Conversion of free magnetic polaron into vortex lattice in quantizing magnetic semiconductors.

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We show that in strong (quantizing) magnetic fields "ordinary" free magnetic polaron in diluted magnetic semiconductors (of type A²MeB₆, where Me = Fe, Mn) exists in the form of vortex lattice quite similar to that in type II superconductors (Abricosov vortex lattice). The region of external parameters (like external magnetic field and temperature), where such lattice exists, is determined from the condition that lattice dimension is less or equal to polaron localization radius.

Diluted magnetic semiconductors (DMS) can be regarded as an ensemble of magnetic impurities Fe, Mn, embedded in the lattice of host A²B₆ semiconductor. The concentration of impurities is such that direct exchange interaction between impurities does not occur so that aforementioned substances is in the paramagnetic phase.

Last decade considerable experimental and theoretical efforts have been spared for investigation of self-localized states of carriers in DMS (see, e.g. [1–5]). Such self-localized state of conduction electron (hole) is called free magnetic polaron (MP) and can be regarded as a region (of polaron radius ρ) of correlated spins of magnetic ions, where the interaction between spins of magnetic impurities is mediated by the electron (hole).

However, existing theories considered the properties of such MPs in magnetic fields (such that ρH = \( \sqrt{\frac{\hbar c}{\epsilon_H}} \) < ρ, ρ is MP localization radius, H is external magnetic field), where diamagnetic effects (Landau quantization) do not manifest themselves (see [3]). It turns out, however, that shape and physical properties of MP may change drastically if we include aforementioned diamagnetic contribution into consideration.

In this paper we show that MP in quantizing magnetic fields exists as a lattice of vortices, very similar to Abricosov vortex lattice in type II superconductors [6]. We have shown that formation of the vortex lattice is energetically favourable as compared to the single MP. Our analysis show that general scenario of vortex lattice formation is as follows. When magnetic field exceeds some threshold value

\[ H_{c1} = \frac{\hbar c}{\epsilon_0} \rho^2, \]  

the initial spherically symmetric "paramagnetic" MP (see [6] for detailed investigation of this MP properties; ρ is a function of magnetic ions concentration, temperature and external magnetic field) looses its spherical symmetry and gains cylindrical one. This "diamagnetic" MP is localized in a plane perpendicular to magnetic field direction (i.e. in the plane of Landau quantization). At further increase of magnetic field this MP splits into several vortices, that tend to organize into vortex lattice [3, 4].

The magnetic field penetrates only to the vortex core in superconductor, giving rise to normal (nonsuperconducting) phase there, the core region of MP consists of coherently oriented correlated spins of magnetic impurities, giving rise to (local) magnetically ordered phase.

At very high magnetic fields \( H \sim H_{c2} \) the "ferromagnetic" cores of the vortices merge so that magnetic impurities do not "need" the electron (hole) to interact with each other. In this region of magnetic fields the amplitude of MP wave function become small so that \( H_{c2} \) can be determined by the usual procedure of linearization [6] of corresponding equation.

In the present paper we give the estimations of \( H_{c1} \) and \( H_{c2} \) rather then detailed (standard) calculation of vortex lattice properties.

Consider first the model of free MP. We start from the Hamiltonian of electron (hole), coupled to subsystem of magnetic ions in DMS. These magnetic ions randomly substitute \( N_l \) cations at the sites \( \vec{R}_j \) (\( j = 1, 2, ..., N_l \)) of a cubic crystal lattice. Under the assumption that corresponding energy band is isotropic and nondegenerate, we write the Hamiltonian of this system in the effective mass approximation

\[ \mathcal{H} = \frac{\vec{p}^2}{2m^*} + g_e \mu_B \vec{H}\vec{S}_e + \sum_{j=1}^{N_l} \left[ -J \Omega \delta \left( \vec{r} - \vec{R}_j \right) \vec{S}_j \cdot \vec{S}_e + \mathcal{H}_j \left( g_e \mu_B \vec{H} \right) \right] + \mathcal{H}_d, \]

(2)
where $\vec{p}, m^*, g_c, \vec{S}_e$ and $\vec{r}$ are momentum operator, effective mass, band g-factor, spin operator, and coordinate of electron (hole); $g_l$ and $\vec{S}_l^i$ are g-factor and spin operator of the magnetic ion localized at lattice site $\vec{R}_l$; $J$ is carrier-ion exchange interaction constant, $\Omega$ is unit cell volume and $\mu_B$ is Bohr magneton. The first two terms in (2) determine the kinetic and Zeeman energy of an electron. The next two terms determine the carrier-ion exchange interaction and the sum of magnetic ions Hamiltonians in the field $\vec{H}$ (see [3] for details).

Choosing electron wave function as a product of coordinate and spin parts and averaging over random impurities positions in a mean field approximation (see [3] for details), we obtain following energy functional for a free magnetic polaron.

\[
E_\sigma = \int \left\{ \frac{1}{2m_\perp} \psi^* \left( \hat{p}_\perp - \frac{e}{c} \hat{A}_\perp \right)^2 \psi + \frac{1}{2m_\perp} \psi^* \left( \hat{p}_\perp - \frac{e}{c} \hat{A}_\perp \right)^2 \psi \right\} d^3r + g_c\mu_B H \sigma + \frac{ni}{2} \int \left[ E_1 (g_l\mu_B H + Q\sigma) - E_1 (g_l\mu_B H) \right] d^3r,
\]

where $\sigma = \pm \frac{1}{2}$ are the eigenvalues of the operator projecting the electron spin onto $\vec{H}$ and

\[
Q(\vec{r}) = -J\Omega |\psi(\vec{r})|^2
\]

is the effective exchange field, $E_1$ depends on the specific type of SMS magnetic ions paramagnetism (see below), $\hat{p}_\perp \equiv -i\hbar \frac{\partial}{\partial r_\perp}$, $\hat{A}_\perp \equiv -i\hbar (\vec{e}_x \frac{\partial}{\partial x} + \vec{e}_y \frac{\partial}{\partial y})$, $\hat{A}_\perp = \vec{e}_x A_x + \vec{e}_y A_y$.

For SMS of type $\Delta S^2-\Delta x M_n B^6$ with Van Vleck paramagnetism $E_1$ has the form

\[
E_{1VV}(x) = \Delta \varepsilon - [(\Delta \varepsilon)^2 + 4x^2]^{1/2},
\]

where $\Delta \varepsilon$ is the splitting of the spin-orbit multiplet of the magnetic ion (see [3] for details). For SMS of type $\Delta S^2-\Delta x M_n B^6$ with orientational paramagnetism we have for $E_1$

\[
E_{1OR}(x) = \frac{1}{\beta} \log \frac{\sinh \left( \left( S + \frac{1}{2} \right) \beta x \right)}{\sinh \left( \frac{\beta x}{2} \right)},
\]

where S is magnetic ion spin, $\beta = (k_B T)^{-1}$.

It is seen that [3] looks like Ginzburg-Landau (GL) functional for superconductors. The difference is more complicated nonlinearity. It is seen that expansion of Eqs (3) and (5) in powers of $|\psi(\vec{r})|^2$ up to $|\psi(\vec{r})|^4$ put formal one-to-one correspondence with GL functional.

Variation of (3) with respect to $\psi^*$ gives following Schrödinger equation for polaron wave function

\[
\frac{1}{2m_\perp} \left( \hat{p}_\perp - \frac{e}{c} \hat{A}_\perp \right)^2 \psi + m_\perp \frac{\partial E_1}{\partial |\psi|^2} \psi = 0.
\]

It is convenient to show the existence of vortex lattice solutions of corresponding differential equations from the side of $H \sim H_{c2}$, where $|\psi(\vec{r})|^2$ is small. For that we linearize (3) (with respect to (5) and (6)) in $\psi$. This gives

\[
\frac{1}{2m_\perp} \left( -i\hbar \frac{\partial}{\partial y} + \frac{\epsilon H_x}{\hbar} \right)^2 \psi + \lambda \psi = 0,
\]

where we choose following gauge of vector potential

\[
A_y = H_x, \quad H \equiv H_z,
\]

\[
\lambda_{VV} = J\Omega m_\sigma \frac{4g_l\mu_B H}{\sqrt{(\Delta \varepsilon)^2 + 4(g_l\mu_B H)^2}},
\]

\[
\lambda_{OR} = -J\Omega m_\sigma S \beta g_l\mu_B H,
\]

$B_S(x)$ is a Brillouin function for spin S:

\[
S B_S(Sx) = \left( S + \frac{1}{2} \right) \coth \left( S + \frac{1}{2} \right) x - \frac{1}{2} \coth \frac{x}{2}.
\]

It is well-known (see, e.g. [9]) that localized solutions of $E_1$ exist if $\lambda$ equals to one of eigenvalues

\[
\lambda = -(n + \frac{1}{2}) \hbar \frac{\epsilon H}{m_\perp c}.
\]

Lowest eigenvalue determines $H_{c2}$ so that we obtain following equations for $H_{c2}$ for the case of Van Vleck

\[
J x l_0 \sigma \frac{4g_l\mu_B H}{\sqrt{(\Delta \varepsilon)^2 + 4(g_l\mu_B H)^2}} = -\frac{1}{2} \hbar \frac{\epsilon H}{m_\perp c}
\]

and orientational paramagnetism

\[
\sigma J x l_0 S B_S(S \beta g_l\mu_B H_{c2OR}) - \frac{\mu_B H_{c2OR}}{\mu} = 0,
\]

\[
\mu = \frac{m_\perp}{m_0}, \quad x_l = n_l \Omega,
\]

where $m_0$ is a free electron mass.
To have feeling of the numerical values of $H_{c2}$ for some specific DMS, we use two examples. First one is Zn$_{1-x}$Fe$_x$Se with Van Vleck paramagnetism of Fe. Its parameters are $[4]$: $m^*_e = 0.14m_0; m^*_h = 1.2m_0; J_e = 0.22eV; J_h = -1.6eV; \Delta \varepsilon = 1.8meV$; unit cell volume $\Omega = 45.6\AA^3$. It is sufficient for our estimations to put $m^*_e, h = m_{e,h}$.

Second one is Cd$_{1-x}$Mn$_x$Te with orientational paramagnetism of Mn. Parameters of this solid solution are following $[1]: m^*_e = 0.096m_0; m^*_h = 0.48m_0; J_e = 0.22eV; J_h = -0.88eV; \text{lattice constant } a = 6.48\AA$; unit cell volume $\Omega = 68.06\AA^3$.

It is seen from (11a) that this equation has solution only if $J\sigma < 0$, i.e. for vortex lattice to occur for electron MP ($J_e > 0$), we should have $\sigma = -1/2$; for hole MP $\sigma = 1/2$. We have from (11a)

$$\frac{1}{\sqrt{1 + 4h_{c2V}^2}} = \frac{1}{4}\frac{\Delta \varepsilon}{\mu g_x|J\sigma|},$$

$$h = \frac{g_1\mu_B H}{\Delta \varepsilon}.$$  \hspace{1cm} (12)

Since $\Delta \varepsilon/J << 1$, the solution of (12) is at $h >> 1$. In this case we have from (12)

$$H_{c2V} = (1.7 \cdot 10^4 \text{ Tesla}) \mu x_1|J_0|, \hspace{0.5cm} J_0 = J/1eV$$  \hspace{1cm} (13)

It was shown earlier $[3]$ that in Zn$_{1-x}$Fe$_x$Se electron cannot autolocalize. So, we give estimate of $H_{c2}$ for hole only. From (12) (at typical value $x_1 = 4\%$) we obtain, that for hole $H_{c2V} \approx 1300$ Tesla.

The solution of Eq. (11) exists at $J\sigma > 0$. In dimensionless variables

$$\frac{g_1\mu_B H}{S\mu Jx_1} = h, \hspace{0.5cm} \frac{3k_B T}{JS(S+1)\mu x_1} = \tau$$

equation (11) can be rewritten as

$$h_{c2OR} = B_{S} \left( \frac{3h_{c2OR}}{\tau (S+1)} \right)$$

Its asymptotic values are as follows

$$k_B T_e = \frac{J}{3} S(S+1)\mu x_1,$$
$$g_1\mu_B H_{c2OR}(T = 0) = J S\mu x_1.$$  \hspace{1cm} (14)

The "universal" (i.e. independent of $J$ and $x_1$) temperature dependence of $H_{c2OR}$ is reported in Fig.1. Our estimations show that electron cannot autolocalize also in orientational DMS Cd$_{1-x}$Mn$_x$Te. Equation (14) permits to estimate $H_{c2OR}^h$ from above. Taking into account that MP in orientational DMS can be formed at $x_1 > 17\%$, we obtain (for $S = 5/2$ and $x_1 = 20\%$) for hole $H_{c2OR}^h \approx 1800$ Tesla.

![FIG. 1. "Universal" temperature dependence of $H_{c2}$ for orientational DMS.](image-url)

The situation with $H_{c1}$ is quite similar to that in type II superconductors. In this case MP plays a role of single vortex. Our analysis show that at $H < H_{c1}$ MP exists in 3D spherically symmetrical form while at $H > H_{c1}$ it has 2D character being localized in the plane perpendicular to the direction of the external magnetic field. So, for $H_{c1}$ estimation it is sufficient to consider spherically symmetrical MP, substituting its radius of localization to Eq. (10).

Since at $H \sim H_{c1}$ we should keep nonlinearity, we cannot solve Eq. (12) analytically. However, MP localization radius $\rho$ can be quite accurately calculated variationally with the trial MP wave function in the simplest possible form $[3]$

$$\psi = \left( \frac{2}{\pi \rho^2} \right) \frac{1}{2} \exp \left( -\frac{r^2}{\rho^2} \right).$$  \hspace{1cm} (15)

In Van Vleck DMS such variational calculation had been done in $[4]$. For $H_{c1}$ we obtain from (13)

$$H_{c1} = \frac{87.4 \text{ Tesla}}{\rho_0^2}, \hspace{0.5cm} \rho_0 = \rho \sqrt{\frac{\pi}{2}} \left( \frac{\Delta \varepsilon}{J}\right)^{\frac{1}{2}}$$  \hspace{1cm} (16)

For $x_1 = 4\%$ variational calculation $[3]$ gives $\rho_0 = 0.75$ and $H_{c1V}^V = 155$ Tesla.

Thus at $x_1 = 4\%$ vortex lattice for hole MP in Van Vleck DMS possibly occurs in wide range of magnetic fields $155$ Tesla $< H < 1300$ Tesla.

We have for $H_{c1}$ in the case of orientational DMS

$$H_{c1} = \frac{6000 \text{ Tesla}}{\rho_0^2}, \hspace{0.5cm} \rho_0 = \rho \sqrt{\frac{\pi}{2}} \left( \frac{1}{12} \right)^{\frac{1}{2}}$$  \hspace{1cm} (17)
For $x_l = 20\%$ and $T = 10K \, \rho_0 = 14$ and $H_{c1 OR}^h = 30$ Tesla.

Thus at $x_l = 20\%$ and low temperatures vortex lattice for hole MP in orientational DMS possibly occurs for magnetic fields $30$ Tesla $< H < 1800$ Tesla. This interval is by order of magnitude the same as that in Van Vleck DMS. The difference is that in orientational DMS we may ”adjust” (e.g. getting lower) critical fields by temperature.

We have shown that quantizing magnetic field ”forces” free spherically symmetric MP in DMS to split into the vortex lattice very similar to that in type II superconductors. Vortex lattice possibly exists at magnetic fields much higher than those for type II superconductors. It occurs for $J\sigma < 0$ for Van Vleck DMS and for $J\sigma > 0$ for orientational ones. The values of $H_{c1}$ and $H_{c2}$ for orientational DMS can be ”adjusted” by temperature, which is impossible for the Van Vleck DMS. This permits to hope, that vortex lattice can be detected more easily in DMS with orientational paramagnetism. As to Van Vleck DMS, in spite of the fact that $H_{c1}$ and $H_{c2}$ are high, they are accessible by modern experimental equipment. We think also, that it is possible to find Van Vleck DMS, where considered phenomena can occur at lower magnetic fields.

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