\frac{1}{2m^*}\left(\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}(\boldsymbol{r})\right)^2 + V_M(z) + eFz\right] \psi(z) = E\ \psi(z), \tag{2}$$

where $m^* = 0.067\ m_e$ is the effective mass of the electron localised in the GaAs material, e is magnitude of electron charge, c is the speed of light in vacuum and $\boldsymbol{p}$ is the momentum operator. $\boldsymbol{A}(\boldsymbol{r})$ represents the vector potential term of magnetic field and in the Landau gauge it is defined as $\boldsymbol{A}(\boldsymbol{r}) = (0,\ -Bz,\ 0)$.

The Schrödinger equation is solved to get the eigen energy-E and wavefunction-$\psi(z)$ within the effective mass and envelope wave function approximations and by employing the diagonalization method. This method proposed by Xia and Fan [52] and based on the expanding the electron wave function-$\psi(z)$ to trigonometric orthonormal functions which are the solution of square quantum well within rigid walls. The wave function is given as below:

$$\psi(z) = \left(\frac{2}{L}\right)^{1/2} \sum_n C_n \sin\left(\frac{n\pi z}{L} + \frac{n\pi}{2}\right), \tag{3}$$

where n stands for the number of contributing term and C_n is the expansion coefficient. The limit value of the series expansion is determined by getting close enough to the true value of the electron energy in the investigated level. As a result of the experiments, it is observed that the value of $n = 200$ provided sufficient convergence. Besides the width of infinite well L is chosen as 200 nm which is very larger than the localisation width of ground state wave function to get rid of the boundary effects of the well.

Once the energy eigenvalues and wave functions are obtained, then the optical properties can be calculated with the help of expressions given in literature. In the present paper, the electronic and optical properties such as OACs and RRICs are examined in the absence and presence of external electromagnetic fields. For the calculation of OACs and RRICs, one need to know the transition energy-ΔE, between the energy of first excited state (E_1) and ground state (E_0), and the dipole moment matrix elements of first two states given as $M_{ji} = |\psi_j(z)|ez|\psi_i(z)|\ ,\ i,\ j = 0,\ 1$. The values and responses of ΔE and M_{10} while the external electromagnetic fields are exerting are represented in the coming section.

The analytical expressions for the linear ($\beta^1(\omega)$), third-order nonlinear ($\beta^3(\omega, I)$), and total ($\beta(\omega, I)$) OACs for the lowest lying first two levels are given by [49–51]:

$$\beta^{1}(\omega) = \omega\sqrt{\frac{\mu_0}{\varepsilon_R}}\left[\frac{|M_{10}|^2\sigma_\nu\hbar\,\Gamma_{10}}{(\Delta E - \hbar\,\omega)^2 + (\hbar\,\Gamma_{10})^2}\right], \tag{4}$$

$$\beta^{3}(\omega, I) = -\omega\sqrt{\frac{\mu_0}{\varepsilon_R}}\left(\frac{I}{2cn_r\varepsilon_0}\right)\frac{|M_{10}|^2\sigma_\nu\hbar\,\Gamma_{10}}{[(\Delta E - \hbar\,\omega)^2 + (\hbar\,\Gamma_{10})^2]^2}$$
$$\left\{4|M_{10}|^2 - \frac{|M_{11} - M_{00}|^2[3\Delta E^2 - 4\Delta E\hbar\,\omega + \hbar^{2}(\omega^2 - \Gamma_{10}^2)]}{\Delta E^2 + (\hbar\,\Gamma_{10})^2}\right\}, \tag{5}$$

$$\beta(\omega, I) = \beta^{1}(\omega, I) + \beta^{3}(\omega, I), \tag{6}$$

where ε_0 and μ_0 are the dielectric constant and permeability of medium, respectively and ε_R is the real part of the permittivity. $\Gamma_{10} = 1/\tau_{10}$ is the damping term related with time of interaction process (τ_{10}). n_r signifies the refractive index of the system and σ_ν represents the density of electrons contributing to the intersubband transition. ω denotes the frequency of incident photon energy while I displays the strength of incident photon, and it is defined as $I = (2n_r/\mu_0 c)|E(\omega)|^2$.

The formulations for the linear, third-order nonlinear and total RRICs corresponding to the transitions between ground and first excited state can be written as below [49–51]:

$$\frac{\Delta n^{(1)}(\omega)}{n_r} = \frac{\sigma_\nu|M_{10}|^2}{2n_r^2\varepsilon_0}\left[\frac{\Delta E - \hbar\,\omega}{(\Delta E - \hbar\,\omega)^2 + (\hbar\,\Gamma_{10})^2}\right], \tag{7}$$

$$\frac{\Delta n^{(3)}(\omega, I)}{n_r} = -\left(\frac{\sigma_\nu|M_{10}|^2}{4n_r^2\varepsilon_0}\right)\frac{\mu_0 cI}{[(\Delta E - \hbar\,\omega)^2 + (\hbar\,\Gamma_{10})^2]^2}$$
$$\times\left\{\begin{array}{l} 4(\Delta E - \hbar\,\omega)|M_{10}|^2 - \dfrac{|M_{11} - M_{00}|^2}{\Delta E^2 + (\hbar\,\Gamma_{10})^2} \\ \quad [(\Delta E - \hbar\,\omega)(\Delta E(\Delta E - \hbar\,\omega) - (\hbar\,\Gamma_{10})^2) - (\hbar\,\Gamma_{10})^2(2\Delta E - \hbar\,\omega)] \end{array}\right\}, \tag{8}$$

$$\frac{\Delta n(\omega, I)}{n_r} = \frac{\Delta n^{(1)}(\omega)}{n_r} + \frac{\Delta n^{(3)}(\omega, I)}{n_r}. \tag{9}$$

3. Results and discussion

The potential distribution of MMS function and related electronic and optical character in the absence and presence of electric and magnetic fields are presented here. The numerical calculations for the electron placed within the conduction band of GaAs/AlGaAs hetero structure are performed with the following physical constants and fixed parameters: $e = 1.602 \times 10^{-19}$ C, $m_e = 9.1 \times 10^{-31}$kg, $\hbar = 1.056 \times 10^{-34}$ Js, $\sigma_v = 3 \times 10^{22}$ m^{-3}, $n_r = 3.2$, $\mu_0 = 4\pi \times 10^7$ Hm^{-1}, $\varepsilon_R = 12.5$, $\varepsilon_0 = 8.854 \times 10^{-12}$ Fm^{-1}, $\tau_{10} = 0.14$ ps, and $I = 0.01\,\mathrm{MW/cm^2}$. The depth of MMS potential well introduced in Equation (1) is taken as $V_0 = 75$ meV and potential function parameters are chosen as $A = 1$, $B = -0.5$, $\eta = 0.01$ nm^{-1}.

Figure 1 shows the spatial distribution of the MMS potential function and the probability of the ground-state wave function with its corresponding energy in the absence (dashed lines) and presence (solid lines) of external electromagnetic fields. As explained in the theory section with the usage of diagonalization method, the outer ends of Möbius well is considered as infinite barriers and spatial extent of the well is taken as 200 nm in the calculations. Figure 1(a) displays the effect of electric field. Electric field widens the well and carries up it to higher energies by playing a remarkable role in spatial dependency. As shown in Figure 1(b), the application of a magnetic field also expands and raises the well; however, the influence of the magnetic field at 15 T is not as great as the effect of the electric field at 50 kV/m. Although the changes in potential profile are significant, the modifications on the probabilities of the ground state wave function in the presence of electromagnetic fields are very small. These slight changes can be attributed to the hyperbolic form of potential. As here, one-sided rigid wall hyperbolic potentials do not cause strong confinement as double-sided confinement potentials, such as square, and triangle wells. Furthermore, this potential presents a considerable depth around -300 meV for $(0 < z < 2$ nm) and it increases rapidly to higher values for $z > 2$ nm. This prompt increase in the edge of the confining potential limits considerably the spatial expanding of the wave functions. Per consequent the confinement due to the geometrical shape of the potential is preponderant compared to that coming from electric and magnetic

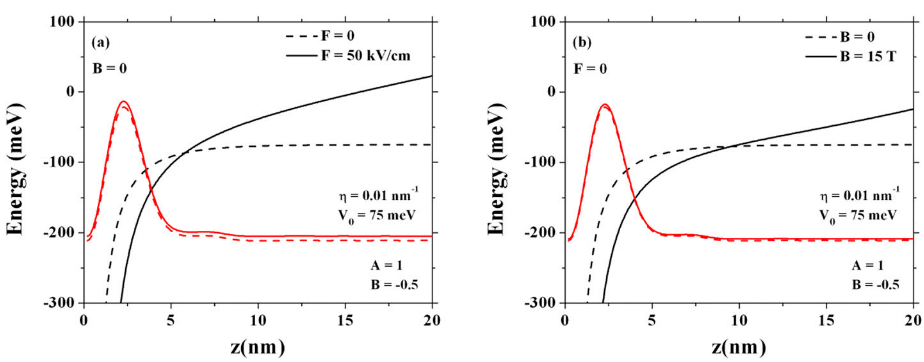

Figure 1. Potential profiles of MMS potential with a depth of 75 meV (black lines) and probability distributions of ground state wave function (red lines) together with their corresponding eigen energies in the absence of electromagnetic field (dashed lines) and in the presence of (a) 50 kV/cm electric field, (b) 15T magnetic field.

field changes. As can be noticed from Figure 1(a,b), the effects of external electromagnetic fields on the ground state energies are more pronounced in the far parts of the well. Another important point is that the wave function is localised with high probabilities in the first quarter of the well where there is a strong confinement region.

The variations in the transition energies between the ground state and first exited state and dipole matrix elements of these states while electromagnetic fields are increasing are presented in Figure 2. A linear increase in the energy differences with an augmented electric field can be seen in Figure 2(a). The variation curve of dipole moment matrix elements with the increasing electric field application looks almost linear. Influence of the strengthening magnetic field on the transition energy differences and dipole moment matrix elements is drawn in Figure 2(b). The linear increase in the magnetic field values leads to an accelerating rise in the energy differences between the first excited state and the ground state. The change in the dipole moment matrix with the application of a magnetic field display a linear increase. It is possible to say that, the application of electric as well as magnetic fields causes a high amount of energy differences in the transition energies. In addition, as shown in Figure 1(a,b), the augmentation of electric and magnetic fields slightly enlarges the width of the potential well especially in its bottom. This enlargement produces more spread of the ground and first excited wave functions and leads to an increase of their overlap, per consequent the dipole matrix rises as shown in Figure 2. The energy levels are sensible to the geometric change in the confining potential. In case of incrementing the electric and magnetic fields, the first and ground energy levels increases, but the excited state has a faster augmentation compared to ground one which explain the increase of the energy transition $(E_1 - E_0)$ as observed in Figure 2(a,b).

The responses of total OACs to the applied external electric and magnetic field is drawn in Figure 3(a,b). Not only the increasing electric field but also the magnetic field result in strong blue shifts with rising magnitudes in the total OACs. Because the transition energy and dipole matrix element given

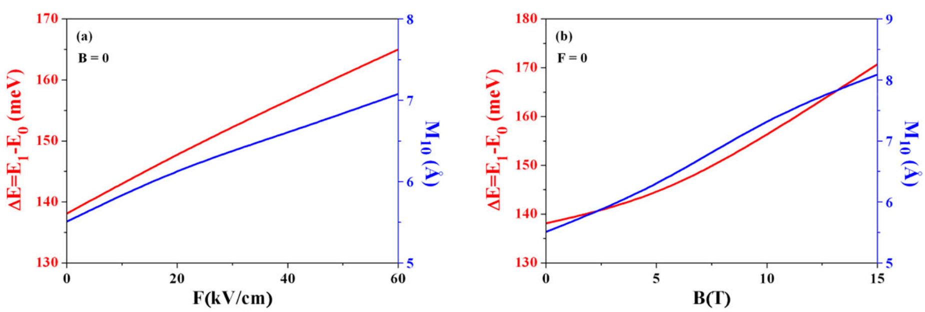

Figure 2. The changes in the transition energies and dipole moment matrix elements between first exited state and ground state as a function of (a) electric field and (b) magnetic field.

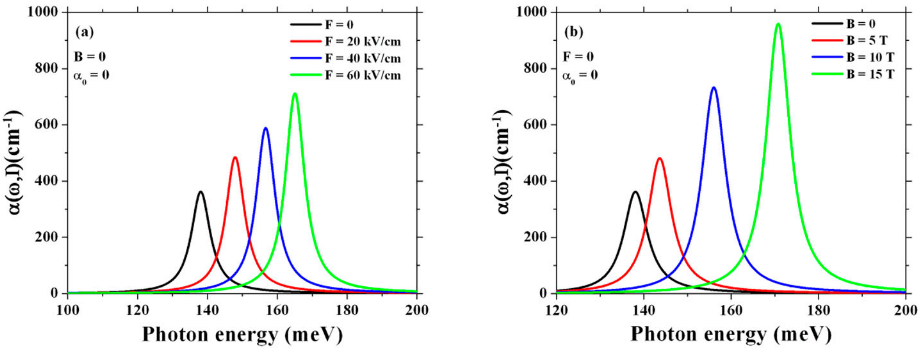

Figure 3. The variations of total OACs as a function of incident photon energy with the application of (a) electric field and (b) magnetic field.

in Figure 2, determine the position and amplitude of the resonance peak, respectively and here the increases in both are seen with increasing electromagnetic field. Furthermore, we remark that the amplitudes of each (OAC) in Figure 3(a,b) are comparable for low intensities of magnetic field ($B < 5\ T$). However, for high values of B, the $(\mathrm{OAC})_{\max}$ reaches large absorptions. For instance, for $F = 60$ kV/cm, $(\mathrm{OAC})_{\max}$ is equal 700 cm^{-1}, but it is around 950 cm^{-1} for $B = 15\ T$. This is explained by examining Figure 2(a,b). In fact, we can observe that the dipole matrix element increases rapidly with magnetic field and at $B = 15\ T$ it gets higher value than that obtained in Figure 2(a) by increasing the electric field.

We pictured the variations in the RRICs in the presence of an external electric field in Figure 4(a) and a magnetic field in Figure 4(b). The augmentation in both electric and magnetic fields cause a strong blue shift in the RRICs by strengthening the magnitudes of RRIC peaks as a consequence of the increases in the transition energy differences and dipole moment matrix elements.

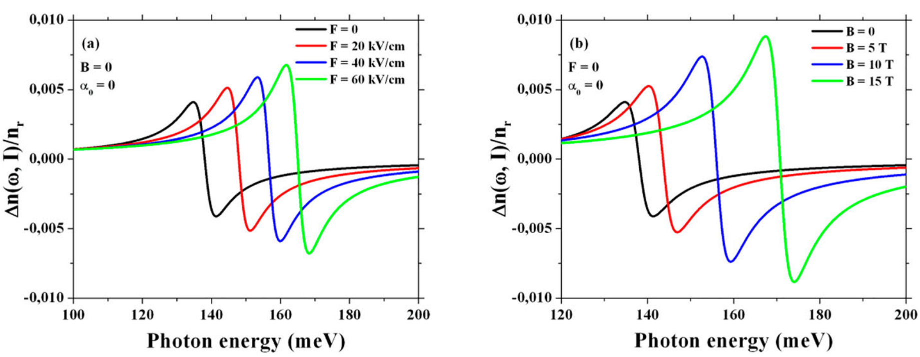

Figure 4. The changes in the RRICs as a function of incident photon energy with the varying (a) electric field and (b) magnetic field.

4. Conclusion

Optical absorption coefficients and relative refractive index changes of a modified Möbius squared potential well are investigated. For that, the Schrödinger equation is solved within effective mass and envelope wave function approximations. Optical properties are obtained with the knowledge of energy eigenvalues and wave functions by employing compact density matrix approach. The findings display that, both the peaks of total optical absorption coefficients and relative refractive index changes occur at significantly higher incident photon energies with augmented magnitudes while the electric and magnetic fields are getting stronger. The paper presents the possibility of responsively controlling the nonlinear optical properties by modified Möbius squared potential under external electromagnetic fields. We expect that the results given here will be useful in the studies of the optical properties of nanostructures confined with exponential-type potentials.

Disclosure statement

No potential conflict of interest was reported by the author(s).

Data availability statement

No data associated in the manuscript.

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