Donor-assisted resonant electron tunneling in double-barrier heterostructures under tilted magnetic fields: A theoretical study

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Abstract. A theoretical study of the current-voltage characteristics of a double-barrier heterostructure doped with a layer of shallow donors in the middle of the well and subjected to a magnetic field tilted with respect to the growth direction is reported. The parent materials are assumed to possess simple cubic lattices, the electronic structure of the system is modeled by means of a one-band tight-binding Hamiltonian, and the current is evaluated employing the Keldysh nonequilibrium formalism. The results reveal the magnetocompression of the donor wavefunction, in good qualitative agreement with the experimental report of Patanè et al [Phys Rev Lett 105 236804 (2010)].

1. Introduction

High magnetic fields can be employed to probe sensitively and noninvasively features of the quantum states of low-dimensional structures embedded in a solid [1]. In particular, in magnetotunneling spectroscopy (MTS) an applied magnetic field perpendicular to the current permits mapping the momentum probability distributions of a nanostructure in the plane perpendicular to the current [1, 2], thereby yielding information about the shape and size of its wavefunctions. Recently, MTS has been applied to the study of the compression effected on the wavefunction of a donor by an applied magnetic field parallel to the current [3] and the stretching caused on the wavefunction of a quantum dot by a focused femtowatt laser beam [4]. Hence, this technique is a valuable aid in the design of nanostructures tailored for specific tasks [5].

In MTS experiments the target nanostructure is either located within the quantum well defined by two tunnel barriers [2, 3] or within a single tunnel barrier [2, 4]. In either configuration, the current-voltage (I – V) characteristic curves exhibit weak features associated with resonant electron tunneling (RET) through quasi-bound states of the nanostructure. Moreover, in the first configuration the I – V curves exhibit strong peaks at higher voltage associated with RET through quasi-bound states of the metastable quantum well. Momentum probability density maps can be extracted from the behaviour of the current intensities associated with these features as functions of the perpendicular magnetic field strength.

In previous reports, it was shown that a simple theoretical methodology, based on a one-band tight-binding Hamiltonian and the Keldysh nonequilibrium formalism [6], can reproduce
the features of the experimental $I - V$ characteristics of double-barrier heterostructures (DBHs) under perpendicular and parallel magnetic fields [7] and $\delta$-doped DBHs under perpendicular magnetic fields [8]. In the latter study, it was demonstrated that the momentum probability density associated with the donor ground state can be quantitatively extracted from the theoretical data. In the present report, this methodology is applied to the case of a $\delta$-doped DBH under a tilted magnetic field, with a view to reproducing the experimental observations of [3] on the magnetocompression of the donor wave function.

2. Methodology

The bare DBH is described by the one-band tight-binding Hamiltonian.

$$\hat{H} = \sum_i \epsilon_i^0 c_i^\dagger c_i + \sum_{i,j} v_{ij}^0 c_i^\dagger c_j$$  \hspace{1cm} (1)

where $\epsilon_i^0$ is the site energy, $v_{ij}^0$ is the hopping energy between sites $i$ and $j$, and the summation is understood to be performed over neighboring sites only. Taking the $z$ axis as the direction of the current, i.e. the DBH growth direction, the perpendicular component of the magnetic field $B_z\hat{z}$ is introduced into the Hamiltonian (1) by means of the Peierls gauge transformation of the hopping energies [9].

$$v_{ij}^0 \rightarrow v_{ij}^0 \exp \left[ i \frac{e}{\hbar} \mathbf{A} \left( \frac{1+1'}{2} \right) \cdot (1-1')a \right]$$  \hspace{1cm} (2)

where $\mathbf{A} = B_z y \hat{k}$ is the vector potential, $I$ and $I'$ are the position vectors of neighboring sites $i$ and $j$, $a$ is the lattice parameter, and $e$ and $\hbar$ have the usual meanings. On the other hand, the presence of the parallel component $B_x \hat{y}$ is taken into account by means of the substitution.

$$\epsilon_i^0 \rightarrow \epsilon_i^0 + (n + 1/2)\hbar\omega_i$$  \hspace{1cm} (3)

where $n = 0, 1, 2, \ldots$ and $\omega_i = eB_z/m_i^*\hbar$ are the Landau index and cyclotron frequency, respectively, with $m_i^*$ being the in-plane ($xy$) electron effective mass.

Assuming that the parent materials possess simple cubic lattices and performing a Fourier transform employing the appropriate Cunningham points [10], the field-dressed three-dimensional (3D) Hamiltonian (1) is reduced to an effective 1D Hamiltonian with dressed energies that depend on the in-plane wave vector $\mathbf{k} = k_x \hat{i} + k_y \hat{j}$, given by,

$$E_i(\mathbf{k}) = \epsilon_i + 2v_i[\cos(k_x a) + \cos(k_y a)]$$  \hspace{1cm} (4)

where $\epsilon_i$ and $v_i$ are the site and hopping energies in the effective 1D lattice, with $i = W, B, I$ for well, barrier or interface sites, respectively. The height of the potential barrier is given by [11] $\Delta E = (\epsilon_W - \epsilon_B) + 2(v_W - v_B)$.

Neglecting the band-bending effect due to the charge accumulation layers that arise at each interface in the real structure, the voltage bias is included in the site energies $\epsilon_i$ by means of a linear interpolation of the voltage $V$ between the two barriers. The presence of the hydrogenic donor in the quantum well is taken into account by including in the site energies the Coulomb term $\epsilon_i^c = -e^2/4\pi\epsilon_0 r_{i0}$, where $r_{i0} = |\mathbf{r}_i - \mathbf{r}_0|$ is the distance between the impurity located at the middle of the quantum well and the electron on site $i$, and $\epsilon_{0,i}$ is the value of the dielectric constant at site $i$.

Employing the Keldysh formalism [6] it can be shown that the average current induced in the system at 0K is given by [12],

$$I = \frac{4\pi^2 e^2 \rho_W^2}{\hbar} \int_{\mu_R}^{\mu_L} \frac{\rho_L(h\omega)\rho_R(h\omega)}{[\Gamma(h\omega)]^2} d(h\omega)$$  \hspace{1cm} (5)
where the subscripts $L$ and $R$ refer to the injector and collector located to the left and right of the structure, respectively, $\rho_L(\hbar\omega)$ and $\rho_R(\hbar\omega)$ are the densities of states, $\Gamma = (1 - g_{LL}^a g_{RR}^a W^2)/(1 - g_{LL}^r g_{RR}^r W^2)$, with $g_{LL}^a$ and $g_{RR}^r$ being the advanced and retarded Green functions, and $\mu_L$ and $\mu_R$ are the chemical potentials, with $\mu_L > \mu_R$. $\mu_L$ will be referred to as the Fermi energy.

3. Results and discussion

The lattice constant, dielectric constant and electron effective mass were assumed to be the same at all sites and equal to the ones of GaAs, $a = 0.282\,\text{nm}$, $\epsilon_0 = 12.5$ and $m^* = 0.067m_0$, with $m_0$ being the free electron mass. The hopping energy between any two sites was evaluated by means of the formula $v^0 = \hbar^2/2m^*a^2$, yielding $v^0 = 7.179\,\text{eV}$. The Fermi energy was taken to be 100meV, which corresponds approximately to the injector doping chosen in ref. [3]. The structural parameters of the DBH were also taken from ref. [3] (barrier height of 300meV and barrier and well widths of 5.7nm and 9.0nm, respectively).

Each frame of Figure 1 displays the $I$-$V$ characteristic curves of the structure for several values of $B_x$ at a fixed value of $B_z$. The shoulder that appears at $B_x = 0$ T and develops into a broad peak as $B_x$ increases, henceforth to be called $D$, is associated with RET through the ground state of the donor [3, 8]. At higher voltage there appears a strong peak (not shown) associated with RET through the lowest subband of the quantum well [3, 8]. It is observed that feature $D$ shifts to lower bias and its current intensity $I_D$ decreases monotonically with $B_x$.

Each curve of Figure 2 shows the normalized dependence of $I_D$ on $B_x$, extracted from the data in the corresponding frame of Figure 1. It is clearly appreciated that $I_D$ is the less sensitive to $B_x$ the higher the strength of $B_z$, in qualitative accordance with the experimental results of [3].

However, the decrease of $I_D$ with $B_x$ in the theoretical plots is observed to be much slower than in the experimental ones. As discussed in [7], the parallel field increases the hopping energy whereas the perpendicular field decreases it. Hence, the overestimation of the peak current produced by the model must be due to an underestimation of the effect on the hopping of the perpendicular field in relation with the one of the parallel field. This can be attributed,
at least in part, to the nearest-neighbor approximation, which enters directly in Equation (2),
but not in Equation (3).

Figure 2. Dependence of the normalized donor peak current on the strength of the perpendicular component of the magnetic field. Each plot is extracted from the data in the corresponding frame of Figure 1.

At $B_z = 0$ T, the plot of $I_D$ versus $B_x$ should furnish a cut of the donor probability density in momentum space $|\Psi(k_y)|^2$ in the direction of the field $[2, 3]$. Indeed, in [8] it was shown that a plot of $\sqrt{I_D}$ versus $B_x$ can be fitted accurately to a Lorentzian, revealing the 1s-like nature of the donor wavefunction. On the other hand, the model calculations presented in [3] indicate that the behaviour of $I_D(B_x)/I_D(0)$ at increasing strengths of $B_z$ exhibited in Figure 2 can be attributed to the compression of the donor wavefunction effected by the field.

4. Concluding remarks

The present simplistic model is appropriate for the qualitative prediction of the effects of applied perpendicular and parallel magnetic fields, and combination thereof, on the $I$-$V$ characteristics of undoped and $\delta$-doped DBHs. In particular, this model is able to account for the magnetocompression of a donor wavefunction. This provides confidence in its more general utility for predicting the spatial characteristics of the quantum states of nanostructures under other applied perturbations.

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