Fermion-magnon bound states in strong magnetic field: Analysis of the extended Hubbard model

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Numerical calculations of the bound state energies of a delocalized fermion and magnons in a strong magnetic field are presented. An analysis has been done in the framework of an extended Hubbard model, strictly speaking, a Kondo-like model. One of the characteristic feature of such a model is an "anti"-Nagoka behavior which is unusual for strongly correlated fermion systems. In the case of a weak doping, when the free fermion interaction can be ignored, the dependence of magnetization on the magnetic field should exhibit a step-like behavior. Steps are mostly of the same amplitude, which is proportional to the concentration of electrons (holes). The critical values of the magnetic field are accompanied by giant absorption (irradiation) of magnons. The effect discussed below would most likely be found in $3d$-compounds with a moderate value of the antiferromagnetic exchange constant J.

Such bound states are not typical of the Emergy model given by the Hamiltonian

$$H = -t_{pd} \sum_{<\vec{R},\vec{r}>,\sigma} (p^+_{r\sigma} d_{R\sigma} + d^+_{R\sigma} p_{r\sigma}) + \sum_{\vec{R}} (\varepsilon_d n^d_R + U_d n^d_{R\uparrow} n^d_{R\downarrow})$$

$$\times \sum_{\vec{r}} (\varepsilon_p n^p_r + U_p n^p_{r\uparrow} n^p_{r\downarrow}). \qquad (1)$$

Here $p^+_{r\sigma}$, $d^+_{R\sigma}$ ($p_{r\sigma}$,$d_{R\sigma}$) are hole (spin projection σ) creation (annihilation) operators at the sites of p and d sublattice, denoted by $\vec{r}$ and $\vec{R}$, respectively. We assume that these sublattices are inserted into each other as in the case of CuO_2 layers. The single hole on-site energies, ε_p and ε_d, and the on-site Coulomb repulsions, U_p and U_d, along with the kinetic energy term (p–d hybridization), define one of the simplest versions of the Emery model which seriously considers both p and d states, takes directly into account hybridization of p and d orbitals, and, certainly, the on-site correlations are also included in it. However, these advantages are not compensated by its complexity.

If the inequalities $\varepsilon = \varepsilon_p - \varepsilon_d \gg t_{pd}$ and $U_d \gg \varepsilon$ hold, then the low-energy states in the extended Hubbard model are associated with d-sites which are singly occupied:

$$n^d_R = \sum_\sigma n^d_{R,\sigma} = 1.$$

A perturbation theory is usually applied to transform Hamiltonian (1). The contribution of the second-order perturbation theory is the Kondo-like interaction H_p of a p-hole with its neighboring d-holes:

$$H_p = (\tau_1 + \tau_3) \sum_{\vec{R},\vec{a}_1 \neq \vec{a}_2} X^{\alpha 0}_{\vec{R}+\vec{a}_1} Z^{\beta\alpha}_{\vec{R}} X^{0\beta}_{\vec{R}+\vec{a}_2} + (\tau_2 + \tau_3) \sum_{\vec{R},\vec{a}} Z^{\alpha\beta}_{\vec{R}+\vec{a}} Z^{\beta\alpha}_{\vec{R}}$$

$$- \tau_3 \sum_{\vec{R},\vec{a}_1 \neq \vec{a}_2} X^{\alpha 0}_{\vec{R}+\vec{a}_1} X^{0\alpha}_{\vec{R}+\vec{a}_2} , \qquad (2)$$

where the Hubbard notation is used: operator $X^{\sigma 0}$ ($X^{0\sigma}$) creates (annihilates) a hole at the p site with the spin projection σ, whereas $Z^{\alpha\beta}$ alters the spin projection $\beta \to \alpha$ of a hole. Lattice vectors $\mathbf{a}_i$ connect the nearest sites of d and p sublattices. The energy parameters τ_i are defined as follows:

$$\tau_1 = \frac{t^2_{pd}}{\varepsilon}, \quad \tau_2 = \frac{t^2_{pd}}{U_p + \varepsilon}, \quad \tau_3 = \frac{t^2_{pd}}{U_d - \varepsilon} . \qquad (3)$$

The terms contained in Hamiltonian (2) are interpreted as a direct p–p hopping term (third term), Kondo-like hopping term (first term), and AFM p–d exchange (second term). The contribution of the fourth-order perturbation theory is the AFM exchange interaction H_d between d-holes:

$$H_d = J \sum_{\langle \vec{R},\vec{R}' \rangle} Z^{\alpha\beta}_{\vec{R}} Z^{\beta\alpha}_{\vec{R}'} , \qquad (4)$$

where J may be related to the parameters of the initial model (1):

$$J = \frac{t^4_{pd}}{\varepsilon^2} \left(\frac{4}{2\varepsilon + U_p} + \frac{2}{U_d} \right). \qquad (5)$$

The operator in Eq. (4) can be rewritten in the conventional form of a spin dot product ($S = \frac{1}{2}$):

$$Z^{\alpha\beta}_{\vec{R}} Z^{\beta\alpha}_{\vec{R}'} = 2\vec{S}_{\vec{R}} \vec{S}_{\vec{R}'} + \tfrac{1}{2} .$$

Glazman and Ioselevich[3] have analyzed a ferromagnetic state instability in the special case $U_d \to \infty$, $U_p = 0$ of the Kondo-like model (2). A single p-hole should move against a well-defined hypothetical FM background of d-holes and should be able to be bound to spin excitations (magnons) against this background. In Ref. 3 a variational approach was used to calculate the energy spectrum of quasiparticles consisting of a hole and several magnons. The conclusion that the bottom of the quasiparticle energy band tends to drop with an increase in the number of magnons appears to be valid. Later the exact solutions for a composite system hole + magnon in a class of Kondo-like models[4,5] have given a good reason to believe, that the p hole tends to arrange the d spins that surround it paramagnetically.

The excitation spectra of a single p hole depend on the total spin S of the system.

It is suitable to introduce the quantum number n, i.e., the number of magnons as compared to the saturated magnetization case: $n = S_{\max} - S$. The bottom of the upper band corresponding to $n=0$ is situated at the Brillouin cell corners. Lying below is the energy band characterized by $n=1$. Its bottom is placed at the Brillouin cell center. Such an alteration repeats itself with an increasing number of magnons and is accompanied by monotonic decrease in energy of a composite state of the p hole and magnons. Below we denote this energy by $e_h^{(n)}$. It is likely that $e_h^{(n)}$ which decrease monotonically with n, goes asymptotically (in the thermodynamic limit $n \to \infty$) to the energy level of the true ground state arranged by a single hole. the interaction of magnons with the external magnetic field h contributes the following n-dependent term: $e_m^{(n)} = 2\mu_B hn$. A competition of $e_h^{(n)}$ and $e_m^{(n)}$ results in a hole energy: $e^{(n)} = e_h^{(n)} + e_m^{(n)}$, which selects a finite optimal n. It is noteworthy that all the quantities $e^{(n)}$, $e_h^{(n)}$, and $e_m^{(n)}$, are defined on the manifold of integer n's. The situation described above is summarized qualitatively in the inset in Fig. 1.

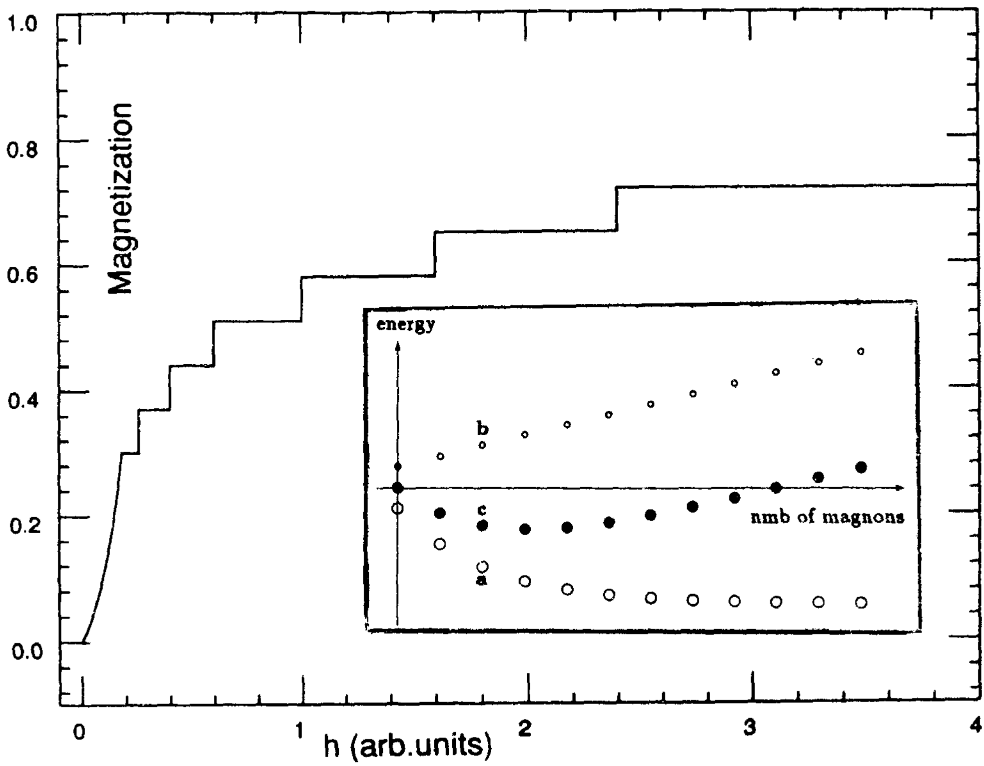

FIG. 1. Magnetization vs magnetic field (shown schematically). Transformation of a step-like behavior to a continuous one is explained in the test. In inset: a) $e_h^{(n)}$ vs n (shown schematically); b) $e_m^{(n)}$ vs n (tangent slope $= 2\text{gm}_B h$); c) $e^{(n)}$ vs n; $e_h^{(0)}$ and $e_m^{(0)}$ are taken arbitrarily. Any exchange interaction between d-spins is ignored.

If a linear size of a hole-magnon polaron is smaller than a hole spacing, then a polaron gas is believed to be weakly interacting. The interaction of composite holes due to the exchange by magnons is strongly suppressed in the case of hole localization by substitutional impurities like Sr in $La_{2-x}Sr_xCuO_4$ at a small Sr concentration.

Reconstruction of a hole polaron structure occurs when the external field reaches one of its critical values h_{cr}, which is accompanied by a change of the magnon number

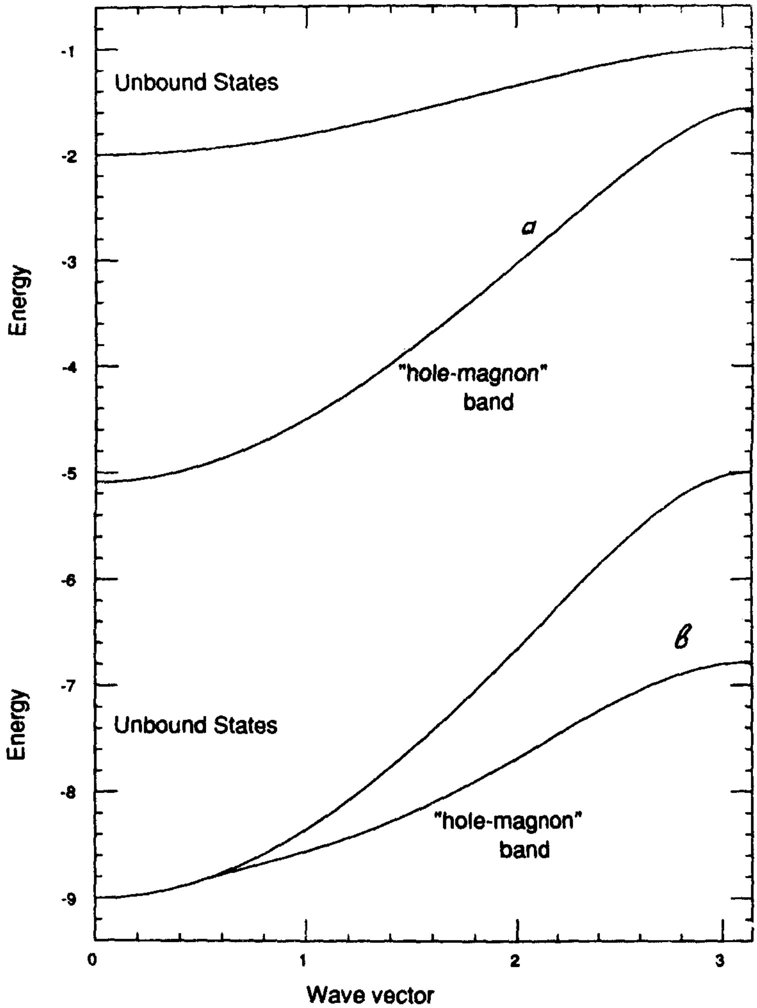

FIG. 2. Energy spectrum of hole + 1 magnon state ($\tau_1 = 1$, $\tau_2 = 0.5$, $\tau_3 = 0.5$). The continuum of unbound states lies above the band of bound states (a, $J = 0.25$). Strong exchange interaction (b, $J = 2$) favors hole-magnon decoupling. The magnon energy is computed as compared with the FM background. The contribution of the Zeemann energy is omitted.

n by unity in each hole polaron. The magnetization-vs-magnetic field curve should exhibit a set of discontinuities. The amplitudes are the same at any h_{cr} and proportional to the hole concentration. A magnetization curve can thus be used to measure the concentration of doped holes. A step-like behavior of magnetization is shown in Fig. 1. Linearly, thermal fluctuations and polaron interaction make the curve in Fig. 1 smoother. Hence, in a sufficiently small magnetic field, when the linear size of a hole-magnon polaron is of the same order of magnitudes larger than the hole spacing, a step-like curve of the magnetization vs magnetic field changes to a smooth curve.

Although the dynamics of absorption (irradiation) of a magnon by a polaron is beyond our interests here, we predict the appearance of giant, probably incoherent, ferromagnetic waves.

So far we have ignored the AFM Heisenberg interaction (4), which changes the magnetic behavior but not radically. First, a FM background is assumed to be stabilized by the finite external field. For a square lattice the field h_F favoring the FM arrangement of d-spins $\frac{1}{2}$ is given by $h_F = 4J/\mu_B$. At the field h above h_F any free magnon has the following excitation spectrum: $E(\mathbf{q}) = \Delta + 4J \times [1 + \frac{1}{2}(\cos q_x + \cos q_y)]$, where $\mathbf{q}$ belongs to the Brillouin cell of d sublattice and $\Delta = 2\mu_B(h - h_F)$ coincides with the tangent slope of curve b (Fig. 1, inset).

Second, there are changes in curve a (Fig. 1, inset) which appears to be well-defined for integer n's limited from above by n_{up}. This occurs because localization of a free FM magnon with a polaron leads to the loss of the exchange energy proportional to J. If the difference $\varepsilon_h^{(n+1)} - \varepsilon_h^{(n)}$ is on the order of the magnon bandwidth, then any new magnon after the nth magnon cannot be captured by a hole and goes into the bulk. Formally, the changes in Fig. 1 are completed if the function $\varepsilon_h^{(n)}$ is assumed to be equal to $\varepsilon_h^{(n_{up}}$ in the "nonphysical" region $(n > n_{up})$. A step-like behavior of the magnetization curve may be observed above h_F. Consisting of n_{up} steps, it is smooth below h_F.

The role of the exchange interaction in restricting the number of magnons captured by a hole is illustrated by the results of numerical calculations. These calculations were performed for the alternative p–d chains which described by the Hamiltonian $H_p + H_d$. The region of stability of hole + 1 magnon bound state can be determined analytically.[2)]

Figure 2b shows the energy gain due to a hole-magnon decoupling which occurs at sufficiently large J. The two-magnon case was investigated by using a simple version of the Lanczos method (for its application to strongly correlated systems see Ref. 6). It is noteworthy that even with a small value of the exchange constant ($J = 0.25$) the loss of energy during decoupling according to the scheme hole + 2 magnons → hole + 1 magnon + free magnon, is very small (cf. Fig. 3).

Below we summarize the results of our study.

1. Two-band systems, like those described by the Emery model, behave unusually if the external field is strong. Magnetization-vs-magnetic field curve displays a set of steps of the same amplitude, which is proportional to the hole concentration.

2. Steps at the magnetization curve disappear at sufficiently small values of the

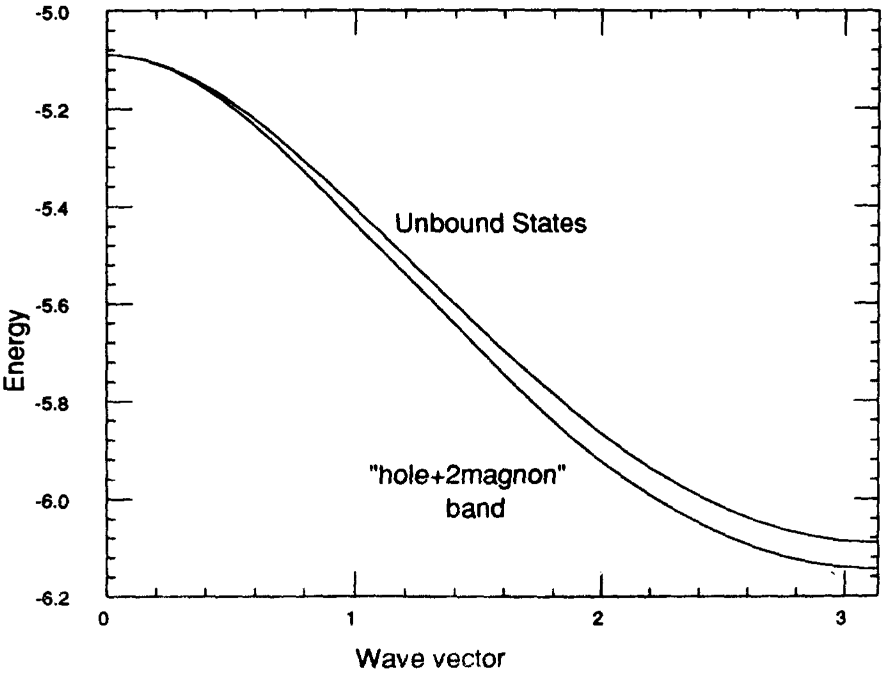

FIG. 3. Hole + 2 magnons ($\tau_1 = 1$, $\tau_2 = 0.5$, $\tau_3 = 0.5$, $J = 0.25$). Unbound states correspond to at least one free magnon.

magnetic field. This occurs either when the external field is less than the exchange field h_F or when the linear size of a hole + magnons polaron exceeds the hole spacing.

3. The exchange interaction favors the escaping of magnons for composite quasi-particles, so the number of captured magnons in a polaron is restricted from above.

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[1)] Our terminology originates with copper oxides, but we have in mind a more general situation.
[2)] For this purpose the equations derived in Appendix A of Ref. 4 can be used with small modification coming from a magnon hopping term.

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