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Finite parabolic quantum wells under crossed electric and magnetic fields: a double-quantum-well problem

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Abstract. We show that, in the framework of the effective-mass approximation, an electron confined in a finite parabolic quantum well under crossed electric and magnetic fields can behave as a double-quantum-well system. These homogeneous crossed fields are such that the magnetic field is parallel to the heterostructure layers and the electric field is applied perpendicular to the magnetic field. For a suitable choice of both fields, the electron is confined to a double-quantum-well effective potential.

1. Introduction

Homogeneous crossed electric and magnetic fields are powerful tools that permit us to make desired changes in the trajectories of charged particles. They have been used as a velocity filter in early atomic physics experiments [1, 2], as well as in the study of the chaotic behaviour of the electron trajectories of Rydberg atoms [3] nowadays. The recent advances in the fabrication and characterization of semiconductor heterostructures have shown that the quantum wells in superlattice heterostructures are well simulated by a finite parabolic potential [4, 5]. In semiconductor research, quantum tunnelling is a fundamental effect. For instance, wave-function tunnelling through potential barriers is related to electronic transport phenomena [6]. New electronic devices have been developed that are based on quantum tunnelling phenomena. In general, these semiconductor devices are related to double-barrier resonant quantum tunnelling (DBRT) [7] as well as double-quantum-well tunnelling (DQWT) systems [8]. In the present work, we study the behaviour of an electron confined in a finite parabolic quantum well (FPQW) subjected to external homogeneous crossed electric and magnetic fields. We will show that for suitable values of the applied fields, this system can simulate the double-quantum-well (DQW) problem.

This work is organized in the following manner. In the second section, we develop the theoretical model and, on the basis of numerical results, we discuss in the third section the special features of the bound state of the system. Finally, we conclude by discussing the main results of this work and some possible applications.

2. Theory

We consider a homogeneous magnetic field $\boldsymbol{B} = (0, 0, B)$ applied parallel to the heterostructure layers, so that in Landau's gauge, the vector potential can be written as

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$\boldsymbol{A} = (0, xB, 0)$. The homogeneous external electric field $\boldsymbol{E} = (-F/e, 0, 0)$ is perpendicular to the magnetic field, where F is a positive constant and e the modulus of the electron charge. In the framework of the effective-mass approximation, the Hamiltonian of an electron confined in a FPQW subjected to the above crossed electric and magnetic fields can be written as

$$\hat{H} = \frac{(p_x^2 + p_z^2)}{2m^*} + \frac{(p_y + exB)^2}{2m^*} + V(x) - Fx \tag{1}$$

where m^* is the effective mass and the confining FPQW potential V is given by

$$V(x) = \frac{m^*\omega^2 x^2}{2}\Theta(L - |x|) + \frac{m^*\omega^2 L^2}{2}\Theta(|x| - L) \tag{2}$$

where Θ is the Heaviside step function and the FPQW width and height are $2L$ and $V_0 = m^*\omega^2 L^2/2$ respectively. If the total energy of the system is E, and assuming free-electronic lateral transport, the wave function can be written as

$$\Psi(\boldsymbol{r}) = \exp(\mathrm{i}(k_y y + k_z z))\psi(x).$$

The resulting Schrödinger equation corresponding to equation (1) gives the following differential equation for $\psi(x)$:

$$-\frac{\hbar^2}{2m^*}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + U_{eff}(x)\psi = \left(E - \frac{\hbar^2 k_z^2}{2m^*}\right)\psi \tag{3}$$

where we define the effective potential U_{eff} as

$$\begin{aligned} U_{eff}(x) \equiv{}& \frac{m^*\Omega^2}{2}\left[(x - x_c)^2 - x_c^2\right]\Theta(L - |x|) \\ &+ \frac{m^*\omega_B^2}{2}\left[(x - x_0)^2 - x_0^2 + \frac{\omega^2 L^2}{\omega_B^2}\right]\Theta(|x| - L) + \frac{\hbar^2 k_y^2}{2m^*} \end{aligned} \tag{4}$$

where $\omega_B = eB/m^*$ is the cyclotronic frequency,

$$\Omega \equiv \sqrt{\omega^2 + \omega_B^2}$$

and the points x_c and x_0 are defined respectively as

$$x_c \equiv (F - \hbar k_y \omega_B)/(m^*\Omega^2) \tag{5}$$

$$x_0 \equiv (F - \hbar k_y \omega_B)/(m^*\omega_B^2). \tag{6}$$

Notice that since Ω is greater than ω_B, x_c is smaller than x_0. In this work, we assume that the electronic charge is shifted in the positive x-direction, since, by construction, the electric field points in the opposite direction. In other words, for non-zero external electric field, the probability of finding the electron as $x \to -\infty$ is smaller than that as $x \to \infty$. The wave-function solution of the Schrödinger equation (3) satisfying this asymptotic boundary condition is the following:

$$\psi(x) = \begin{cases} c_1 U(a_\eta, -\eta) & -\infty < x \leqslant -L \\ c_2 U(a_\xi, \xi) + c_3 V(a_\xi, \xi) & |x| \leqslant L \\ c_4 H(a_\eta, \eta) & L \leqslant x < \infty \end{cases} \tag{7}$$

where the c_i $(i = 1, 2, 3, 4)$ are constants to be determined from the boundary conditions. The function H is defined as

$$H(a, x) \equiv U(a, x) + \mathrm{i}\Gamma\left(\frac{1}{2} - a\right)V(a, x)$$

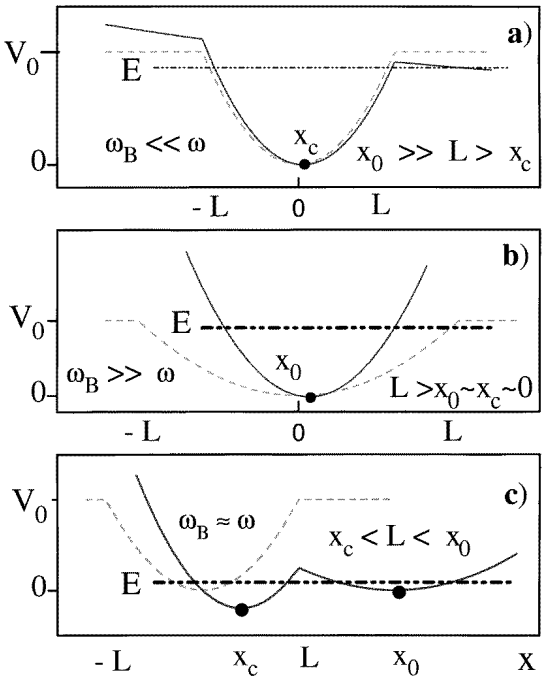

Figure 1. (a) shows that in the limit of strong electric field, U_{eff} is a single well. In this case U_{eff} presents three turning points. Due to tunnelling through the barrier centred at $x = L$, the states of U_{eff} are quasi-bound. Otherwise, as U_{eff} has a finite depth, only a finite number of quasi-bound states with $E < U_{eff}(L)$ can oscillate inside the well. Notice that in this case the ground-state energy can have positive values. (b) shows U_{eff} in the limit of strong magnetic field. In this case U_{eff} is a single well with infinite parabolic confinement; the related parameter frequency is very close to ω_B. Notice that in this case the ground-state energy can have positive values. These bound states are very similar to Landau-like states. (c) shows that as $x_c < L < x_0$, U_{eff} exhibits a double-quantum-well slope which is composed from two parabolic wells connected by a barrier centred at $x = L$. Notice that in this case the points x_0 and x_c at which U_{eff} has minimum values satisfies the inequality $x_0 < L < x_c$. The double-quantum-well states are such that the energy of the electron is below the top of the barrier ($E < U_{eff}(L)$) and the related wave function can oscillate in two distinct wells. Notice that in this case the ground-state energy can have negative values.

where Γ is the gamma function [9], and where the functions $U(a, z)$ and $V(a, z)$ are the Weber parabolic cylinder functions [9] with the following arguments and parameters:

$$\eta(x) = \sqrt{\frac{2m^*\omega_B}{\hbar}}(x - x_0) \tag{8}$$

$$a_\eta = \frac{-1}{\hbar\omega_B}\left(E - \frac{\hbar^2 k_z^2}{2m^*} - U_{eff}(x_0)\right) \tag{9}$$

$$\xi(x) = \sqrt{\frac{2m^*\Omega}{\hbar}}(x - x_c) \tag{10}$$

$$a_\xi = \frac{-1}{\hbar\Omega}\left(E - \frac{\hbar^2 k_z^2}{2m^*} - U_{eff}(x_c)\right). \tag{11}$$

Matching the wave function and the first derivative at $x = \pm L$, we obtain the transcendental equation for the energy spectrum. It is given by the following secular equation:

$$\begin{vmatrix} -U(a_\eta, -\eta_-) & U(a_\xi, \xi_-) & V(a_\xi, \xi_-) & 0 \\ \frac{\sqrt{\Omega}}{\sqrt{\omega_B}}U'(a_\eta, -\eta_-) & U'(a_\xi, \xi_-) & V'(a_\xi, \xi_-) & 0 \\ 0 & U(a_\xi, \xi_+) & V(a_\xi, \xi_+) & U(a_\eta, \eta_+) \\ 0 & U'(a_\xi, \xi_+) & V'(a_\xi, \xi_+) & \frac{\sqrt{\Omega}}{\sqrt{\omega_B}}U'(a_\eta, \eta_+) \end{vmatrix} = 0. \tag{12}$$

In the above determinant, $\eta_\pm \equiv \eta(\pm L)$, $\xi_\pm \equiv \xi(\pm L)$ and we denote as W' the first derivative of any Weber function W with respect to the argument. For non-zero electric field, the electron tunnelling for $x > L$ is related to quasi-bound states. On the basis of this, the solution of the above transcendental equation (12) lies in the energy complex plane. In order to solve equation (12), we need first to understand the behaviour of the effective potential U_{eff} as the electric and magnetic field varies.

Figure 1(a) shows that, in the limit of weak magnetic field, U_{eff} is a single well where the electronic confinement is related to quasi-bound states. In this case, U_{eff} presents three turning points, and E, the solution of equation (12), is complex; that is, $E = \Re[E] + \mathrm{i}\,\Im[E]$. The level width $\Im[E]$ is related to tunnelling through a barrier centred at $x = L$, and only a finite number of quasi-bound states with $\Re[E] < U_{eff}(L)$ can oscillate inside the well. In this situation, U_{eff} resembles a FPQW under an external electric field [10]. In the opposite limit, that of strong magnetic field (see figure 1(b)), the cyclotronic confinement dominates. U_{eff} is a single well with infinite parabolic confinement; the related parameter frequency is very close to ω_B. These bound states are very similar to Landau-like states. In the two above special situations the ground state of the system is related to a single well. For a review of the main system properties in the above limiting cases, see the work of Cury, Celeste and Portal [11] and that of Wang and Chuu [12]. However, for intermediate values of both magnetic and electric fields, the behaviour of U_{eff} can be very peculiar. For magnetic and electric fields such that $x_c < L < x_0$, U_{eff} exhibits a DQW slope (see figure 1(c)). In this case, U_{eff} is composed of two parabolic-like wells connected by a barrier centred at $x = L$. The points x_0 and x_c are such that $U_{eff}(x_c)$ and $U_{eff}(x_0)$ are minimum values of U_{eff}. So, if the energy of the electron is below the top of the barrier ($E < U_{eff}(L)$), the related wave function can oscillate in two distinct regions.

Figure 2(a) shows for fixed values of F and k_y the behaviour of the effective potential as the external magnetic field varies. This figure shows that there is a maximum value for the magnetic field, $B = B_{max}(F, k_y)$, for which double-quantum-well states can survive. It occurs only if the applied magnetic field is less than B_{max}. Otherwise, figure 2(b) shows for fixed values of B and k_y that there is a minimum value for the external electric field $F = F_{mim}(B, k_y)$ for which U_{eff} exhibits double-quantum-well states if the external electric field is greater than F_{min}. The critical fields B_{max} and F_{min} are given respectively by

$$B_{max} \equiv \omega\frac{m^*}{e}\left[\sqrt{\frac{FL}{2V_0} + \left(k_y L\frac{\hbar\omega}{4V_0}\right)^2} - k_y L\frac{\hbar\omega}{4V_0}\right] \tag{13}$$

$$F_{min} \equiv 2\frac{V0}{L}\left[\left(\frac{\omega_B}{\omega}\right)^2 + k_y L\frac{\hbar\omega_B}{2V_0}\right]. \tag{14}$$

In general, the double-well spectrum is quasi-degenerate. If the wells are not correlated, the spectrum is completely degenerate. However, wave-function tunnelling through the barrier

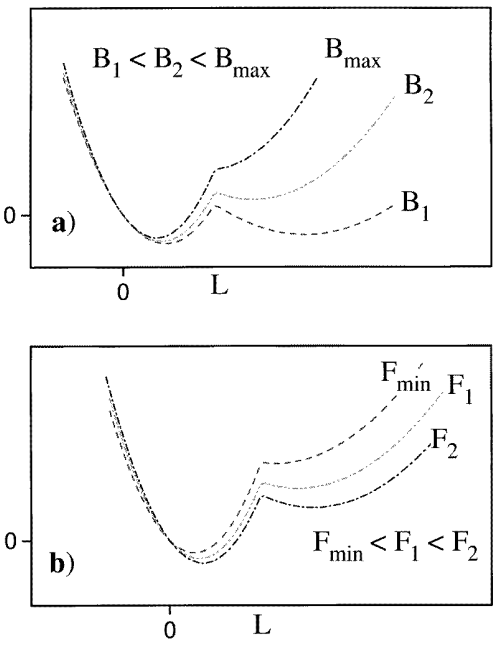

Figure 2. (a) shows that U_{eff} cannot exhibit a double-quantum-well state for magnetic field greater than $B = B_{max}(F, k_y)$ (see equation (13)). (b) shows that U_{eff} behaves as a double-quantum-well potential if the applied electric field is less than a minimum value, $F = F_{min}(B, k_y)$ (see equation (14)).

that connects the two wells can remove this degeneracy [13]. In other words, if $\bar{E}$ is the eigen-energy related to the single-well case, a gross estimate for the double-quantum-well eigen-energy is

$$E \to E_{\pm} = \bar{E} \pm \Delta E/2$$

where ΔE is the energy shift due to tunnelling. The values of $U_{eff}(L)$, $U_{eff}(x_c)$ and $U_{eff}(x_0)$ are very sensitive to variation in the parameters L, V_0, F and B. So, if the height or the width of the barrier is large, the spectrum can become completely degenerate.

3. The ground state

We assume that $k_y = k_z = 0$ in the ground state. An algorithm for calculating the spectrum of the ground state related to a DQW requires that the initial guess $\bar{E}$ used in solving the transcendental equation (12) in the complex plane is such that

$$U_{eff}(L) > \Re\{\bar{E}\} > \min\{U_{eff}(x_c), U_{eff}(x_0)\}$$

where $\min\{a, b\}$ is the smaller of a and b. However, for these states the level width is sharper. So for these double-well spectra we can neglect the imaginary part of E and solve equation (12) in the real plane. In this last step it is advisable to use the uniform asymptotic expansion to Weber functions [14] in order to minimize some numerical instabilities. In this work, we assume a semiconductor heterostructure of $Ga_{1-x}Al_xAs$–GaAs with an aluminium concentration x such that the height V_0 of the QW barrier is 150 meV, the width of the FPQW is $2L = 300$ Å and the effective mass m^* is 0.0667 times the rest electronic mass m_0. Using these QW parameters and adopting an applied electric field of $F = 62.5$ kV cm^{-1} $< F_{min}$ we solve equation (12) numerically for three different values of the applied magnetic field $B < B_{max}$.

For the magnetic field $B = 8.75$ T, figure 3(a) shows the behaviour of the ground- and first-excited-state wave functions ψ_- (solid line) and ψ_+ (dashed line) respectively. In this

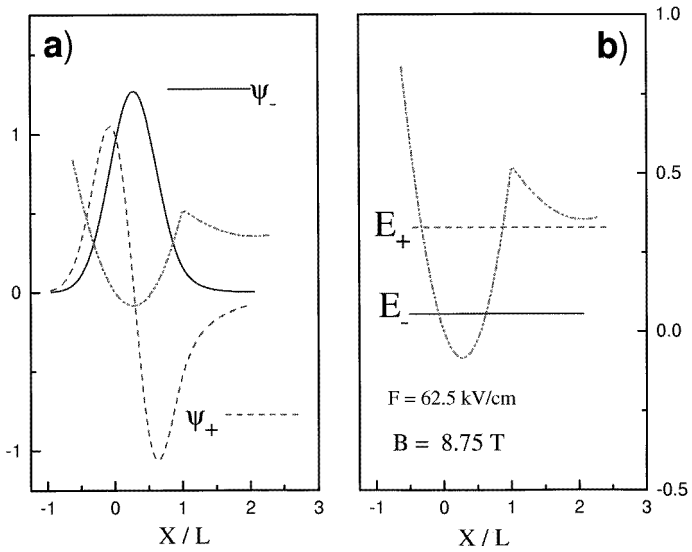

Figure 3. For a QW of width $2L = 300$ Å, effective mass $m^* = 0.0667m_0$ and $V_0 = 200$ meV, and applied electric and magnetic fields $F = 62.5$ kV cm^{-1}, $B = 8.75$ T respectively, (a) shows the ground- and first-excited-state wave functions ψ_- (solid line) and ψ_+ (dashed line) respectively and the effective potential U_{eff} (dotted line) in units of the barrier height V_0, while (b) shows, in units of V_0, E_-, the ground-state energy (solid line), E_+, the first-excited-state energy (dashed line), and the effective potential U_{eff} (dotted line).

case, the barrier that connects the two wells is large, so these wells cannot be correlated, and ψ_- and ψ_+ are located in the region delimited by the FPQW. Figure 3(b) shows E_-, the ground-state energy (solid line), E_+, the first-excited-state energy (dashed line), and the effective potential U_{eff} (dotted line) in units of the barrier height V_0. Notice that both eigen-energies are below the minimum $U_{eff}(x_c)$, so it is not possible for there to be strong correlation between the two wells and $\Delta E = E_+ - E_-$, the level separation, is large.

However, for an applied magnetic field of $B = 7.06$ T, correlation between the two wells starts to become important; figures 4(a) and 4(b) show these results. In this situation, the wave-function behaviour is very peculiar. Figure 4(a) shows that ψ_-, the ground-state wave function (solid line), is strongly localized in regions close to the origin. On the other hand, ψ_+, the first-excited-state wave function (dashed line), is appreciable in regions far from the origin; in other words, in the first excited state the electron has a great probability of being found close to the point $x = x_c$ where U_{eff} has a minimum. The left-hand vertical axis of figure 4(b) gives the energy scale in units of the barrier height V_0, where E_- is the ground-state energy (solid line), E_+ is the first-excited-state energy (dashed line) and U_{eff} is the effective potential (dotted line). Notice that both eigen-energies are above both minimum effective-potential values $U_{eff}(x_0)$ and $U_{eff}(x_c)$. The right-hand vertical axis of figure 4(b) shows on an enlarged scale E_- and E_+ (in units of V_0). Notice that $\Delta E = E_+ - E_-$, the energy separation, is very small. In this case, the two wells can exhibit correlation. This DQW ground-state energy has a value close to the ground-state energy related to a single equivalent parabolic well centred at $x = x_c$. In the same manner, the DQW first-excited-state energy has a value very close to the ground-state energy of an effective single parabolic well centred at $x = x_0$. This is interesting, because two very close eigen-energies have related wave functions exhibiting very different behaviour.

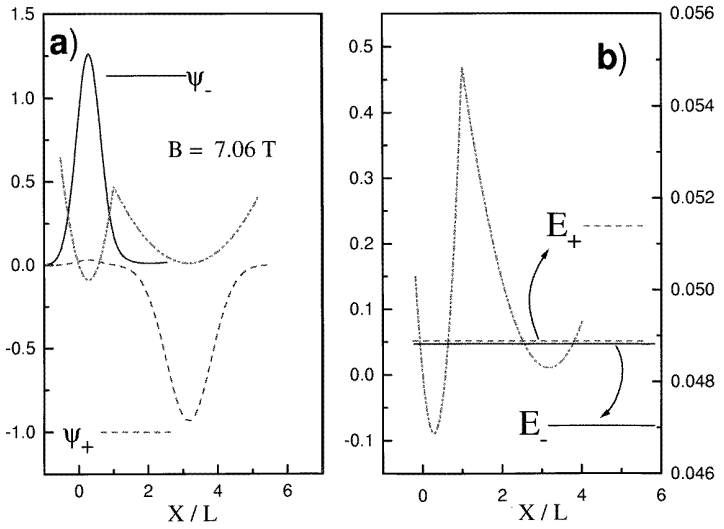

Figure 4. For the same heterostructure parameters as for figure 3 but an applied magnetic field of $B = 7.06$ T, (a) shows that ψ_-, the ground-state wave function (solid line), is strongly localized in regions close to the origin and ψ_+, the first-excited-state wave function (dashed line), is shifted to regions far from the origin, while in (b) the left-hand vertical axis shows, in units of V_0, E_-, the ground-state energy (solid line), E_+, the first-excited-state energy (dashed line), and the effective potential U_{eff} (dotted line) (notice that $\Delta E = E_+ - E_-$, the energy separation, is very small) and the right-hand vertical axis shows, in units of V_0 and on an enlarged scale, E_- and E_+ (notice that, in this case, the two wells can exhibit correlation).

On decreasing the strength of the magnetic field to $B = 6.40$ T, the wave functions ψ_- and ψ_+, related to ground and first excited states respectively, are shifted to regions far from the origin; this is shown in figure 5(a). Notice that for these states the probability of finding the electron in regions delimited by a FPQW is very small. Figure 5(b) shows that, in this case, the ground E_--states and first excited E_+-states are below the effective-potential minimum $U_{eff}(x_c)$. So the two wells do not exhibit correlation.

4. Conclusions

In this work, we have shown that a finite parabolic QW under crossed electric and magnetic fields can behave as a double-quantum-well system. The effective potential exhibits DQW behaviour for suitable choices for both fields (see equations (13) and (14)). The calculation of this double-quantum-well spectrum is not trivial (see equation (12)). In this way, a numerical algorithm was developed in order to solve the exact transcendental equation (12) for energy eigenvalues. We showed that the energy spectrum degeneracy can be removed by wave-function tunnelling through the barrier that connects the two wells (see figures 4(a) and 4(b)). We showed that the wave-function behaviour is very sensitive to changes in the applied fields (see figures 3, 4 and 5). For instance, if the applied fields are such that the two wells are strongly correlated, it is possible to have high electronic charge density in both wells for electrons having very close eigen-energies (see figures 3(a) and 3(b)). Finally, we would like to note that in the present model the potential U_{eff} is very similar to the double-well effective potential related to the electronic spin system in the presence of an external magnetic field [15, 16]. On the basis of this analogy, we think that the present

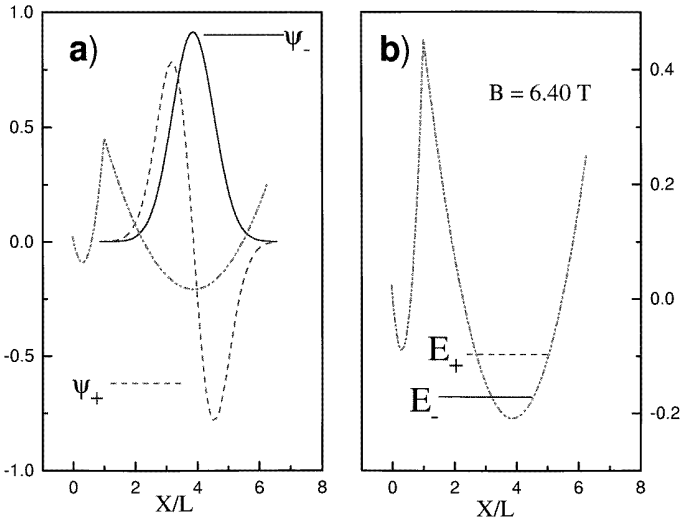

Figure 5. For the same heterostructure parameters as for figure 3 but an applied magnetic field of $B = 6.40$ T, (a) shows the ground- and first-excited-state wave functions ψ_- (solid line) and ψ_+ (dashed line) respectively and the effective potential U_{eff} (dotted line) in units of the barrier height V_0, while (b) shows (in units of V_0), E_-, the ground-state energy (solid line), E_+, the first-excited-state energy (dashed line), and the effective potential U_{eff} (dotted line).

model can behave as a new heterostructure electronic device. In other words, these abrupt changes in electronic charge-density shape as the external fields vary can be used as a *binary mechanism* in an electronic memory. These *binary-like states* can be accessed by varying the external applied electric and magnetic fields.

Acknowledgments

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