Tunneling and time-dependent magnetic phase transitions in a bilayer electron 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 a time-dependent magnetic phase transition from the usual unpolarized ground state to spin-polarized one, we have calculated the tunneling dynamics between the two quantum wells when an external bias is applied. Due to the nonlinear effective-mass equation, it is found that the charge dynamically trapped in both wells produces a reaction field that modifies the system resonant condition. In this way, we have shown the possibility of having another kind of tunneling oscillations between both quantum wells after an optical excitation of the sample.

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I. INTRODUCTION

The search for systems that exhibit unusual spin instabilities is an area of active research. These instabilities illustrate the qualitatively improved 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 restrict the phase space available for electron-electron scattering enhancing the potential for interesting phase transitions. 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.

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.[2] In addition to this, tunneling experiments in low-dimensional systems have demonstrated a capability to probe electron-electron interactions. Recently, it was found that tunneling of electrons into two-dimensional (2D) systems in a magnetic field displays characteristics of a pseudogap created by Coulomb interactions among electrons.[3]

In addition, and given the spin properties of quantum Hall systems, Chan *et al.*[4] explored whether tunneling could also prove useful for revealing effects of electronic spins. For spin-polarized quantum Hall states, they described that tunneling from a 3D electrode occurs at two distinct rates that differ by up to two orders of magnitude. The dependence of the two rates on temperature suggested that slow in-plane spin relaxation creates a bottleneck for tunneling of electrons. Considering Skyrmion excitations, a theory of tunneling between a metal and a partially spin-polarized two-dimensional electron system has been recently presented by McDonald.[5] Recently, a nonequilibrium population of spin-up and spin-down states in quantum well structures has been achieved applying circularly polarized radiation. The spin polarization results in a directed motion of free carriers in the plane of a quantum well perpendicular to the direction of light propagation.[6]

The tunneling rate values between two parallel 2D electron gases have been recently investigated as a function of the carrier density and temperature.[7] In such an experiment, the carrier densities in both semiconductor layers were independently controlled by two different applied biases. From a theoretical point of view, the electron dynamics between parallel two-dimensional electron gases has been studied in a coupled quantum well system.[8] Considering a Hartree potential, and using a time-dependent wave function for the charge density in the semiconductor growth direction, the tunnelling 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 tunneling current in a bilayer electron system.[8]

However, we know that the 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.[9] One of the most important approaches to the electron many-body problem is the local-density approximation (LDA) of the density-functional theory.[10] 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.[9] 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. We have considered time-dependent magnetic phase transitions, from the usual unpolarized ground state to a spin-polarized one and vice versa,

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generated by an external pulsed electromagnetic radiation. In such a case, we shall show that the system resonant condition can be strongly modified due to effective spin-dependent exchange-correlation potential. Consequently, the possible effects of electronic spins in a two-dimensional electron system could be also investigated by performing tunnelling 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 to an 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[11]

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

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 the Poisson equation

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

where ε is the GaAs dielectric constant and n_s is the carrier sheet density. In the exchange-correlation potential $V_{\rm xc}^{\sigma}$ for our calculations we use the parametrization of the $V_{\rm xc}^{\sigma}$ potential for the 3D electron gas obtained by Ceperley and Adler[12]

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

where $i=U$ (unpolarized) or $i=P$ (polarized). The parameters in the previous expressions, as used by Radtke, Tamborenea, and Dar Sarma,[9] 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 $\beta_2^P=0.2611$. This parametrization of the exchange-correlation potential for the uniform electron gas in three dimensions does not depend on the widths and heights of the potential barriers. However, the LSDA can describe the inhomogeneous electron gas that exists inside quantum well structures. This $V_{\rm xc}$ potential has been employed to study spin instabilities in coupled quantum wells and spin effects in parabolic quantum wells. 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 wavefunction form.

In our model, we have considered an external pulsed electromagnetic radiation with a certain period $T_{\rm em}$. It is well known that spin-polarized electrons can be generated by polarized light. We have considered a periodic magnetic transition as a function of the external pulsed radiation period $T_{\rm em}$ in a coupled double quantum well system. Then, the time-dependent exchange-correlation potential is

$$V_{\rm xc}(t)=g(t)V_{\rm xc}^{U}+[1-g(t)]V_{\rm xc}^{P}, \tag{4}$$

where the $g(t)$ function is given by

$$g(t)=\sum_{n=1,3,5,\ldots}\sum_{m=2,4,6,\ldots}\left[\Theta\left(t-n\frac{T_{\rm em}}{2}\right)-\Theta\left(t-m\frac{T_{\rm em}}{2}\right)\right] \tag{5}$$

Θ being the Heaviside function. We should point out that if $t=nT_{\rm em}/2$ or $t=mT_{\rm em}/2$ in Eq. (5) a magnetic phase transition occurs.

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 become $j\,\delta z$ 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 Crank-Nicholson method.[13] The wave-packet propagator $e^{-i\,\delta t H}$ is replaced by the rational approximation $(1-i\,\delta t H)/(1+i\,\delta t H)$. In the Cranck-Nicholson approach, it is difficult to estimate the minimum value of δt required to guarantee a specified accuracy. In addition, we have checked our results by using the split-step method. In the split-step approach, the wave packet is advanced in time steps δt short enough that the algorithm $e^{-i\,\delta t T/2}e^{-i\,\delta t U}e^{-i\,\delta t T/2}$ can be applied to the generator. *T* and *U* are the Hamiltonian kinetic and potential terms. In each time step δt, the algorithm propagates the wave packet freely for $\delta t/2$, applies the full potential interaction, then propagates freely for the remaining $\delta t/2$. The split-step algorithm is stable and norm preserving and it is well suited to time-dependent Hamiltonian problems.[14] However, execution of this algorithm requires relatively long times and large storage. In addition, we have also solved the Poisson equation associated to V_H using another tridiagonal numerical method for each *t* value.[13]

In the tunneling experiments,[7] 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 centred 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. In practice, we will not have a perfectly symmetrical double well potential in absence of an external applied bias. We have also assumed a slightly asymmetric wave function that is created in the center of both quantum wells at $t=0$. The obtained dynamical evolutions of the different initial wave packets are identical. If an interlayer voltage *V* is applied, the bottom of both quantum wells are shifted a quantity equal to eV.

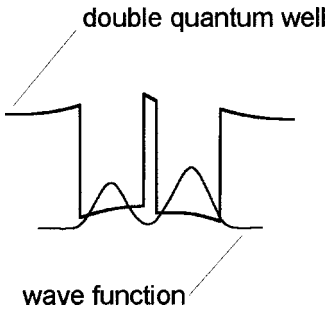

FIG. 1. Conduction-band potential and wave function. We have taken an initial 2D electron sheet density equal to $n_s = 6.0 \times 10^{11}$ cm^{-2}.

Figure 1 shows the amplitude of the wave function $|\psi|^2$ and the conduction-band potential. The unpolarized ground state has been considered. We have numerically integrated Eqs. (1)–(3) using an initial 2D electron sheet density equal to $n_s = 6.0 \times 10^{11}$ cm^{-2} for both quantum wells. In Fig. 1, we have taken an applied voltage equal to 15 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 that consists of two 100-Å-wide GaAs quantum wells separated by a barrier of thickness equal to 20 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.

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

$$P_{a,b}(t) = \int_a^b dz |\psi(z,t)|^2, \tag{6}$$

where $[a,b]$ are the quantum well limits. In Fig. 2, we have plotted the probability density $P_{a,b}$ in left quantum well versus time. The total probability density in both quantum wells has been taken to be 1. In our calculations, the unpolarized ground state and periodic magnetic transitions from the usual unpolarized ground state to a spin-polarized one ($T_{\rm em} = 100$ fs) have been considered. We have taken an initial 2D electron sheet density equal to $n_s = 6.0 \times 10^{11}$ cm^{-2} and an applied bias equal to 14 mV. The existence of tunneling oscillations between the two quantum wells is clearly shown in Fig. 2.

In Fig. 2, we can notice that an averaged value for the amplitude of the tunneling oscillations can easily be calculated. In Fig. 3, we have plotted the averaged amplitude value of the tunneling oscillations versus V for different spin polarizations and electron densities. We have considered the unpolarized ground state and a periodic magnetic transition as a function of an external period ($T_{\rm em} = 100$ fs). For both magnetic 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 tunneling 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

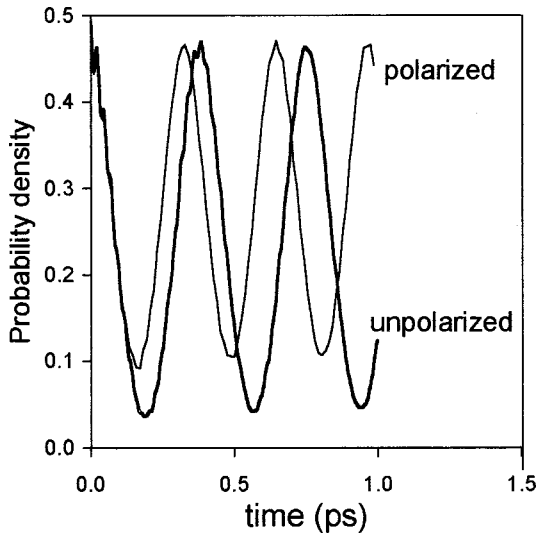

FIG. 2. Probability density in the left quantum well ($P_{a,b}$) versus time for the unpolarized ground state and for periodic magnetic transitions ($T_{\rm em} = 100$ fs). We have taken an initial 2D electron sheet density equal to $n_s = 6.0 \times 10^{11}$ cm^{-2}.

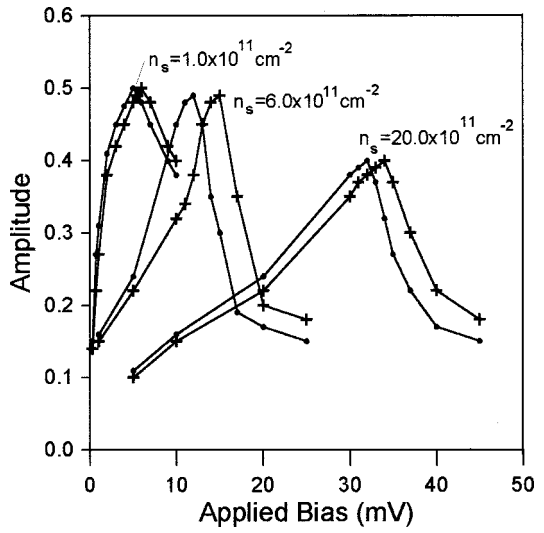

FIG. 3. Amplitude of the tunneling oscillations versus V. We have taken different spin polarizations and a 2D electron sheet density equal to $n_s = 6.0 \times 10^{11}$ cm^{-2}. Crosses: the unpolarized ground state. Circles: time-dependent spin-polarized magnetic phase ($T_{\rm em} = 100$ fs).

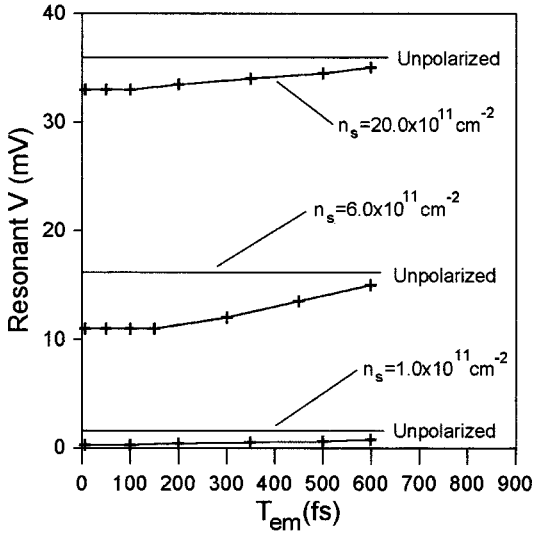

FIG. 4. Resonant V versus T_{em} at different sheet density values. We have also plotted the unpolarized resonant V values (horizontal lines).

of the applied voltage (resonant V) for both unpolarized and time-dependent spin-polarized phases.

In Fig. 4, we have plotted the position of the tunnelling peaks (resonant V) versus T_{em} at different electron sheet density values. We have considered periodic magnetic transition as a function of the external pulsed radiation period at different electron sheet density values. Up to a certain value of $T_{\mathrm{em}}=100$ fs, we have found that the V curve has a minimum. In contrast, and in the case of $T_{\mathrm{em}}>100$ fs, it is found that the amplitude peak position is increased if we increase T_{em}. Such a result can be easily explained as follows. In Fig. 3, it is clearly shown that the time-dependent exchange-correlation potential, $V_{\mathrm{xc}}(t)$, determines the dynamical evolution of our electron wave function. Increasing the T_{em} value, the time-dependent potential filling up in both quantum wells is also modified. As a result, the amplitude peak position is also increased. In addition to this, we know that the initial symmetric charge density will oscillate between both wells with a $\tau=0.5$ ps tunneling period in the absence of an external electromagnetic radiation. If the electromagnetic radiation period is much smaller than the tunneling oscillation period (in our case, $T_{\mathrm{em}}<\tau/5$), the obtained dynamical evolutions of different electron wave packets are identical. In such a case, the amplitude peak position has a near constant value.

In Fig. 4, we note the existence of the studied effect. The shift in the amplitude peak position at high and low electron densities is smaller than in the $n_s=6.0\times10^{11}$ cm^{-2} case. We shall explain this result considering both Hartree and exchange-correlation effects on the carrier dynamics. The 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 both V_{xc}^P and V_{xc}^U potentials can be neglected. At low electronic densities the exchange-correlation potential can also be neglected, $V_{\mathrm{xc}}\rightarrow 0$. At $1.0\times10^{11}<n_s<20.0\times10^{11}$ cm^{-2}, the time-dependent

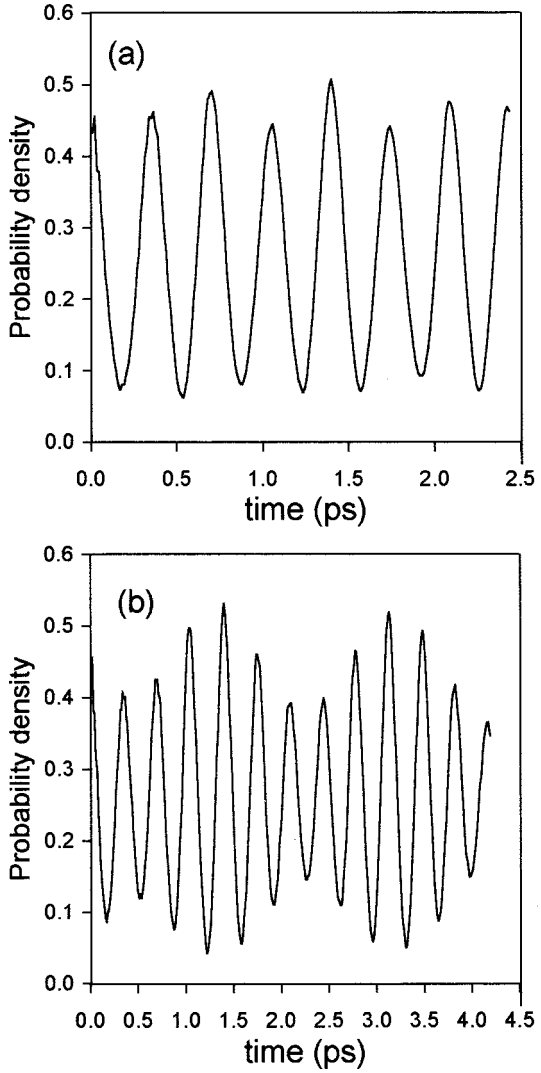

FIG. 5. Probability density in the left quantum well ($P_{a,b}$) versus time at $V=14$ mV. We have taken an initial 2D electron sheet density equal to $n_s=6.0\times10^{11}$ cm^{-2}. (a) $T_{\mathrm{em}}=0.2$. (b) $T_{\mathrm{em}}=1.0$ ps.

exchange-correlation potential becomes important and the wave-function dynamics is given by two different competing potentials. In such a case, an important shift in the amplitude peak position has been obtained.

In Fig. 5, we have plotted the amplitude of the tunneling oscillations versus t at $n_s=6.0\times10^{11}$ cm^{-2} (Fig. 5). We have considered a periodic magnetic transition as a function of the external pulsed radiation period ($T_{\mathrm{em}}=0.2$ and 1.0 ps). The radiation period is of the same order of magnitude as the tunneling oscillation period. Then, we have obtained a time-varying probability density with an amplitude which is also oscillating with time. The amplitude period is given by the electromagnetic radiation period. In this way, we have shown the possibility of having another kind of tunneling oscillations between both quantum wells after an optical excitation of the sample.

In summary, in this work we have numerically integrated in space and time a nonlinear effective-mass Schrödinger equation in a bilayer electron system. Electron-electron inter-

action effects have been considered in our model through a Hartree potential and the local spin-density approximation. We have considered time-dependent magnetic phase transitions, from the usual unpolarized ground state to a spin-polarized one and vice versa, generated by an external pulsed electromagnetic radiation. As a result, a shift in the position of the tunneling peak has been obtained due to the time-dependent potential form of the local-spin-density approximation. In addition to this, and at certain charge-density values and electromagnetic radiation periods, we have obtained a time-varying probability density with an amplitude which is also oscillating with time. Consequently, we have shown the possibility of having another kind of tunneling oscillations between both quantum wells after an optical excitation of the sample. In this way, the possible effects of electronic spins in a two-dimensional electron system could be also investigated by performing tunneling current measurements.

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