Magnetic phase transitions and time-dependent tunneling in a coupled quantum well system

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In this work, we have numerically integrated in space and time the effective-mass nonlinear Schrödinger equation for an electron wave packet in a bilayer electron system. Considering both polarized and unpolarized magnetic phases, we have calculated the tunneling dynamics between the two quantum wells when an external bias is applied. In our coupled quantum well system, we have considered a magnetic phase transition from the usual spin-polarized ground state to an unpolarized one. We have found the possibility of having a shift in the position of the resonant tunneling peak when the magnetic phase transition occurs.

I. INTRODUCTION

The search for systems that exhibit unusual spin instabilities is an area of active research. These instabilities illustrate the qualitatively new state of matter that may result in simple systems through the presence of electron-electron interactions. In addition, they lead to interesting phases with unique potentially useful properties. One class of systems considered for serious exploration has been single and double quantum well structures at low electronic density. These low-dimensional structures restricts the phase space available for electron-electron scattering enhancing the potential for interesting phase transitions. Devices of ultrapure modulation-doped $GaAs/Ga_{1-x}Al_xAs$ heterostructures may be fabricated with precisely controlled dimensions. Recently, Das Sarma and Tamborenea[1] have predicted an antiferromagnetic phase transition to occur in double quantum well heterostructures. They studied the magnetic instabilities of semiconductor quantum wells within the local-density approximation to both density-functional and Hartree-Fock theories. In addition to this, calculations of novel magnetic instabilities in semiconductor double quantum wells have been also presented by Reboredo and Proetto.[2]

From an experimental point of view, we note that at least an experimental group has investigated the possibility of an antiferromagnetic phase transition by performing resonant inelastic light-scattering measurements on double quantum well structures.[3] In the last few years, the physics of strongly coupled two-dimensional (2D) electron gases have attracted considerable interest for possible 2D-2D tunneling devices.[4] With the application of parallel and perpendicular magnetic fields to such bilayer heterostructures, a variety of new phenomena has been observed at several electron sheet densities. In the experiments, most magnetotransport measurements on double quantum wells have been for high magnetic fields perpendicular to the growth plane, where the electronic kinetic energy is quenched and Coulomb interactions dominate.[5,6] In such a case, interesting phenomena arise from the combined effect of tunneling and electron-electron interactions.[7] In addition, and when the magnetic field is applied in the growth plane, recent work has also investigated the magnetotransport properties in which case single-particle tunneling dynamics dominate the interactions between both electron semiconductor layers.[8] At zero magnetic field, many-body interactions in such low-dimensional electronic systems have also been the object of a great attention.[9]

The tunneling between two parallel 2D electron gases have been recently investigated as a function of the carrier density and temperature.[10] In such an experiment, the carrier densities in both semiconductor layers were independently controlled by two different applied biases. In this way, Turner *et al.*[10] investigated the zero-field differential tunneling conductance as a function of the applied interlayer voltage. From a theoretical point of view, the electron dynamics between parallel two-dimensional electron gases has recently studied in a coupled quantum well system.[11] Considering a Hartree potential, and with the using of a time-dependent wave function for the charge density in the semiconductor growth direction, the tunneling rate values between the two quantum wells have been obtained at different electron sheet densities. Due to nonlinear effects, there is a possibility of having a suppression of the tunnelling current in a bilayer electron system.[11]

However, we know that Hartree theory neglects contributions to the energy beyond the exchange term and is therefore expected to overestimate the electron-electron potential value in a quantum well system.[12] One of the most important approaches to the electron many-body problem is the local-density approximation (LDA) of the density-functional theory.[13] The LDA formalism is based on the self-consistent solution of the Kohn-Sham equation coupled with the Poisson equation and a local exchange-correlation potential. In order to study the different populations of the spin orientations on double quantum wells, a generalization of the local-density approximation has been recently introduced.[12] The local-spin-density approximation (LSDA) is also based on the self-consistent solution of the Schrödinger-like Kohn-Sham equation. The main technical difference between LSDA and LDA is that the effective exchange-correlation potential in LSDA depends on the local spin polarization as well as the electron density.

In view of the above comments and from a theoretical point of view, in this work we shall study the time-dependent evolution of an electron wave packet considering the LSDA in a coupled quantum well system. The method of calculation will be based on the discretization of space and time for the carrier wave functions. As the sheet density is raised, we have considered a magnetic phase transition from the usual

spin-polarized ground state to an unpolarized one. In such a case, we shall show that the system resonant condition can be strongly modified due to effective spin-dependent exchange-correlation potential. In this way, the possible antiferromagnetic phase transition[3] could be also investigated by performing resonant tunneling current measurements.

II. MODEL

In order to study the charge-density dynamics in the structure growth direction, we need to solve the time-dependent Schrödinger equation associated with an spinless electron in a double quantum well potential. Assuming translation symmetry of the system in the xy plane perpendicular to the growth direction z, the wave function ψ will be given by the nonlinear Schrödinger equation[14]

$$i\hbar\frac{\partial}{\partial t}\psi(z,t)=\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}+V_H(|\psi|^2)+V_{\rm xc}^{\sigma}(|\psi|^2)+V_{\rm qw}(z)\right]\psi(z,t), \tag{1}$$

where m^* is the GaAs electron effective mass and $V_{\rm qw}(z)$ is the double quantum well potential. The V_H and $V_{\rm xc}^{\sigma}$ terms are the self-consistent Hartree and exchange-correlation potentials, respectively. The V_H term is the potential given by the electron-electron interaction in the heterostructure region. Such a many-body potential is given by Poisson's equation

$$\frac{\partial^2}{\partial z^2}V_H(z,t)=-\frac{e^2 n_s}{\varepsilon}|\psi(z,t)|^2, \tag{2}$$

where ε is the GaAs dielectric constant and n_s is the initial carrier sheet density. In the exchange-correlation potential $V_{\rm xc}^{\sigma}$, σ denotes the spin orientation, which can be up $(+)$ or down $(-)$. In our calculations we use the parametrization of the $V_{\rm xc}^{\sigma}$ potential for the 3D electron gas obtained by Ceperley and Adler,[15]

$$V_{\rm xc}^{i}=\frac{d^i}{r_s}+\gamma^i\frac{1+\frac{7}{6}\beta_1^i\sqrt{r_s}+\frac{4}{3}\beta_2^i\eta_s}{(1+\beta_1^i\sqrt{r_s}+\beta_2^i r_s)^2}, \tag{3}$$

where $i=U$ (unpolarized) or $i=P$ (polarized). The parameters in the previous expressions, as used by Radtke, Tamborenea, and Das Sarma,[12] are $d^U=-1.2218$, $d^P=-1.5393$, $\gamma^U=-0.1423$, $\gamma^P=-0.0843$, $\beta_1^U=1.0529$, $\beta_1^P=1.3981$, $\beta_2^U=0.3334$, and $\beta_2^P=0.2611$. Finally, we should point out that in Eq. (1) the V_H and the $V_{\rm xc}$ potentials are wave-dependent quantities. Such a result is given by Eqs. (2) and (3), where both V_H and $V_{\rm xc}$ depend on the wave-function form.

Now we discretize time by a superscript ϑ and spatial position by a subscript j. Thus, $\psi\rightarrow\psi_j^{\vartheta}$. The various z values becomes $j\,\delta z$ in the conduction band, where δz is the mesh width. Similarly, the time variable takes the values $\vartheta\,\delta t$, where δt is the time step. In this way, and to treat the time development, we have used a unitary propagation scheme for the evolution operator obtaining a tridiagonal linear system that can be solved by standard numerical methods.[16] In addition, we have also solved Poisson's equation associated with V_H using another standard tridiagonal numerical method for each t value.[16]

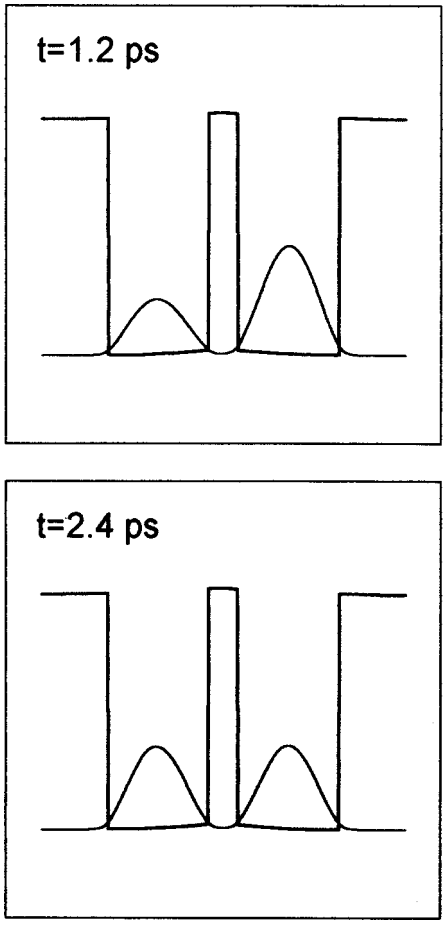

FIG. 1. Conduction-band potential and wave function at different times. We have taken an initial 2D electron sheet density equal to $n_s=1.0\times10^{11}\,\mathrm{cm}^{-2}$ and an applied bias equal to 0.5 mV.

In the tunneling experiments,[10] the carrier densities in both semiconductor layers were independently controlled by two different applied biases. Taking this into account, we have taken two Gaussian wave packets centered in both quantum wells as our initial wave function. In our model, we have an initial symmetric wave function, i.e., both Gaussian wave packets are identical. If an interlayer voltage V is applied, the bottom of both quantum wells are shifted a quantity equal to eV.

In Fig. 1, it is shown the amplitude of the wave function $|\psi|^2$ and the conduction band potential at several times. We have numerically integrated Eqs. (1)–(3) using an initial 2D electron sheet density equal to $n_s=1.0\times10^{11}\,\mathrm{cm}^{-2}$ and $n_s=3.0\times10^{11}\,\mathrm{cm}^{-2}$ for the two quantum wells. In Figs. 1 and 2, we have taken an applied voltage equal to 0.5 mV. Then, the equations are numerically solved using a spatial mesh size of 0.5 Å and a time mesh size of 0.2 a.u. and a finite box (4000 Å) large enough as to neglect border effects. We have considered a GaAs/$Ga_{1-x}Al_xAs$ double quantum well system which consists of two 140-Å-wide quantum wells separated by a barrier of thickness equal to 40 Å. The barrier height is taken to be 220 meV. At $t=0$, we have assumed a symmetric wave function that is created in the center of both quantum wells.

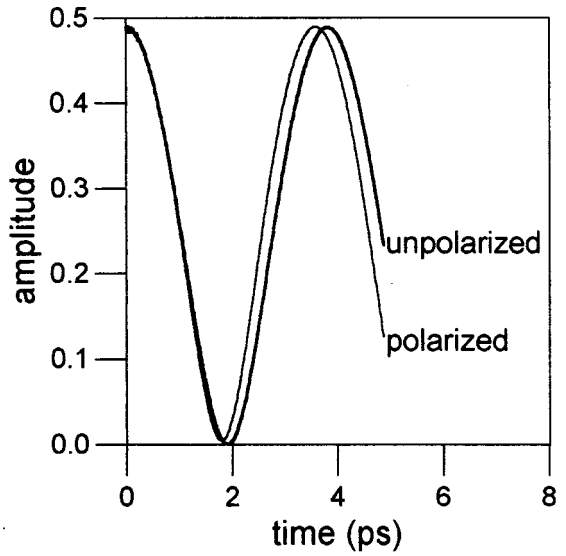

FIG. 2. Probability density in the left quantum well (P_{ab}) vs time for different spin polarizations. We have taken an initial 2D electron sheet density equal to $n_s = 0.1 \times 10^{11}\,\mathrm{cm}^{-2}$ and applied bias equal to 0.5 mV.

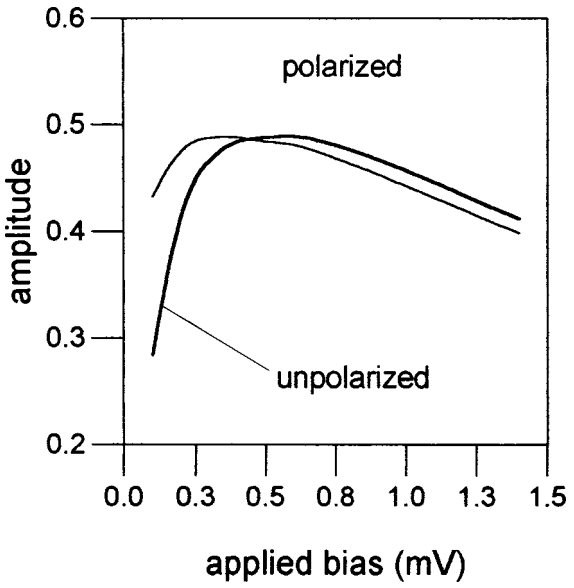

FIG. 3. Amplitude of the tunneling oscillations vs V. We have taken different spin polarizations. We have taken an initial 2D electron sheet density equal to $n_s = 0.1 \times 10^{11}\,\mathrm{cm}^{-2}$.

III. RESULTS AND DISCUSSION

The numerical integration in time allows us to obtain the probability of finding the charge density $P_{a,b}$ inside a quantum well region $[a,b]$ at any time t:

$$P_{a,b}(t) = \int_a^b dz |\psi(z,t)|^2, \tag{4}$$

where $[a,b]$ are the quantum well limits. In Fig. 2, we have plotted the probability density $P_{a,b}$ in the left quantum well versus time. The total probability density in both quantum wells has been taken to be 1. In our calculations, two different spin polarizations have been considered. We have taken an initial 2D electron sheet density equal to $n_s = 0.1 \times 10^{11}\,\mathrm{cm}^{-2}$ and an applied bias equal to 0.5 mV. The existence of the tunneling oscillations between the two quantum wells is clearly shown in Fig. 2.

In Fig. 3, we have plotted the amplitude of the tunneling oscillations versus V for different spin polarizations. We have considered a ferromagnetic transition as a function of the electron density n_s in a coupled doubled quantum well system. As in the 3D case, a fully polarized phase is expected at low density and a normal unpolarized phase a high density. For our particular choice of parameters,[2,12] we have assumed that the transition occurs around $n_s \sim 1 \times 10^{10}\,\mathrm{cm}^{-2}$ at zero temperature. For both spin-polarized and unpolarized phases we have found that the amplitude of the tunneling oscillations is increased as we increase V up to a certain value of the applied voltage (Fig. 3). Such a result can be easily explained as follows. The electron energy levels of both wells are exactly aligned at $V=0$. Therefore, if $V \sim 0$ the charge density will oscillate between both wells with a certain tunnelling period. If V is increased, the amplitude of the oscillations will also be increased due to the field-induced tunneling process. However, we know that if the potential difference between both wells is higher than the level splitting, the resonant condition is not obtained, and then the tunneling process is not allowed. Such an effect is clearly shown in the numerical data plotted in Fig. 3. We have found the existence of oscillations up to a certain value of the applied voltage (resonant V) for both spin-polarized and unpolarized phases. Taking into account the relation between the tunneling amplitude and the electric current we can see that our results are consistent with the experimental data obtained by Eisenstein, Pfeiffer, and West[6] and by Turner *et al.*[10] In the experiments, the authors found a peaked tunneling conductance at $V \sim 0$ in absence of applied magnetic field. In our model, the peak characteristics is given by the amplitude peak position (Fig. 3).

In Fig. 4, we have plotted the position of the tunneling peaks (resonant V) versus the electron sheet density. We have considered a magnetic phase transition from the usual

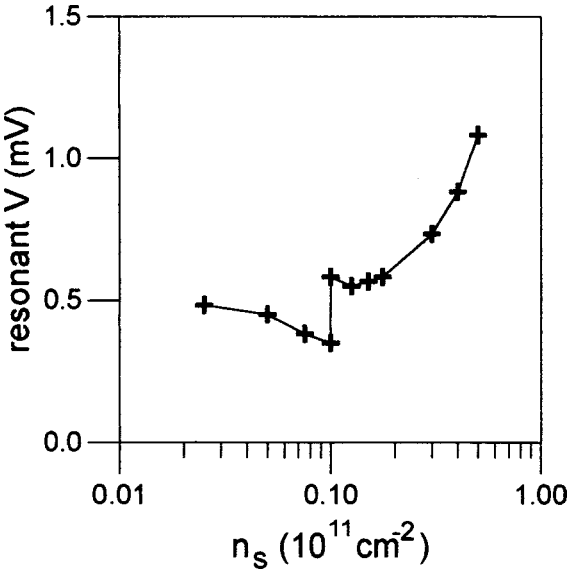

FIG. 4. Resonant V vs electronic sheet density n_s. We have considered a magnetic phase transition at $n_s = 0.1 \times 10^{11}\,\mathrm{cm}^{-2}$.

spin-polarized ground state to an unpolarized one at $n_s = 0.1\times10^{11}\,\mathrm{cm}^{-2}$. In Fig. 4, we note two new effects. First, the amplitude peak position is shifted to a higher resonant V value at $n_s = 0.1\times10^{11}\,\mathrm{cm}^{-2}$. Second, at high n_s values the resonant applied bias is strongly increased as we increase n_s. This shift in the amplitude peak position can be easily explained as follows. At $n_s = 0.1\times10^{11}\,\mathrm{cm}^{-2}$ we have calculated the resonant applied bias considering both polarized and unpolarized ground states (Fig. 4). Consequently, we have used in Eq. (3) two different exchange-correlation potentials (V_{xc}^{P} and V_{xc}^{U}), respectively. As a result, a shift in the position of the tunneling peak is obtained due to the potential form of the local spin-density approximation.

Let us study the second effect. In Fig. 4, we have found that the peak position is strongly increased as we increase the 2D sheet density ($n_s > 0.125\times10^{11}\,\mathrm{cm}^{-2}$). We shall explain this result considering the Hartree potential effect on the carrier dynamics, Eq. (1). The nonlinear dynamics of an electron that is localized in our double quantum well system is determined by two different competing potentials V_H and V_{xc}. At high electron densities, the Hartree potential dominates and we have field-induced tunneling oscillations due to the existence of a potential difference between both wells. Such a potential value is given by the ratio between eV and the electron-electron potential in the coupled quantum well system. Consequently, the resonant V value is increased as we increase n_s.[11] In addition, and at low electronic densities ($n_s < 0.1\times10^{11}\,\mathrm{cm}^{-2}$), the exchange-correlation potential becomes important when the total electron charge density is located in one quantum well and our nonlinear dynamics is given by two different competing potentials.

In summary, in this work we have numerically integrated in space and time a nonlinear effective mass Schrödinger equation in a double quantum well system. Electron-electron interaction effects have been considered in our model through a Hartree potential and the local spin-density approximation. We have considered a magnetic phase transition from the usual spin-polarized ground state to an unpolarized one at $n_s = 0.1\times10^{11}\,\mathrm{cm}^{-2}$. When the magnetic phase transition occurs, we have found the possibility of having a shift in the position of the resonant tunneling peak. In this way, the possible antiferromagnetic phase transition[3] could be also investigated by performing resonant tunneling current measurements.

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