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Ferromagnetism mediated by the upper Hubbard band in selectively doped GaAs/AlGaAs structures

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We consider in detail the indirect exchange between Mn ions imbedded to GaAs/AlGaAs quantum wells where the barriers are doped by acceptor impurity supported by the carriers of the upper Hubbard band supplied by barriers acceptors. A special attention is paid to an interplay between strong delocalization of the carriers within the upper Hubbard band (allowing exchange between well separated ions) and relatively weak coupling of these carriers with Mn ions. It is shown, that, despite of the latter factor, the values of Curie temperatures can for such structures be as high as room temperatures.

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Introduction. A lot of attempts were made to fabricate 2D ferromagnetic structure on the base of Mn dopants within GaAs–AlGaAs quantum wells [1]. Since the direct exchange between Mn magnetic ions is negligibly weak, the ferromagnetism was expected to be supported by indirect exchange mediated by holes supplied by Mn acceptors. The important problem here is related to the fact that Mn plays a role in magnetism only being in the substitutional Ga position where Mn is an acceptor. However at significant degree of doping (preferable for high Curie temperatures) many Mn dopants occupy interstitial positions where they play a role of donors thus leading to strong charge disorder. As a result, the holes suffer strong localization and the indirect exchange is weak. In our recent paper, [2], we, however, have shown (both theoretically and experimentally), that at relatively weak degrees of doping, when Mn mostly occupy substitutional positions and the disorder is weak, we deal with virtual Anderson transition, allowing delocalization of the holes within the impurity band. As a result, we have observed relatively high Curie temperatures (~ 100 K) at weak degrees of doping. Note, however, that in this case we still need samples with very low degree of any background disorder.

To prevent the localization of the holes by Mn-introduced disorder, in several papers [3] it was suggested to place the Mn delta-layer outside of the quantum well (occupied by holes). In this case the holes were not strongly affected by the charge disorder in Mn delta layer and the indirect exchange was possible. However an inevitable payment in this case is a small tunneling transparency between the delta-layer and the quantum well.

Here, we will present another realization allowing effective indirect exchange for the case of weak Mn doping (see Fig. 1). It is related to the role of the upper Hubbard band of Mn centers which can be occupied provided the AlGaAs barrier is doped by an acceptor impurity. As it is known, the metal-insulator transition in the upper Hubbard band takes place at much weaker concentrations than for single-occipied dopants. Thus we can expect that the indirect exchange (and thus ferromagnetism) can take place for concentrations even less than were used in [2]. Moreover, the limitations on the background disorder are not as strong as implied in [2].

However, it is easily understood that the Coulomb interaction between the hole from the upper Hubbard band with Mn ion (equal to the binding energy of the hole) is much weaker than for the one known for the lower Hubbard band. Indeed, the binding energy for the upper Hubbard band is typically by an order of magnitude lower than for the lower Hubbard band. Thus the indirect exchange via the states of the upper Hubbard band is also to be expected to be weaker than for the lower band. Thus to make a decisive conclusion concerning the role of the effect of the upper Hubbard band on the magnetic properties of the structure we need detailed experimental estimates of all the factors relevant for support of ferromagnetic state.

Discussion. Although earlier [2] we have given semiqualitative estimates for 2D RKKI, here we need somewhat more detailed ones in a view of the factors mentioned above. As it is known, the indirect exchange is supported by a coupling of the potential of magnetic ion j to Friedel oscillations of mobile electron density

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resulting from the interference of incoming plane wave and scattering state produced by the ion i (and vice versa). Recall that scattering state resulting from the incoming plane wave $\psi_i = \exp i\mathbf{k}\mathbf{R}$ scattered by ion i, with a position $\mathbf{R}_i$ is given as

$$\psi_s = \frac{f}{(-iR)^{1/2}} e^{i(\mathbf{k}\mathbf{R}_i - kR)}, \tag{1}$$

where

$$f = -\frac{m}{\hbar^2 (2\pi k)^{1/2}} \int d^2\rho J e^{ik\rho}, \tag{2}$$

J is the exchange scattering potential for the delocalized mode by the magnetic ion. The result of interference, $\psi_i \psi_s^* + \psi_i^* \psi_s$ is given as

$$\frac{2^{1/2} f}{R^{1/2}} \left\{ \cos[\mathbf{k}(\mathbf{R} - \mathbf{R}_i) - kR] + \sin[\mathbf{k}(\mathbf{R} - \mathbf{R}_i) - kR] \right\}. \tag{3}$$

Here we have assumed that the effective radius of J is small. To obtain local electron density at the point $\mathbf{R} = \mathbf{R}_j$ we should sum Eq. (3) over $\mathbf{k}$. In particular, the result of summation over the angle variable φ of the cosine term gives

$$\int_0^{2\pi} d\varphi Re \exp(ikR_{ij}(\cos\varphi - 1)) = \cos(kR_{ij}) J_0(|kR_{ij}|), \tag{4}$$

where φ is $\angle(\mathbf{k}, \mathbf{R}_{ij})$, J_0 is the Bessel function. As for the sin term, we note that at small kR it can be neglected. Then, in what follows we will show that the dominant contribution to the final result corresponds to $kR = \pi$. As it can be seen, the result of integration of the sin term over φ is equal to zero. Thus, in what follows we will restrict ourselves with cosine term. Thus we obtain for the modification of the electron density in a position of the ion J resulting from the ion i by summation over all of the modes. Then, the coupling energy between ions i and j is

$$U_{ij} = -\mathbf{S}_i \mathbf{S}_j \frac{2^{1/2}}{R^{1/2}} \frac{m}{\hbar^2 (2\pi k)^{1/2}} \bar{J}^2 a^4 \times \\ \times \int dk g(k) f_k \cos(kR_{ij}) J_0(|kR_{ij}|), \tag{5}$$

where f_k is the distribution function while g is the density of states while $\bar{J}$ is the magnitude of the exchange integral between the localized spin and the delocalized mode and a is the effective radius of the corresponding exchange potential. In our case all of the hole states within the band are occupied and $f = 1$. Unfortunately, we have no detailed information concerning the delocalized states resulting from the virtual Anderson transition. Although we expect that the corresponding modes (or their wave packets) can be described by some plane waves with isotropic spectrum, we do not know the energy and wave vector dependence of the effective mass and of density of states. However, we can conclude that the upper limit for k is given by $\pi/\bar{R}$ where $\bar{R}$ is a typical distance between Mn atoms. Correspondingly, for the exchange between the neighboring magnetic ions the maximal value of the factor kR_{ij} in the exponent is estimated as π. For such a case the integral over k in 5 for $g(k) = Ck$ (which is typical for isotropic spectrum of plane waves in 2D where $C = 2\pi^{-2}$) gives $\sim 2.5C/\bar{R}^2 > 0$ which corresponds to a ferromagnetic type of the exchange. Actually, one can expect that the density of states decays near the limiting value of k and thus the upper limit for $k\bar{R}$ can be even less than π. However for the angular factor given by Eq. (4) (which is positive except of a small interval of k) one still expects a positive sign of the integral over k almost irrespective to the form of $g(k)$.

The final estimate gives

$$U_{ij} \sim \frac{2^{1/2} \cdot 2.5}{(2\pi)^{5/2}} \bar{J}^2 \frac{a^4 \pi m}{\bar{R}^2 \hbar^2}. \tag{6}$$

Basing on the estimates given in [4] for T_c of square plane lattice (the number of neighbors equal to 4),

$$T_c = \frac{2U}{\ln 2} \tag{7}$$

we finally obtain

$$T_c \sim \frac{2.5}{2(\pi)^{3/2} \ln 2} \bar{J}^2 \frac{a^4 m}{\bar{R}^2 \hbar^2}. \tag{8}$$

One notes that the first factor is ~ 0.5. Thus assuming $a \sim \bar{R} \sim 10^{-6}$ cm we obtain as a very rough estimate $T_c \sim \bar{J}^2 10^{15}$ erg. Correspondingly, even for $\bar{J} \sim 6$ meV (which is reasonable estimate for the binding energy of the upper Hubbard band) we can obtain $T_c \sim 300$ K. Thus one can conclude that the kinetic factor resulting from effective delocalization of carriers within the upper Hubbard band can dominate over the relative weakness of the exchange coupling of these carriers within the Mn ion.

Note that in our considerations we have assumed that all barrier acceptors supply their holes to form A^+ centers. However, in general it is not a case. As it was noted in [5], if the barrier acceptor is close enough to the interface between the well and the barrier, there is a possibility to form so-called $\tilde{A}^0$ center which is just a complex of the acceptor within the barrier and hole in the well coupled to this acceptor. The energy of such a complex can be lower than the energy of A^+ center. It can be shown that for dilute structures the relation between A^+ and $\tilde{A}^0$ centers is controlled by the following inequality:

$$U_{A^+} + \frac{e^2}{\kappa[r^2 + (d_w/2 + d_b)^2]^{1/2}} \geq U_{\tilde{A}^0}. \quad (9)$$

Here, d_w is a width of the well (it is assumed that the dopants are within the center of the well), d_b is a distance of the negatively charged barrier acceptor (A^- center) from the interface, r is a distance between the two acceptors along the plane of the structure, U_{A^+} is the binding energy of A^+ center while $U_{\tilde{A}^0}$ is the binding energy of $\tilde{A}^0$ center.

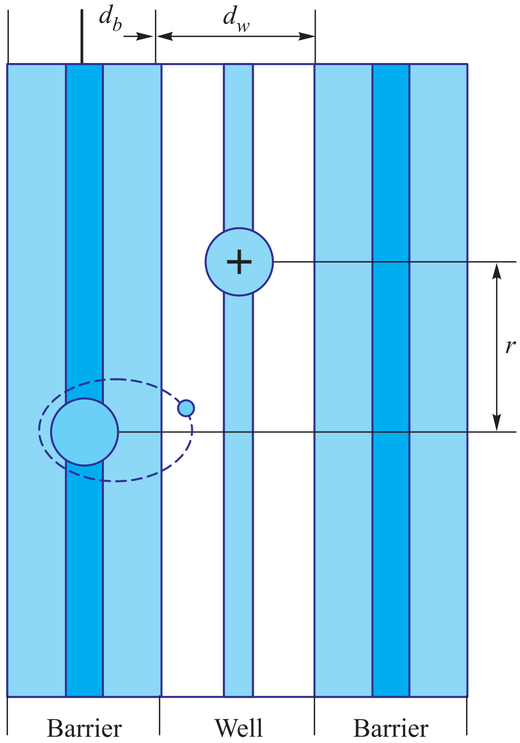

Fig. 1. Schematic picture of the structure discussed above

When this inequality holds, then A^+ center is formed, otherwise we deal with $\tilde{A}^0$ center. In principle, basing on this inequality we could easily calculate densities of states for A^+ and $\tilde{A}^0$ centers. However, in realistic situations one can not restrict himself by only interactions within A^+ and $\tilde{A}^0$ complexes due to partial overlapping of the potentials of the corresponding complexes. Nevertheless, qualitatively we can conclude that for large d_b the binding energy of $\tilde{A}^0$ complex is too small and almost all barrier acceptors supply their holes to form A^+ centers. Contrary, for small d_b one expects that practically no A^+ centers are formed and all the holes supplied by the barrier acceptors are localized near the interface. It is clear that in the latter case the exchange of these holes with Mn ions in the center of the well is weak and no enhancement of the ferromagnetism of the sort discussed above is possible. Thus, by a proper choice of d_w and d_b we can control the ferromagnetic properties of the structure. An interesting possibility can be provided by external gate which could shift the charge distribution within the well thus varying a relation between A^+ and $\tilde{A}^0$ centers and, correspondingly, the efficiency of the indirect exchange.

We would like also to emphasize that, while the magnetic properties are supported by Mn acceptors within the well, the nature of the barrier acceptors is of no matter. At the same time it could be of interest to study structures where the barrier acceptors are also of a magnetic nature (Mn ions). When the values of d_b are not too big, one can expect that the exchange between Mn barrier acceptors with holes of $\tilde{A}^0$ centers could still support ferromagnetic phase (see, e.g., [3]). If at the same time the concentration of A^+ centers in the wells is still high enough, one expect an interesting co-existence of two ferromagnetic phases with different parameters.

Finally, we note that in course of selective doping one should take care to prevent any additional factor enhancing the disorder. To say, one should initially introduce Mn dopants to the well and only after that introduce dopants to the barrier. Otherwise, the procedure of doping the barrier can lead to a distortion in positions of Mn in the well.

Conclusion. To conclude, we have shown that – despite of relatively strong charge disorder within GaAs/AlGaAs structures where the wells are doped by Mn while the barriers – by some other acceptor defects, these structures can exhibit relatively large Curie temperatures at small Mn concentrations (of the order of $10^{12}\,\mathrm{cm}^{-2}$).

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