Quasi-two-dimensional magnetic polaron: an exact self-consistent approach

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The energy and wavefunction of a quasi-two-dimensional magnetic polaron in semimagnetic semiconductors are calculated by solving a non-linear Wannier equation. A self-consistent solution is presented including exactly the structure factor of the system. We found that the magnetic polaron energy is strongly dependent on temperature and well width. Good agreement is obtained with experimental results for the CdMnTe/CdTe system.

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The free energy is:

\[ \mathcal{F} = \frac{1}{\beta} \ln \left[ \text{Tr}(e^{-\beta \mathcal{H}}) \right] \]
where $H = H_0 + H_{\text{spin}}$. The trace operation is performed over the electronic as well as the spin states of the system. In a system in contact with a thermal reservoir, the free energy tends to a minimal value, so that the equilibrium condition in this case is given by $\delta F = 0$, subject to the normalization condition for the wave function $\langle \Psi | \Psi \rangle = 1$. After performing the corresponding functional derivatives, we are left with the effective equation:

$$
\left[ H_0 - \alpha \sum_j \langle \vec{s} \cdot \vec{S}_j \rangle \delta(\vec{r} - \vec{R}_j) \right] |\xi\rangle = \lambda |\xi\rangle,
$$

(4)

where $\lambda$ is a Lagrange multiplier arising from the normalization condition and

$$
\langle \vec{s} \cdot \vec{S}_j \rangle = \frac{\operatorname{Tr}_{\{s_j S_j\}} \left\{ e^{-\beta(\xi)|H_{\text{spin}}|\xi} \right\}}{Z} = \frac{1}{\beta} \frac{\partial \ln Z}{\partial K_j},
$$

(5)

$$
Z = \operatorname{Tr}_{\{s_j S_j\}} \left\{ e^{-\beta(\xi)|H_{\text{spin}}|\xi} \right\},
$$

(6)

$$
K_j = \alpha n |\xi(R_j)|^2.
$$

(7)

Here, $n$ is 1 or 3 depending on whether we are considering electron-ion or hole-ion exchange and $Z$ is the partition function corresponding to the exchange term of the Hamiltonian. After calculating $Z$ we obtain the following approximate result for the spin correlation function, valid for temperatures roughly below $100^\circ K$:

$$
\langle \vec{r}_e | n \vec{k} \rangle = f_n(z_e) \frac{e^{i\vec{k} \cdot \vec{r}_e}}{\sqrt{A}} u_n(\vec{r}_e),
$$

(9)

$$
\langle \vec{r}_h | m \vec{k} \rangle = g_m(z_h) \frac{e^{i\vec{k} \cdot \vec{r}_h}}{\sqrt{A}} u_h(\vec{r}_h),
$$

(10)

where $\vec{r} = (\vec{r}, z)$. Now, we propose a solution built up from this set of individual electron and hole states

$$
|\xi\rangle = \sum_{n,m,k} \phi^{nm}(\vec{k}) |nm\vec{k}\rangle.
$$

(11)

In terms of the new amplitude $\phi^{nm}(\vec{k})$, the effective equation takes the form

$$
E_{\text{MP}}(\vec{k}) \phi^{nm}(\vec{k}) - \sum_{n',m',\vec{k}'} \langle nm | V^C_{\vec{k},\vec{k}'} | n'm' \rangle \phi^{n'm'}(\vec{k}') = \lambda \phi^{nm}(\vec{k}).
$$

(12)

The effective interaction term $V^C$ is the sum of the Coulomb term $V^C$ and the exchange term $V^{\text{spin}}$. The explicit expressions are

$$
\langle nm | V^C_{\vec{k},\vec{k}'} | n'm' \rangle = \frac{-e^2/2z}{|| \vec{k} - \vec{k}' ||} A \int dz_e \int dz_h f_n^*(z_e) g_m^*(z_h) e^{-||\vec{k} - \vec{k}'||z_e - z_h}|f_n(z_e)g_m(z_h)|,
$$

(13)

$$
\langle nm | V^{\text{spin}}_{\vec{k},\vec{k}'} | n'm' \rangle = \frac{-5z\alpha N_0}{4A^2} \int d^2 \rho_e \int d^2 \rho_h \int dz_e \int dz_h f_n^*(z_e) g_m^*(z_h) B_{5/2} \left[ \frac{\alpha n}{2} \langle \xi|\delta(\vec{r}_h - \vec{R}_j)|\xi\rangle \right] e^{-i\vec{k} \cdot (\vec{r}_e - \vec{r}_h)} f_{n}(z_e)g_m(z_h),
$$

(14)

where $\bar{z}$ is the effective concentration of Mn ions and $N_0$ is the number of cation sites per unit volume in the crystal. Once these interaction terms have been calculated we can solve Eq. (12) self-consistently and use the solution $\phi^{nm}(\vec{k})$ to calculate the MP energy given by

$$
E_{\text{MP}} = -\frac{\partial}{\partial \beta} \ln \operatorname{Tr}_{\{s_j S_j\}} \left\{ e^{-\beta(\xi)|H_{\text{spin}}|\xi} \right\}.
$$

(15)

This energy represents the gain in binding energy of the polaron, i.e. the spin exchange contribution to the total energy, which is exactly the entity that is measured. In order to simplify the calculations we take into account only one bound state for the electron and one for the hole ($n = m = 1$).
In Fig. 1 we display the well width and temperature dependence of the polaron energy. A rapid decrease of the energy with increasing temperature is observed. We also find a maximum in the MP energy for varying well width (independent of temperature) at 10 Å. Figure 2 is a contour plot corresponding to Fig. 1. This figure displays better the region of high stability of the polaron complex. The MP energy strongly depends on the carrier wavefunction in the sense that if the probability of finding the electron (or hole) in the magnetic region increases, so does the MP energy. It is for this reason that the polaron energy vanishes rapidly with increasing well width. This feature is correctly reproduced by our calculation.

In Fig. 3 we compare our theoretical results with available experimental data (at fixed temperature). The polaron energy, $E_{\text{MP}}$, as a function of the well width is shown in Fig. 3 (temperature is $T = 1.6$ K). The open circles represent experimental data taken from Ref. 8. The agreement is excellent except for the 6 Å QW. The reason for this disagreement is evident since interface roughness and well width fluctuations in the range of one monolayer should be very important for QW's of such small nominal well width. These inhomogeneities are responsible for the formation of islands (totally confined regions) with the obvious increase of binding energy. Therefore we conclude from the experimental result for $E_{\text{MP}}$ for the 6 Å QW, reported in Ref. 8, that it cannot be taken as an ideal QW as in our calculations. Our calculated $E_{\text{MP}}$ are in excellent agreement (within the error bars) with the experimental results. This confirms that our computational method is reliable for semimagnetic QWs. As a final verification, we show in Fig. 4 the comparison of our results with experimental data [8] for a 12 Å well width as a
function of the temperature. As it should be the MP energy goes rapidly to zero as the temperature increases due to the increasing magnetic disorder of the Mn ions at high temperature. A good agreement between our results and experiment is obtained over the 25 K temperature range reported.

In conclusion, we developed a new computational approach to address the problem of the magnetic polaron in quantum well heterostructures with semimagnetic semiconductor compounds. We showed the high accuracy of the results obtained by comparing them with available experimental results for quantum well with non-magnetic wells.

The computed magnetic polaron energies agree quantitatively with experiments. This calculational method appear to be adequate to include more realistic considerations, i.e. valence-band mixing effects, about the physics of these interesting systems.

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