Comment on "Effects of Disorder on Ferromagnetism in Diluted Magnetic Semiconductors"

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In a recent Letter, Berciu and Bhatt [1] have presented a mean-field theory of ferromagnetism in III-V semiconductors doped with Mn [2]. The approach starts from uncorrelated Mn impurity states, which overlap to form an impurity band (IB). We argue here that this approach is not appropriate for (Ga,Mn)As containing 1–5% Mn. There is also a sign error in Ref. [1]. After correcting this error, mean-field theory no longer yields stable ferromagnetism for the system sizes used.

For the overlap matrix elements between hole impurity states, Ref. [1] gives $t(r) = 2E_b\,(1 + r/a_B)\,e^{-r/a_B}$ with hole binding energy E_b and Bohr radius a_B. The calculations are done with $t(r) > 0$. We have reproduced the numerical results of Ref. [1], for example, the dotted curves in the inset in Fig. 1 give the Mn and hole spin polarizations for three impurity configurations with a Mn concentration of $x = 0.05$ and $p = 0.1$ holes per Mn, using 200 Mn spins. These are evidently the same parameters as used for Fig. 3 of Ref. [1].

However, the overlap matrix elements $t(r)$ should be negative, as we show now, using the sign convention of Ref. [1]. For a parabolic valence band, the Hamiltonian for a hole and two impurities at $\mathbf{R}_A$ and $\mathbf{R}_B$ reads $H = p^2/2m^* + V_A(\mathbf{r}) + V_B(\mathbf{r})$ with $V_i(\mathbf{r}) = -e^2/\epsilon|\mathbf{r} - \mathbf{R}_i|$ where $i = A, B$. m^* is the effective mass and ϵ is the dielectric constant. The hydrogen-like Hamiltonian for a single impurity is $H_i = p^2/2m^* + V_i(\mathbf{r})$. Let ψ_i be the ground state of H_i with energy $E_b < 0$. The overlap matrix element between ψ_A and ψ_B is $t \equiv \langle\psi_B|H|\psi_A\rangle$, which we can also write as $t = \langle\psi_B|\,H_A + V_B(\mathbf{r})|\psi_A\rangle = E_b\langle\psi_B|\psi_A\rangle - \langle\psi_B|e^2/\epsilon|\mathbf{r} - \mathbf{R}_B|\,|\psi_A\rangle$. Since the wave functions ψ_i are real and positive, we obtain $t < 0$.

The sign change in $t(r)$ inverts the *highly asymmetric* IB. With the correct sign the IB has a long tail to negative hole energies (positive electron energies), resulting from strongly bound states. Fig. 1 shows the density of states (DOS) for $x = 0.05$ with 200 Mn impurities. The subband structure is due to the finite system size. We find that the IB width (independent of the sign of t) is about 18 eV, and thus much larger than the gap of GaAs. Furthermore, the IB strongly overlaps with the valence band. These results show that the IB picture is not appropriate. The reason is that there are typically many Mn impurities within the range over which $t(r)$ falls off, *i.e.*, the system is *not* weakly doped [3].

With the corrected $t(r)$ the Fermi energy no longer lies in a region of very large DOS as in Ref. [1], but in the band tail close to the conduction band edge, as shown in Fig. 1 for $p = 0.1$. Average Mn and hole spin polarizations for $x = 0.05$ and $p = 0.1$ are shown in the inset. The maximum Curie temperature is only about 20 K and the stability of the ferromagnetic state strongly depends on the impurity configuration. If ferromagnetism is found at all, the hole polarization is at most 0.05. For the numerical parameters this means that only a *single* hole spin is flipped, suggesting large finite-size effects.

To conclude, the impurity-band approach is not applicable to (Ga,Mn)As containing a few percent of Mn. However, it should be valuable for weak doping. We would like to thank J. König, M. Raikh, and J. Schliemann for interesting discussions.

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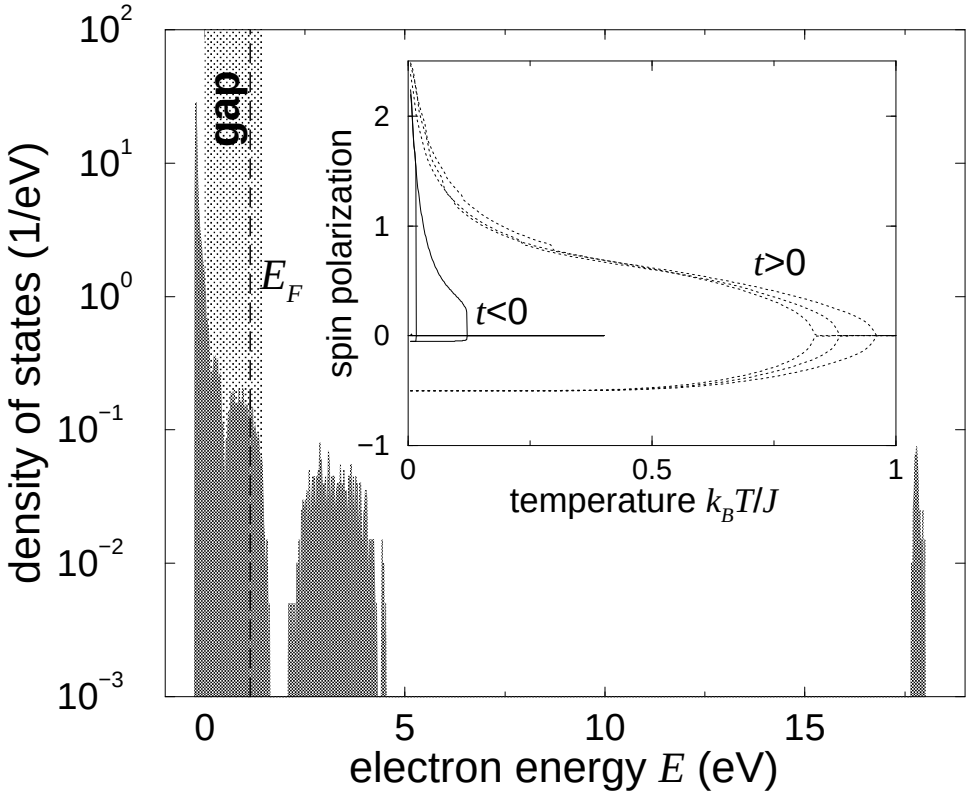

FIG. 1. Density of states per Mn impurity as a function of *electron* energy relative to the valence band top for $x = 0.05$, averaged over 100 configurations of 200 Mn impurities (dark gray area). The light gray bar denotes the GaAs gap. The dashed line shows the Fermi energy for $p = 0.1$. Inset: Average Mn (positive) and hole (negative) spin polarizations for the same parameters. The dotted curves have been obtained with overlap matrix elements $t(r) > 0$ as in Ref. [1], the solid curves with the correct $t(r) < 0$, each for three configurations.