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ON FERMION-MAGNON BOUND STATES IN STRONG MAGNETIC FIELD: ANALYSIS OF THE EXTENDED HUBBARD MODEL

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Numerical calculations of bound state energies of a delocalized fermion and magnons in 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'-Nagaoka behaviour unusual for strongly correlated fermion systems. In the case of a weak doping, when the free fermion interaction can be neglected, the dependence of magnetization on 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 accompaned with giant absorption (irradiation) of magnons. Most likely, the effect discussed below is better to look for in $3d$-compounds with a moderate value of antiferromagnetic exchange constant J.

Recently the experimental discovery of high-T_c superconductivity (SC) invoked a great interest in different versions of a Hubbard model. The crucial prerequisite of high-T_c SC are CuO_2 layers exhibiting antiferromagnetic (AFM) order in Cu sublattice when the doping of holes into the oxygen band is negligible. In this work we discuss properties of strongly correlated fermion systems described by the so-called extended Hubbard model first introduced by Emery [1]. In sufficiently strong magnetic field, near the saturation limit, a doped hole [1)] appears to be in a bound state with a few spin excitations, i.e., magnons on the FM background. This situation is common for several models like $t-t'-J$ model, Kondo-like model, etc. The considered properties are not associated with the subject of SC. Most likely, the effects discussed below cannot be observed in high-T_c SC because of the enormously large value of the exchange field ($J > 0.1eV$).

One of the curious property of the conventional Hubbard model with an infinitely strong on-site repulsion ($U_d \to \infty$) is the Nagaoka phenomenon [2]: a single hole on a half-filled d-band background ($\bar{n}_d = 1$) arranges all the spins ferromagnetically. The energy gain comes from the kinetic energy term favouring the FM background. For large but finite U_d, a competition of the weak AFM interaction and the mentioned above tendency of a hole to create the FM background results in emergence a magnetic polaron. It occupies a finite area, moving after the

[1)] Our terminology originates from copper oxides, but we keep in mind a more general situation hole with spins inside it being arranged ferromagnetically. A conventional AFM background is formed by domains beyond this area.

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

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

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

Here $p^{+}_{r\sigma}, d^{+}_{R\sigma} (p_{r\sigma}, d_{R\sigma})$ are hole (spin projection σ) creation (annihilation) operators on the sites of p- and d-sublattice, denoted by $\vec{r}$ and $\vec{R}$, respectively. We suppose that these sublattices are inserted one into another like in the case of CuO_2 layers. The single hole on-site energies ε_p, ε_d and the on-site Coulomb repulsions U_p, U_d together with the kinetic energy term ($p-d$ hybridization) define one of the simplest version 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 into 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 neighbouring d-holes:

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

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

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

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

The terms entering Hamiltonian (2) are interpreted as a direct p-p hopping term (3rd term), Kondo-like hopping term (1st term) and an AFM p-d exchange (2nd term). The contribution of the fourth order perturbation theory is the AFM exchange interaction H_d between d-holes:

$$H_d = J \sum_{<\vec{R},\vec{R}'>} Z^{\alpha\beta}_{\vec{R}} Z^{\beta\alpha}_{\vec{R}'} \tag{4}$$

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

$$J = \frac{t_{pd}^4}{\varepsilon^2}\left(\frac{4}{2\varepsilon + U_p} + \frac{2}{U_d}\right) \tag{5}$$

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

$Z_{\vec{R}}^{\alpha\beta} Z_{\vec{R}'}^{\beta\alpha} = 2\vec{S}_{\vec{R}}\vec{S}_{\vec{R}'} + \frac{1}{2}$

Glazman and Ioselevich [3] have analysed a ferromagnetic state instability in a special case $U_d \to \infty$, $U_p = 0$ of the Kondo-like model (2). A single p-hole is supposed to move in a well-defined hypothetical FM background of d-holes and be able to be bound to spin excitations (magnons) on this background. In the work [3] a variational approach has been used to calculate the energy spectrum of quasiparticles consisting of a hole and several magnons. The conclusion about a tendency of the bottom of a quasiparticle energy band to low with an increase of the number of magnons looks truthful. 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 p-hole tends to arrange d-spins surrounding it paramagnetically.

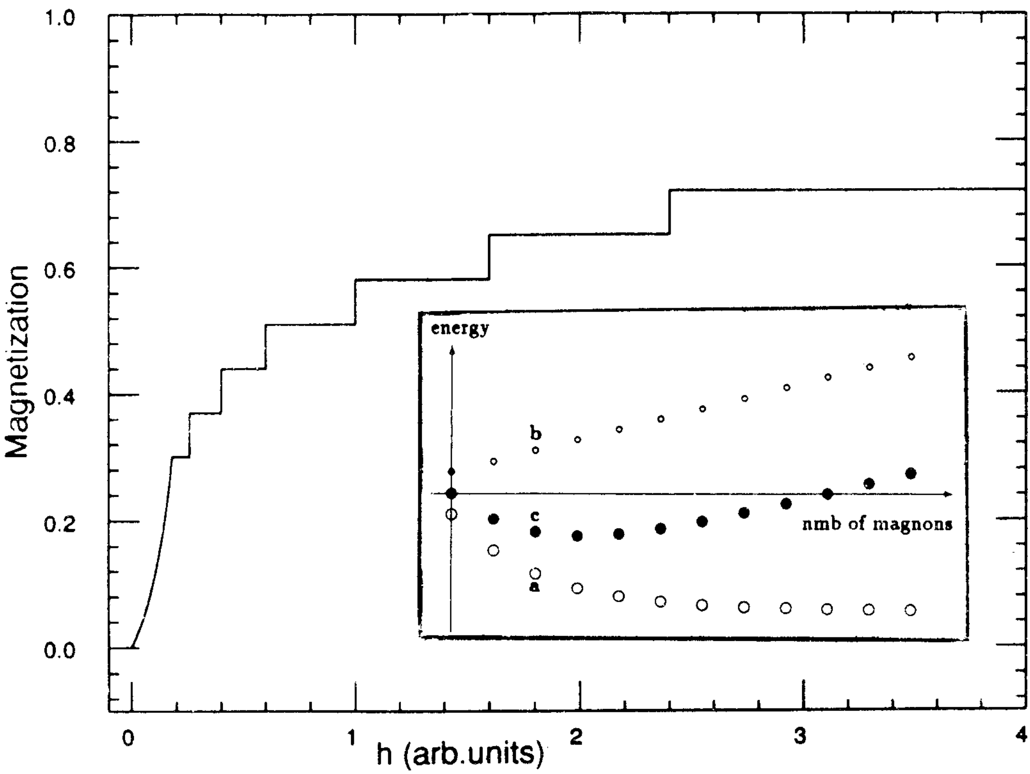

Fig. 1. Magnetization vs magnetic field (shown schematically). Transformation of a step-like behavior to a continuous one is explained in the text. In inset: a) $e_k^{(n)}$ vs n (shown schematically); b) $e_m^{(n)}$ vs n (tangent slope= $2\mu_B h$); c) $e^{(n)}$ vs n; $e_k^{(0)}$ and $e_m^{(0)}$ are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

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 centre. Such an alteration repeats itself with an increasing number of magnons and is accompanied by monotonical lowering the energy of a composite state of p-hole and magnons. Below we denote this energy by $e_h^{(n)}$. Most likely, that $e_h^{(n)}$, decreasing monotonically with n, goes asymptotically (in the thermodynamical limit $n \to \infty$) to the energy level of a 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 above is summarized qualitatively in Fig.1(inset).

If a linear size of a hole-magnon polaron is smaller than a hole spacing, then a polaron gas is beleived to be weakly interacting. The interaction of composite holes owing 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 small Sr concentration.

Reconstruction of a hole polaron structure happens when the external field achieves one of its critical values h_{cr} accompanied by a change of the magnon number n by unity in each hole polaron. Thence, the magnetization vs magnetic field curve should exhibit a set of discontinuities. Their amplitudes are the same at any h_{cr} and proportional to the hole concentration. So, a magnetization curve could be used to measure the concentration of holes under the doping. A step-like behavior of magnetization is shown in Fig.1. Certainly, 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 becomes of the same order or larger than the hole spacing, a step-like behavior of magnetization vs magnetic field changes by smooth one.

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

So far we ignored the AFM Heisenberg interaction (4). It changes a magnetic behaviour but not crucially. *First*, a FM background is assumed to be stabilized by the finite external field. For a square lattice the field h_F favouring 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: $E(\vec{q}) = \Delta + 4J(1 + \frac{1}{2}(\cos q_x + \cos q_y))$, where $\vec{q}$ belongs to the Brillouin cell of d sublattice and $\Delta = 2\mu_B(h - h_F)$ coincides with a tangent slope of the curve **b** (Fig.1,inset).

Second, there are changes in the curve a (Fig.1,inset) which appears to be well-defined for integer n's limited from above by n_{up}. It happens because localization of a free FM magnon within a polaron leads to the loss of the exchange energy proportional to J. So, if the difference $\varepsilon_h^{(n+1)} - \varepsilon_h^{(n)}$ becomes of the order of the magnon bandwidth, then any new magnon after the nth magnon cannot be captured by a hole and goes to the bulk. Formally, the changes in Fig.1 are completed if the function $\varepsilon_k^{(n)}$ is supposed to be equal to $\varepsilon_k^{(n_{up})}$ in the 'non-physical' 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.

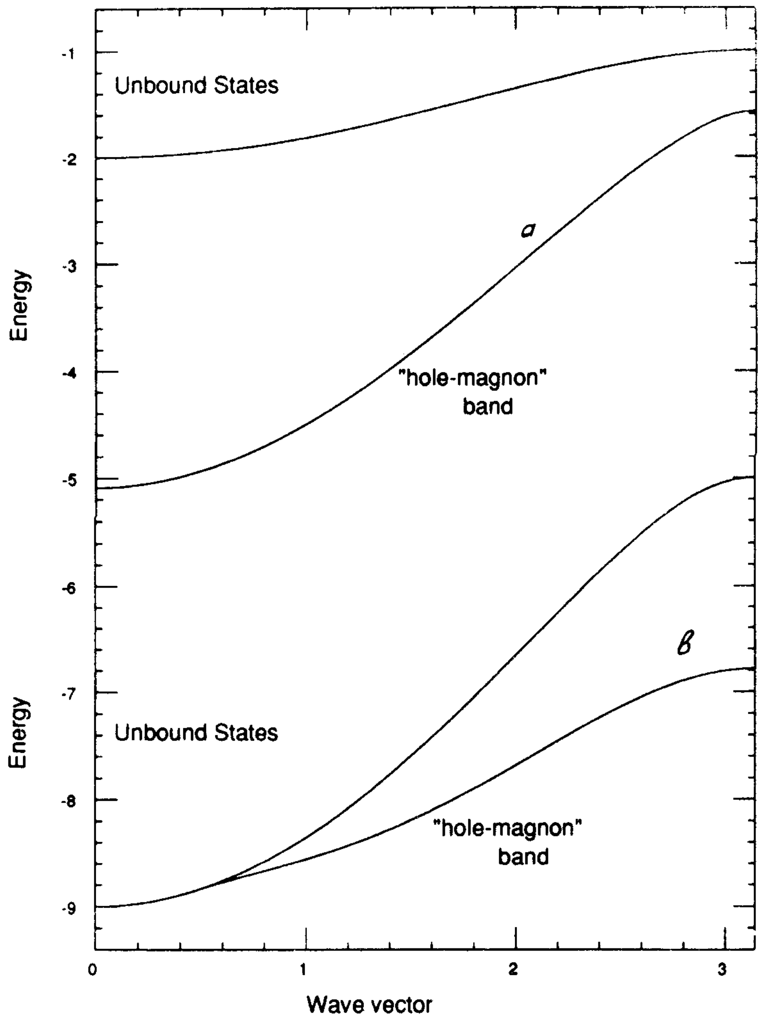

Fig. 2. Energy spectrum of 'hole+1 magnon' bound state ($\tau_1 = 1, \tau_2 = 0.5, \tau_3 = 0.5$). The continuum of unbound states lies above the band of bound states (a, $J = 0.25$). Strong exchage interaction (b, $J = 2$) favours in hole-magnon decoupling. The magnon energy is computed as compared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

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

Fig.2b displays the energy gain due to a hole-magnon decoupling. It happens at sufficiently large J.The two-magnon case has been investigated by means of a simple version of the Lanczos method (for its application to strongly correlated systems see [6]). It is noteworthy that even at the small value of the exchange constant ($J = 0.25$) the loss of energy in the course of decoupling according to the scheme 'hole+2 magnons' → 'hole+1 magnon' + 'free magnon' is very small (cf.Fig.3).

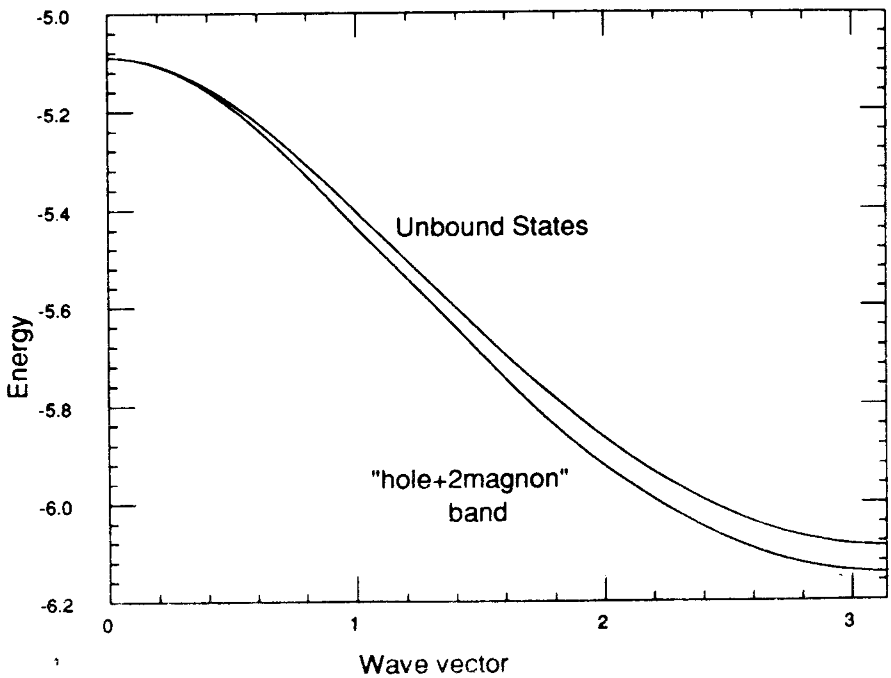

Fig. 3. 'Hole+2 magnons' ($\tau_1 = 1, \tau_2 = 0.5, \tau_3 = 0.5, J = 0.25$). Unbound states correspond to one free magnon at least

Below we resume the results of this work.

1. Two-band systems, like those, described by the Emery model, behave unusually, if the external field is strong. Magnetization vs magnetic field curve should display 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 a magnetic field. It happens 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.

[2)]For this purpose the equations derived in the Appendix A of [4] can be used with small modification coming from a magnon hopping term.

3. The exchange interaction favours the escaping of magnons from composite quasiparticles, so, the number of captured magnons in a polaron is restricted from above.

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