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Bound magnetic polarons in semimagnetic quantum wells

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We examine the position dependence of the binding energy of a hydrogenic impurity in a semimagnetic quantum well. We consider, in particular, a CdTe well confined by (Cd,Mn)Te potential barriers. We show that, due to the penetration of the impurity wave function inside the barrier, at low temperatures, the exchange interaction with the Mn local spins may lead to the formation of a bound magnetic polaron. In such a case, the impurity is more strongly bound at the interface than at the center of the well, in contrast to the situation in nonmagnetic quantum wells.

Semimagnetic superlattices of CdTe-(Cd,Mn)Te have recently been produced by molecular-beam-epitaxy techniques.[1,2] As a result, their basic physical properties have attracted the attention of experimentalists[3,4] and theorists.[5,6] The observation of stimulated emission in (Cd,Mn)Te quantum wells opens the way for interesting and useful device applications of such materials.[7] Unlike III-V superlattices, such as those based on GaAs-(Al,Ga)As, the semimagnetic superlattices may be strongly affected by moderate magnetic fields—$\lesssim 5$ T—and the energy levels of some defects and impurities are strongly temperature dependent.[4] The aim of the present Rapid Communication is to present results of our studies concerning the magnetic field and temperature dependence of energy levels in semimagnetic quantum wells.

We study the energy levels in a CdTe square quantum well of depth V and length L, confined by barriers of $Cd_{1-x}Mn_xTe$. We treat hydrogenic impurities in the isotropic effective-mass approximation. The main distinction between this type of quantum well and the nonmagnetic ones[8] resides in the exchange interaction between the spin of the carrier—electron or hole—and the local moments on the Mn ions in the barrier. Given the uncertainties about conduction- and valence-band offsets, we chose the simplest model capable of yielding qualitatively significant results. The Mn spin polarization in the barriers is treated phenomenologically,[9] although there is some experimental evidence that the interface strongly affects the magnetic properties introducing anisotropies not present in the bulk.[4,6]

Our model Hamiltonian is given by

$$H = H_0 + H_x + H_s \ , \tag{1}$$

where

$$H_0 = \frac{1}{2m}\left[\mathbf{p} + \frac{e}{c}\mathbf{A}\right]^2 + V(z) + V_d(\mathbf{r}) - g\mu\mathbf{B}\cdot\mathbf{s} \ , \tag{2}$$

$$H_x = -J\mathbf{s}\cdot\sum_i \delta(\mathbf{r}-\mathbf{r}_i)\mathbf{S}_i \ , \tag{3}$$

and

$$H_s = \sum_{(ij)} J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j - g_{\mathrm{Mn}}\mu\mathbf{B}\cdot\sum_i \mathbf{S}_i \ . \tag{4}$$

In Eq. (2), $V(z)$ is the conventional symmetric square-well barrier potential,[8] $V_d(\mathbf{r})$ is a defect potential to be defined below, and the other terms have their usual interpretation. Equation (3) describes the exchange interaction between the carrier spins s and the Mn localized spins $\mathbf{S}_i$. Equation (4) describes the magnetic interaction between the Mn spins. In what follows we neglect the orbital effects of the applied magnetic field and treat the spins $\mathbf{S}_i$ as classical vectors oriented in the direction of the applied field and with average magnitude given by

$$S = \tfrac{5}{2} r(x) B_{5/2}(w) \ , \tag{5}$$

where

$$w(B,T) = g_{\mathrm{Mn}}\mu(B + B_x)/k_B[T + T_0(x)] \ . \tag{6}$$

In Eqs. (5) and (6), $r(x)$ and $T_0(x)$ are Mn concentration-dependent parameters, as defined in Refs. 9 and 10, $B_{5/2}(w)$ is the Brillouin function for spin $\frac{5}{2}$, and B_x is an effective field due to the exchange interaction, Eq. (3). The parameters r and T_0 describe phenomenologically the effect of the Mn spin-spin exchange interaction, Eq. (4).

To deal with $H_0 + H_x$ we introduce a simple variational wave function, the spatial part of which is

$$\psi(\mathbf{R},z) = \frac{\eta\sqrt{\alpha}}{\pi^{3/4}} \exp(-\tfrac{1}{2}\eta^2 R^2) \exp[-\tfrac{1}{2}\alpha^2(z-z_0)^2] \ , \tag{7}$$

where $\mathbf{R}$ is the coordinate vector parallel to the interface. This is a three-parameter variational wave function: η describes its extension parallel to the interface, α its extension in the direction perpendicular to the interface, and z_0 defines the position of the maximum of the wave function. The energy is minimized with respect to these three parameters using an iterative algorithm.

From (7), we obtain for the exchange energy, in the mean-field approximation

$$E_x = -\frac{5}{4\sqrt{\pi}} x N_0 J r \int_0^1 dq \int_0^\infty d\xi \exp[-(\xi - \alpha z_0)^2] B_{5/2}(w) \ , \tag{8}$$

where, in Eq. (6),

$$B_x = \frac{1}{2g_{\mathrm{Mn}}\mu} N_0 J \Omega_0 \frac{\eta^2\alpha}{\pi^{3/2}} q \exp[-(\xi - \alpha z_0)^2] \ . \tag{9}$$

In the equations above $\Omega_0 = N_0^{-1}$ is the primitive cell volume of the bulk crystal and x is the Mn concentration. We know from previous works on bound magnetic polarons

in bulk semimagnetic semiconductors that the mean-field approximation employed to obtain Eq. (8) is not quantitatively correct when the carrier wave function is strongly localized.[11] However, our present level of knowledge of the relevant materials parameters for semimagnetic quantum wells does not warrant the use of more sophisticated approximations, which do not qualitatively change the results. For the defect potential we consider the screened Coulomb potential

$$V_d(\mathbf{r}) = -\frac{e^2/\epsilon}{[R^2+(z-z_i)^2]^{1/2}} , \tag{10}$$

with the impurity centered at z_i.

In Figs. 1 and 2, the relevant parameters are as follows: $m = m_0$, the free-electron mass, $V = 40$ meV, $L = 50$ Å, $\epsilon = 10$, $\Omega_0 = 68$ Å^3, $N_0J = 880$ meV, and for the Mn spins $x = 0.1$, $r = 0.43$, and $T_0 = 3.8$ K.[9] With these parameters, we have the case of a model hydrogenic acceptor impurity. We chose them because, in the CdTe-(Cd,Mn)Te superlattices, it is expected that the valence-band offset is smaller than the conduction-band offset. Consequently, physical effects due to the wave-function penetration into the barrier are more pronounced for holes than for electrons. For $x = 0.1$, our value for the potential barrier height corresponds to roughly a 25% valence-band offset. We are perfectly aware that the theoretical description of heavy-hole states in these strained lattice superlattices by simple isotropic hydrogenic models is inadequate. Our aim, however, is to obtain a first estimate of the exchange energy contribution to the acceptor impurity energy and to show that, under certain conditions, it can be significant.

In Fig. 1 we present the impurity energy level as a function of z_i for $T = 1$ and 100 K and also, for comparison, the result for $N_0J = 0$ corresponding to a nonmagnetic quantum well. As is well known, in the latter case the impurity level becomes less strongly bound as z_i moves from the center to the well interface. This is due to the effect of the barrier potential. In a semimagnetic quantum well, however, at low temperatures, the opposite effect may take place corresponding to the formation of a bound magnetic polaron. The nearer the impurity is to the barrier, the greater is the probability of penetration of the bound particle into it and the stronger is the Mn spin polarization induced by the localized carrier spin. In fact, when the impurity is on or very near to the interface the (Cd,Mn)Te barrier becomes a local potential well and the CdTe well becomes a local potential barrier for the appropriate spin direction of the carrier. This can be seen from Fig. 2, where we plot $z_0 - z_i$ as a function of z_i for $T = 1$ K. Both $N_0J \neq 0$ and $N_0J = 0$ cases are shown. When $N_0J \neq 0$, the peak of the wave function lies

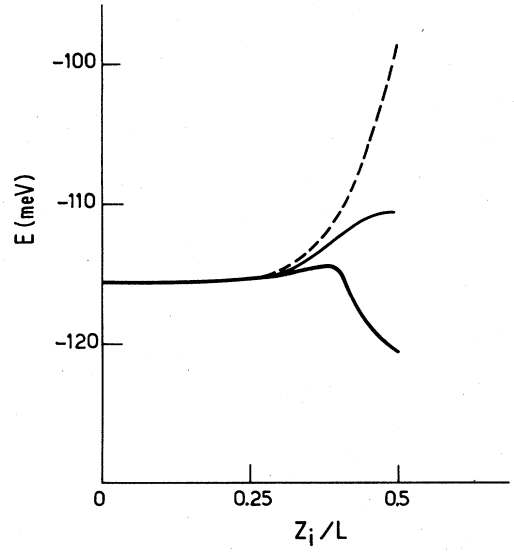

FIG. 1. Impurity energy level as a function of position inside quantum well. Center of the well is $z = 0$; interface with barrier is $z = 0.5$ L. (For other parameters, see text.) Impurity level at $T = 1$ K is the lower curve, at $T = 100$ K is the middle curve, and in the absence of exchange interaction is the dashed curve. Notice that bound-polaron effects are only present when the impurity is near to the interface.

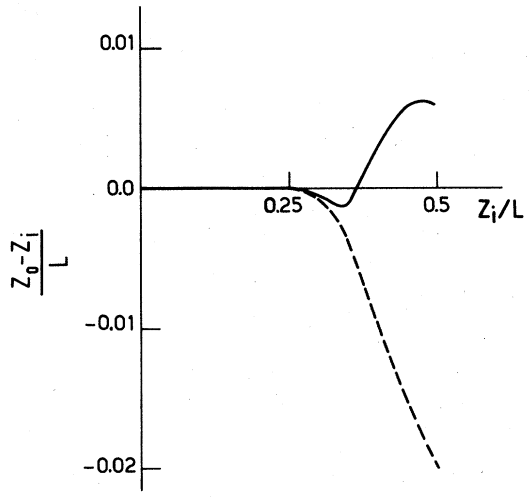

FIG. 2. Position of the maximum of the wave function as a function of the position of the impurity. (For parameters, see text.) The full curve shows the result at $T = 1$ K in the presence of the exchange interaction. The dashed curve shows the result for the nonmagnetic barrier.

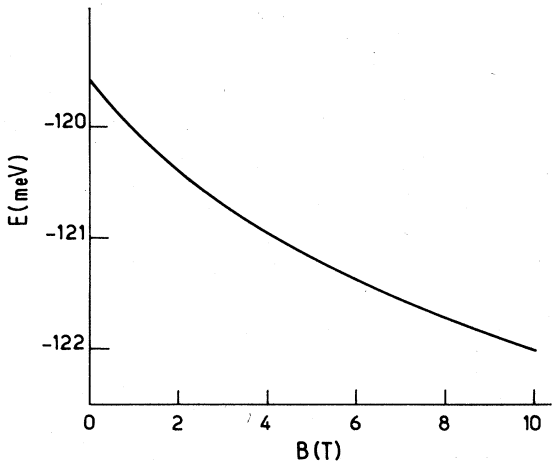

FIG. 3. Magnetic field dependence of the impurity energy level at $T = 5$ K. (For complete set of parameters, see text.) Notice that the total variation, up to 10 T, is of the order of 3 meV.

inside the barrier for the impurity on the interface. The contribution of the barrier energy, in this case, is 23.4 meV, whereas that of the exchange term is -43.2 meV. This shows clearly the formation of a bound magnetic polaron at the interface. For other values of z_i, as the impurity is displaced towards the center of the well, the results approach those of the nonmagnetic case. The strong temperature dependence of these energy levels, due to the temperature dependence of the Mn spin polarization can also be seen from Fig. 1.

In Fig. 3, we have slightly changed the parameters, taking $V=50$ meV, $x=0.3$, $r=0.2$, and $T_0=15$ K. This figure shows the variation with magnetic field, at $T=5$ K, of the energy of an impurity located at the interface. As we can see, it is not strongly dependent upon B. This result suggests that the strong line shifts of the photoemission spectra observed by Zhang *et al.*[4] may not be explained exclusively in terms of the recombination of excitons trapped by charged impurities. Other mechanisms, such as alloy fluctuations, are conjectured in Ref. 4.

In summary, we have shown that for small valence-band offsets in CdTe-(Cd,Mn)Te, of the order of 50 meV or less, we may expect to observe bound magnetic polarons in these superlattices, as in bulk semimagnetic semiconductors, provided the impurities lie sufficiently close to the interface. In a forthcoming publication we will discuss the case of particles trapped by interface defects.

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