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Partial Localization of Correlated Electrons in an Orbitally Degenerate Narrow Band: Spin Dependent Masses, Saturated Ferromagnetism, and the Effective $s-d$ Model

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We determined the localization threshold in a partially filled and doubly degenerate model of correlated electrons. Particular emphasis is put on a non-integer band filling $n \geq 1$, when the system decomposes into the localized and the itinerant subsystems; this situation is described by *an effective s–d model*. A simultaneous transition to the ferromagnetic state is discussed as driven by the Hund rule coupling combined with the effective field coming from the correlations. The dependence of the quasiparticle mass on the spin direction appears naturally in the spin-polarized phase and is attributed to the electron correlation effects, as is also a metamagnetic transition in an applied field. Although the main results were obtained within the saddle point slave-boson approach, their qualitative features are discussed in general terms, i.e. as a transition from quantum-mechanical indistinguishability of particles forming the Fermi fluid to a two-component situation.

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1. Introduction

The longstanding problem [1] of the dual (*localized-itinerant*) nature of correlated electrons has been recently addressed in the context of heavy-fermion systems

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containing $5f$ states due to U ions and termed *the partial localization* [2]. It appears only when the occupancy n_f of the $5f$ states is a noninteger number and exceeds unity, as is expected for uranium containing compounds, even though a relatively strong hybridization of $5f$ states with $6d{-}7s$ states takes place. Therefore, such a decomposition of the quantum-mechanically indistinguishable electrons into two separate subsystems must be accompanied by a phase transition and attributed to the correlation effects such as the Hund rule exchange interaction, particularly when combined with the direct Coulomb (Hubbard) interaction.

The question arises whether such a decomposition can occur also for $3d$ electrons [3, 4]. This is a legitimate question, since the $s{-}d$ model, involving a mixture of localized and itinerant electrons is invoked ad hoc [5], for example for the semiconducting spinels and the manganites, where inequivalent $3d$ states (for example the $d_{x^2-y^2}$ and d_{z^2} orbitals forming $e_{\rm g}$ orbital doublet) appear.

The *partial localization* has been discussed mainly in the model situations [2–4]. In this paper we would like to discuss specific physical properties related to this phenomenon not discussed in detail so far. Namely, we show first that the transformation into the localized-itinerant mixture is often accompanied by a formation of *saturated ferromagnetic* state, i.e. with one spin orientation of carriers at the Fermi level. Secondly, the spin-direction dependence of the mass enhancement, predicted some time ago [6], and confirmed experimentally very recently [7], for the case of $5f$-electron systems, is estimated numerically to see if such interesting effects are observable also for the itinerant $3d$ magnets. Finally, we provide an exact analytic argument how the orbitally degenerate Hubbard model with the Hund rule coupling included, can be transformed into an effective $s{-}d$ model involving the partial localization.

2. The model

We start from the orbitally doubly degenerate version of the Hubbard model containing inequivalent, but spatially isotropic, hopping integrals, $t_{ijl} = t_l$, with the orbital index $l = 1$ or 2. This means that the starting system Hamiltonian is of the form

$$\mathcal{H} = \sum_{\langle i,j\rangle,\sigma}\sum_{l=1}^{2} t_l a^{\dagger}_{il\sigma} a_{jl\sigma} - 2J\sum_i \left(\boldsymbol{S}_{i1}\cdot\boldsymbol{S}_{i2} + \frac{3}{4}\hat{n}_{i1}\hat{n}_{i2}\right) + U\sum_{i,l}\hat{n}_{il\uparrow}\hat{n}_{il\downarrow} + (U-J)\sum_i \hat{n}_{i1}\hat{n}_{i2} - 2\sum_{i,l} S^z_{il}h. \tag{1}$$

In this Hamiltonian the first term is the hopping term, the second expresses the complete form of intraatomic interorbital exchange (the Hund rule coupling), the third describes intraatomic intraorbital Coulomb term (the Hubbard term), the fourth describes the intraatomic interorbital Coulomb term with $n_{il} = \sum_\sigma n_{il\sigma}$ being the number of electrons on site i and orbital l, whereas the last term represents the effect of the external magnetic field. The summation $\langle i,j\rangle$ denotes that over the nearest neighboring sites i and j.

2.1. Slave-boson approach

The method we use is the auxiliary (slave) boson approach, in which each K-particle state on site i is labeled with a boson field $\beta^{(K)\dagger}_{i,l_1\sigma_1,\ldots,l_K\sigma_K}$. In effect, the physical K-electron state located on that site assumes the form

$$|i,l_1\sigma_1,\ldots,l_K\sigma_K\rangle = \prod_{m=1}^{K} a^{\dagger}_{il_m\sigma_m}|0\rangle = \beta^{(K)\dagger}_{i,l_1\sigma_1,\ldots,l_K\sigma_K}\prod_{m=1}^{K} f^{\dagger}_{il_m\sigma_m}|v\rangle, \tag{2}$$

where $|v\rangle$ is the auxiliary vacuum state and $f^{\dagger}$ represents the pseudofermion creation operator. The new Fock space contains states which have no physical meaning. To get rid of them, we have to take into account the following constraints:

$$\sum_{K=0}^{4}\sum_{I_K}\beta^{(K)\dagger}_{i,I_K}\beta^{(K)}_{i,I_K} = 1_i, \tag{3}$$

$$\hat{n}_{il\sigma} = f^{\dagger}_{il\sigma}f_{il\sigma} = \sum_{K=1}^{4}{\sum_{I_K}}'\beta^{(K)\dagger}_{i,I_K}\beta^{(K)}_{i,I_K}, \tag{4}$$

where $I_K = \{l_1\sigma_1,\ldots,l_K\sigma_K\}$ is a multi-index, and primed summation is taken over configurations with (l,σ) state occupied. The first constraint ensures the completeness condition of the basis vector set on each site, the second expresses the equivalence of counting the electrons in terms of either fermions or bosons. This representation was introduced some time ago [8, 9]. It has a drawback in the sense that it does not reproduce the spin-flip part of the full Hund-rule term through the slave bosons [10, 11]. Thus, within this method we can include only the Ising part of that term. In other words, we start not from the full form of the Hamiltonian (2), but from its simplified form without the spin-flip term. In effect, we can rewrite (2) in the form

$$\begin{aligned}\mathcal{H} = &\sum_{\langle i,j\rangle,\sigma}\sum_{l=1}^{2} t_l a^{\dagger}_{il\sigma}a_{jl\sigma} + U\sum_{i,l}\hat{n}_{il\uparrow}\hat{n}_{il\downarrow}\\ &+\sum_{i,\sigma}(U_{\mathrm{a}}\hat{n}_{i1\sigma}\hat{n}_{i2\bar{\sigma}} + U_{\mathrm{p}}\hat{n}_{i1\sigma}\hat{n}_{i2\sigma}) + H_Z.\end{aligned} \tag{5}$$

Here $U_{\mathrm{a}} = U - 2J$, $U_{\mathrm{p}} = U - 3J$, $H_Z = -2\sum_{i,l} S^z_{il}h$.

The Hamiltonian (4), expressed through the new fermion and boson fields with inclusion of the constraints (2) and (3) via the corresponding Lagrange multipliers and the additional renormalizing factors [8, 9], reads now

$$\begin{aligned}\tilde{\mathcal{H}} = &\sum_{l=1}^{2}\sum_{i,j,\sigma} f^{\dagger}_{il\sigma}(t_l\hat{z}^{\dagger}_{il\sigma}\hat{z}_{jl\sigma} - \sigma h\delta_{ij})f_{jl\sigma} + \sum_{i}\sum_{K=2}^{4}\sum_{I_K}\sum_{a,b} U_{l_a\sigma_a l_b\sigma_b}\beta^{(K)\dagger}_{i,I_K}\beta^{(K)}_{i,I_K}\\ &+\lambda^{(1)}_i\left(\sum_{K=0}^{4}\sum_{I_K}\beta^{(K)\dagger}_{i,I_K}\beta^{(K)}_{i,I_K} - 1_i\right) + \lambda^{(2)}_{il\sigma}\left(f^{\dagger}_{il\sigma}f_{il\sigma} - \sum_{K=1}^{4}\sum_{I_K}\beta^{(K)\dagger}_{i,I_K}\beta^{(K)}_{i,I_K}\right),\end{aligned} \tag{6}$$

where the factor renormalizing the hopping term is

$$\hat{z}_{il\sigma} = \frac{1}{\sqrt{1-\hat{n}_{il\sigma}}} \sum_{K=1}^{4} \sum_{\tilde{I}_{K-1}} \beta_{i\tilde{I}_{K-1}}^{\dagger(K-1)} \beta_{iI_K}^{(K)} \frac{1}{\sqrt{\hat{n}_{il\sigma}}}. \tag{7}$$

The factors $1/\sqrt{1-\hat{n}_{l\sigma}}$ and $1/\sqrt{\hat{n}_{l\sigma}}$ ensure the proper Hartree–Fock limit value of $\hat{z}_{l\sigma}$ [8, 9]. The Hamiltonian in the form (5) is used next to construct the partition function expressed as a functional integral over coherent states of the Fermi and Bose fields, in a standard manner [12]. This integral, however, cannot be handled directly, as only bilinear fermionic part can be integrated out exactly. To proceed further, an approximation scheme must be developed. We shall use the saddle--point (mean-field) approximation for the Bose fields (their mean-field amplitudes are defined in Table, and the new labeling of the electron configurations is explicitly specified).

TABLE

Site configurations with $K = 1, \ldots, 4$ electrons and their slave-boson (SB) labeling.

Configuration representation	SB representation	Mean-field value of the Bose field
$\|0\rangle$	$e^{\dagger}\|v\rangle$	e
$\|l\sigma\rangle$	$f_{l\sigma}^{\dagger} p_{l\sigma}^{\dagger}\|v\rangle$	$p_{l\sigma}$
$\|l\uparrow l\downarrow\rangle$	$f_{l\uparrow}^{\dagger} f_{l\downarrow}^{\dagger} d_{l}^{\dagger}\|v\rangle$	d_l
$\|1\sigma 2\sigma\rangle$	$f_{1\sigma}^{\dagger} f_{2\sigma}^{\dagger} d_{\sigma}^{\dagger}\|v\rangle$	d_σ
$\|l\sigma\bar{l}\bar{\sigma}\rangle$	$f_{1\sigma}^{\dagger} f_{2\bar{\sigma}}^{\dagger} w_{\sigma}^{\dagger}\|v\rangle$	w_σ
$\|l\bar{\sigma}\bar{l}\sigma\bar{l}\bar{\sigma}\rangle$	$f_{l\bar{\sigma}}^{\dagger} f_{\bar{l}\sigma}^{\dagger} f_{\bar{l}\bar{\sigma}}^{\dagger} t_{l\sigma}^{\dagger}\|v\rangle$	$t_{l\sigma}$
$\|1\uparrow 1\downarrow 2\uparrow 2\downarrow\rangle$	$f_{1\uparrow}^{\dagger} f_{1\downarrow}^{\dagger} f_{2\uparrow}^{\dagger} f_{2\downarrow}^{\dagger} q^{\dagger}\|v\rangle$	q

2.2. The saddle-point approximation

In the saddle-point approximation all the Bose fields are approximated by their expectation values. This means that the operator quantities $\hat{z}_{il\sigma}$ ($\hat{z}_{il\sigma}^{\dagger}$) reduce to the site-independent real numbers $z_{l\sigma}$, which renormalize the bare hopping integrals t_l and make them explicitly spin-dependent. In result, in the spin-polarized state the effective masses of quasiparticles represented by the pseudo-fermion fields become also spin-dependent. We assume also a rectangular (featureless) form of (bare) density of states in both bands

$$\rho_l(\epsilon) = \frac{1}{W_l} \theta\left(\frac{W_l}{2} - |\epsilon|\right), \tag{8}$$

where θ is the Heaviside step function, and W_l is the bare band width of the l-th band. In what follows we take the limit of zero temperature. Those assumptions allow us to find a closed, analytic expression for the ground-state energy function (per site) of the system, which has the following form:

$$E = -\sum_{l,\sigma} \frac{W_l}{2}$$
$$\times (e p_{l\sigma} + d_l p_{l\bar{\sigma}} + d_\sigma p_{\bar{l}\sigma} + w_{\sigma(l)} p_{\bar{l}\bar{\sigma}} + w_{\bar{\sigma}(l)} t_{\bar{l}\bar{\sigma}} + d_{\bar{l}} t_{l\bar{\sigma}} + d_{\bar{\sigma}} t_{\bar{l}\sigma} + t_{l\sigma} q)^2$$
$$+ \sum_l U_l d_l^2 + U_{\mathrm{a}} \sum_\sigma w_\sigma^2 + U_{\mathrm{p}} \sum_\sigma d_\sigma^2 + \sum_{l,\sigma} (U_{\bar{l}} + U_{\mathrm{a}} + U_{\mathrm{p}}) t_{l\sigma}^2$$
$$+ \left(2U_{\mathrm{a}} + 2U_{\mathrm{p}} + \sum_l U_{\bar{l}} \right) q^2 - \sigma h \sum_l n_{l\sigma}. \tag{9}$$

However, one has to keep in mind that variables in (8) are not independent. First, we write down the mean-field version of the constraints (2) and (3), which are

$$1 = e^2 + \sum_{l,\sigma} (p_{l\sigma}^2 + t_{l\sigma}^2) + \sum_l d_l^2 + \sum_\sigma (w_\sigma^2 + d_\sigma^2) + q^2, \tag{10}$$

and

$$n_{l\sigma} = p_{l\sigma}^2 + d_l^2 + d_\sigma^2 + w_{\sigma(l)}^2 + t_{l\sigma}^2 + t_{l\bar{\sigma}}^2 + t_{\bar{l}\bar{\sigma}}^2 + q^2, \tag{11}$$

where $n_{l\sigma} = \langle f_{il\sigma}^\dagger f_{il\sigma} \rangle$. The squares of the corresponding mean-field amplitudes have the interpretation of probabilities of finding the respective electron configurations. It is the total number of electrons per site, $n = \sum_{l\sigma} n_{l\sigma}$, which is fixed. Thus, when minimizing E we use the following constraint for the band filling:

$$n = \sum_{l,\sigma} (p_{l\sigma}^2 + 3t_{l\sigma}^2) + \sum_l 2d_l^2 + \sum_\sigma (2w_\sigma^2 + 2d_\sigma^2) + 4q^2. \tag{12}$$

Let us note that the Lagrange multipliers do not appear in (8) explicitly, as they are now expressed through the bosonic fields. The functional dependence of the energy on the values of $e, p_{l\sigma}, \ldots, q$ leads to the result similar to those obtained earlier by means of the Gutzwiller ansatz. The quasiparticle mass enhancement is connected to the band narrowing factor $q_{l\sigma} \equiv z_{l\sigma}^2$ by the relation [6]

$$\frac{m_{l\sigma}^*}{m_l} = \frac{1}{q_{l\sigma}}, \tag{13}$$

where m_l is the bare (band) mass in the l-th band, and

$$q_{l\sigma} = (e p_{l\sigma} + d_l p_{l\bar{\sigma}} + d_\sigma p_{\bar{l}\sigma} + w_{\sigma(l)} p_{\bar{l}\bar{\sigma}} + t_{\bar{l}\bar{\sigma}} w_{\bar{\sigma}(l)} + d_{\bar{l}} t_{l\bar{\sigma}} + d_{\bar{\sigma}} t_{\bar{l}\sigma} + t_{l\sigma} q)^2$$
$$/ n_{l\sigma}(1 - n_{l\sigma}) \equiv \gamma_{l\sigma} / n_{l\sigma}(1 - n_{l\sigma}), \tag{14}$$

where the equation defines also the quantity $\gamma_{l\sigma}$, which we refer to as the reduced band narrowing factor. Hence, the mass enhancement factor is spin-dependent in either ferromagnetic metallic (FM) state or in paramagnetic metallic (PM) state in an applied magnetic field. It is pronounced close to the PM→FM phase transition, as discussed below. The ground-state properties of the correlated Fermi liquid are determined, when E is minimized with respect to all Bose fields and with self-consistently adjusted position of the chemical potential for a given band filling n and for the fixed values of parameters: the band widths W_l and the inter-

action parameters U and J, where here we take that $J = 0.25U$. We also assume that $W_1 = 4$, $W_2 = 2$.

3. Discussion of results

In this section we discuss the results obtained by the numerical minimization of the ground-state energy function (8). First, we minimize E with respect to all sixteen slave-field amplitudes, with the constraints (9) and (11) included. This allows us to determine both the ferromagnetic and the paramagnetic solutions. Because the E function has the obvious symmetry with respect to the spin index reversal, we add the symmetry-breaking constraint $n_\uparrow - n_\downarrow \geq 0$ to single out one of the two ferromagnetic minima. However, minimization in the full 16-dimensional parameter space is not always an easy task, especially near the paramagnetic–ferromagnetic phase transition, where those two minima become degenerate. Hence, we restrict a posteriori number of variables by putting some of them equal to zero in accordance with the results of the full minimization procedure. This allows us to improve the numerical accuracy of the obtained solutions.

3.1. Integer band filling, n = 1 and 2

Let us consider first the case of half-filling, $n = 2$, discussed intensively recently by many authors [4] in the context of *orbitally-selective Mott transition* in $Ca_{2-x}Sr_xRuO_4$ system. In Fig. 1 we have plotted the band narrowing factor $q_{l\sigma}$, including, respectively, only the paramagnetic states in the half-filled case (top), and with the ferromagnetic states included for the quarter-filled band case (bottom). In the former case the electrons in the narrower band can become localized in a continuous manner at the critical interaction magnitude $U_{c2} = 3.4$, whereas those in the wider band are still itinerant and localize via first-order transition for $U_{c1} = 3.56$. The intermediate region is then called *partially localized* (PL) phase. Let us note that all displayed phases are of paramagnetic character (no ferromagnetic solution has been found stable). These results are very similar to those of Rüegg et al. [4], but differ from those of van Dongen et al. [4] obtained within quantum Monte Carlo — dynamic mean-field theory (QMC-DMFT) method, where the character of the phase transitions is different.

Next, we examine the quarter-filled case, i.e. $n = 1$ (cf. Fig. 1, bottom), showing the band narrowing factor $q_{l\sigma}$. For this particular situation, the system transforms with the increasing U first discontinuously into an FM state, with the electrons in the narrower band being fully polarized. The wider band is then partially polarized, unlike in the equivalent-band model, with the orbital ordering included [11]. By increasing U further we observe a disappearance of the minority-spin electrons in the wider band, as the system undergoes a transition to the saturated ferromagnetic metallic (SFM) phase. For sufficiently high U, electrons in both bands localize simultaneously, forming ferromagnetic insulating (FI) state. The SFM/FI phase boundary point located at $U/5 = 4.8$ in the lower

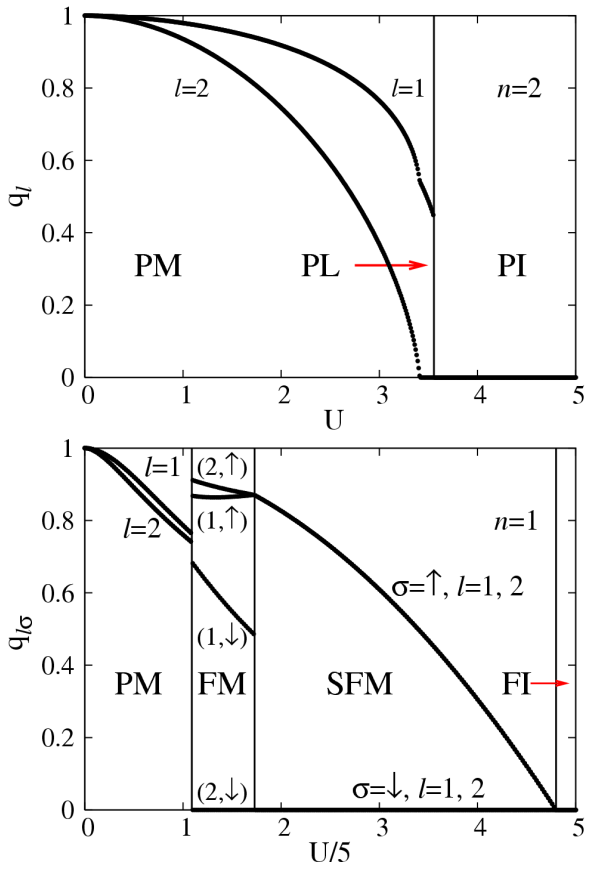

Fig. 1. (top) U dependence of the band-narrowing factors q_1 and q_2, for the half--filling. The phases considered are PM and paramagnetic insulating (PI) as well as the PL phase (see the main text). (bottom) The corresponding plot of $q_{l\sigma}$ for the quarter filling. The phase transitions to the FM, SFM, and FI phases are marked by the vertical lines.

part represents a *quantum critical point*. One should note that SFM–FI phase boundary located at $U = 24$, is quite analogous to the original *Brinkman–Rice quantum critical point* occurring in the nondegenerate band, except that now the transition takes place between the ferromagnetic states. In the present situation the orbital index $l = 1, 2$ replaces the spin quantum number for the nondegenerate case. Explicitly, only the variables $e = d_\uparrow \equiv x$, $p_{1\uparrow}$, and $p_{2\uparrow}$ have non-zero values in SFM state. Thus, we can write down the ground-state energy function E (per site) of SFM state in the following analytic form:

$$E = -Wx^2(1 - 2x^2) + (U - 3J)x^2, \tag{15}$$

where $W = (W_1 + W_2)/2$. This expression is formally identical with that for the single-band case [13]. Minimizing E with respect to x^2, we obtain the physical

ground-state characteristics

$$E = E_{\mathrm{G}} = -\frac{W}{4}\left(1 - \frac{U - 3J}{2W}\right)^2, \tag{16}$$

and

$$q_{l\uparrow} = 1 - \left(\frac{U - 3J}{2W}\right)^2. \tag{17}$$

Equation (16) provides the justification for the corresponding parabolic dependence of $q_{l\uparrow}$ in the SFM state, as shown in Fig. 1 (bottom).

3.2. Partially filled case: n = 1.1 and 1.9

For the band filling slightly larger than 1.0, e.g. for $n = 1.1$, localization in both bands is not possible, as now obviously some double occupancies must be

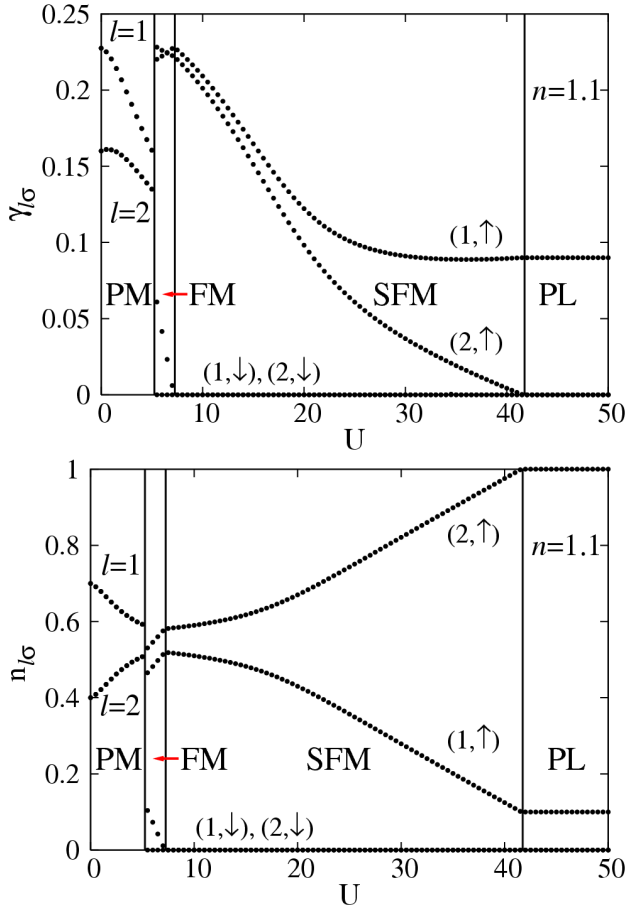

Fig. 2. (top) U-dependence of the reduced band narrowing factor $\gamma_{l\sigma} = q_{l\sigma} n_{l\sigma} \times (1 - n_{l\sigma})$. (bottom) The band occupancies versus U, for $n = 1.1$. The phases and the corresponding boundaries are separated by the vertical lines.

present for an arbitrarily high value of U to fulfill the constraint (11). Guided by the experience gained from the $n = 1$ case, we can make a conjecture about the character of the ground state in the present situation. Thus, with the increasing U we expect that the system should undergo a transition from PM to a ferromagnetic state. This ferromagnetic state, in turn, should become saturated (SFM state) for high enough U resulting in a state of the same kind as that in the ($n = 1$) case. That is, only the variables e, $d_\uparrow$, $p_{1\uparrow}$, and $p_{2\uparrow}$ have non-zero values in this state. However, as now $d_\uparrow^2 - e^2 = 0.1 \neq 0$, we expect that for sufficiently high $U = U_c$ we find $e = 0$, in order to minimize the Coulomb repulsion, and then E is minimized for $p_{1\uparrow} = 0$. Thus, for $U > U_c$ electrons in the narrower band localize, resulting in a simple PL phase, for which all the variables except $d_\uparrow$ and $p_{2\uparrow}$ have non-zero values. In other words, electrons in the narrow band are localized and that band is fully occupied, forming a spin background for itinerant ($1\uparrow$) quasiparticles. Those predictions are confirmed by the detailed numerical analysis. In Fig. 2, top, we have plotted the reduced band narrowing factor $\gamma_{l\sigma}$ instead of $q_{l\sigma}$, as its value is well defined for values of $n_{l\sigma}$ close to zero or unity. In the bottom part of Fig. 2 we have plotted the corresponding occupation numbers. Interestingly enough, we see that, firstly, the FM phase exists in a relatively narrow interval of U, and, secondly, that the SFM–PL transition occurs for rather high value of $U_c \approx 41.5$.

The results obtained for $n = 1.0$ and $n = 1.1$ suggest that for large U the ground state of the system is ferromagnetic. However, with the increasing band filling the character of this state changes as for $n \to 2$ it is no longer favorable as a non-zero value of e should be retained.

Next, we analyze the situation for the band filling $n = 1.9$ (cf. Figs. 3–6). In Fig. 3, left, we display the energies of paramagnetic metallic (PM) and ferromagnetic solutions, respectively, and show that for $U = 3.4$ we have the

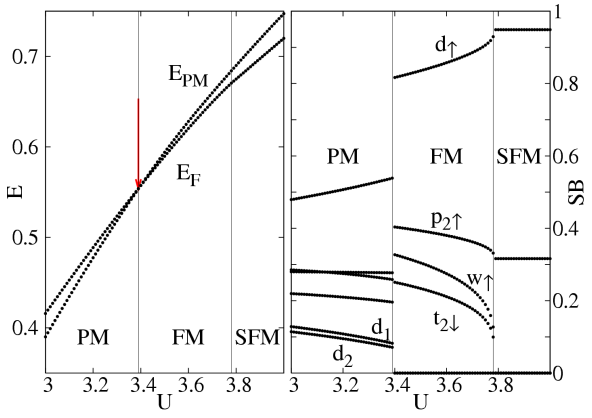

Fig. 3. (left) U dependence of the ground-state energies of PM as well as of ferromagnetic metallic (FM) and saturated ferromagnetic metallic (SFM) solutions. (right) Values of selected slave-boson mean field amplitudes. Phase transitions are marked by the vertical lines.

paramagnetic–ferromagnetic transition. To reveal the nature of those states, let us analyze first the right part of Fig. 3, where some of the slave boson amplitudes are plotted. For $U < 3.4$ we have an ordinary paramagnetic behavior, very much alike in the earlier cases. However, for $3.4 < U < 3.78$ only the variables $p_{2\uparrow}, d_{\uparrow}, w_{\uparrow}$, and $t_{2\downarrow}$ have non-zero values. In other words, we have always one $(2\uparrow)$ electron (forming the spin-background) and one of the four possible configurations for the $l = 1$ orbital. Thus, in this case we also have effectively a one-band behavior, for which in the limit $U > 3.78$ only $p_{2\uparrow}$ and $d_{\uparrow}$ are non-zero, just like for the corresponding PL phase for the $n = 1.1$ case. In this state both $d_1 = d_2 = 0$, even though the system is only partially spin-polarized.

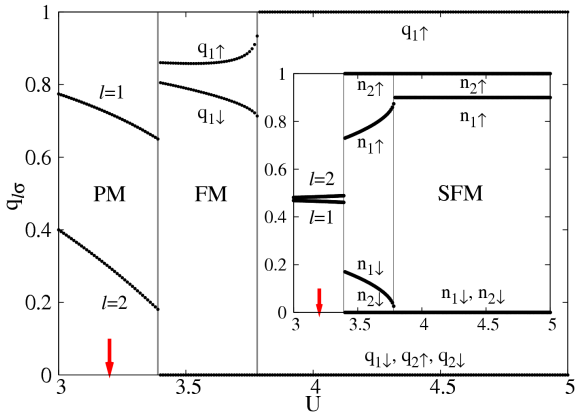

Fig. 4. U dependence of the band narrowing factors $q_{l\sigma}$ for $n = 1.9$. Inset: corresponding occupation numbers. Phase transitions are marked by the vertical lines.

In Fig. 4, we display both the band narrowing factors $q_{l\sigma}$ and the occupancies (cf. the inset). In the PM phase electrons in both bands retain an itinerant character. The PM–F transition represents now also the localization threshold for electrons in the narrower band which becomes completely localized, polarized and forms a spin background with $n_{2\uparrow} = 1$, $n_{2\downarrow} = 0$ (see the inset). Additionally, both the $(1\uparrow)$ and $(1\downarrow)$ electrons remain itinerant for $3.4 < U < 3.78$ composing together with $(2\uparrow)$ electrons a partially localized FM phase, which subsequently transforms into SFM state, where only $(1\uparrow)$ electrons remain itinerant. One should note that the residual $(n-1)$ carriers per site acquire the bare band mass in this state ($q_{1\uparrow} = 1$). This is because the Hubbard interaction vanishes in the SFM state and the hopping is not hampered by the Hund rule interaction.

The PM–FM transition is realized with the increasing amplitude of U. There is however, another possibility, namely, that we can induce it by applying an external magnetic field in the paramagnetic state as shown in Fig. 5. Apart from this transition we expect also that an effective mass of electrons will become then also spin-dependent. To analyze these effects in detail, in Fig. 5 (top part) we have

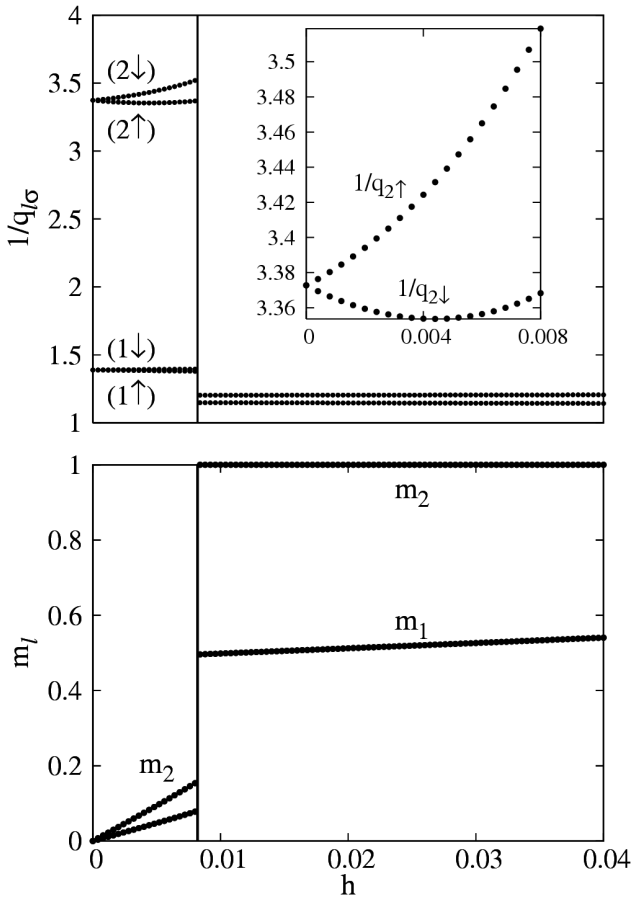

Fig. 5. (top) Applied field-dependent mass enhancements for $n = 1.9$ and $U = 3.2$; (bottom) corresponding orbital dependent spin polarizations ($m_l = n_{l\uparrow} - n_{l\downarrow}$) for both bands. Phase transition is marked by the vertical line. Inset: detailed mass enhancement for the narrower band below the localization threshold.

drawn their enhancement as a function of $h = g\mu_{\mathrm{B}}H_{\mathrm{a}}/2$ for the partially filled-band configuration $n = 1.9$. The masses in the narrower ($l = 2$) band become infinite (i.e. electrons localize) when the system undergoes a *metamagnetic transition* (as shown in the bottom part of the figure). If the model parameter values specified there, are taken in electronovolts, then the metamagnetic field is of the order of 100 T and should diminish fast with $n \to 2$. The ferromagnetic phase is stable even for $n = 1.9$, when the Hund rule is strong enough and overcomes the tendency towards the antiferromagnetism (not discussed here). In the inset to Fig. 5 (top part) we display the masses in the low-field range, and show their nonlinear field dependence. The important feature of the transition in the applied field is that it requires relatively low external perturbation in the range of meV, whereas the

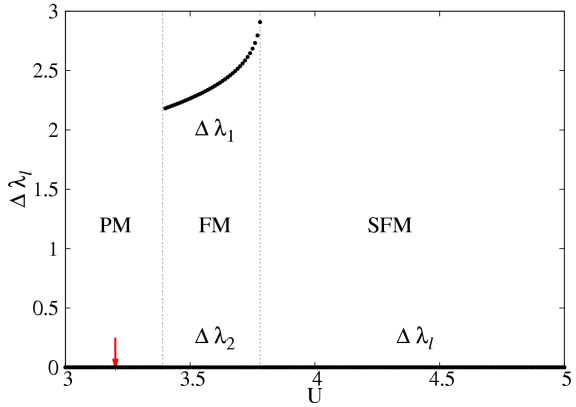

Fig. 6. Plot of $\Delta\lambda_1 \equiv (\lambda_{1\downarrow} - \lambda_{1\uparrow})/J$, $\Delta\lambda_2 \equiv (\lambda_{2\downarrow} - \lambda_{2\uparrow})/J$ vs. U for $n = 1.9$.

corresponding critical interaction U, needed for the transitions displayed in Fig. 2, is in the eV range.

In Fig. 6 we have determined the effective exchange field acting on the correlated electrons. It originates from the explicitly spin-dependent constraint (3), and is related to the Lagrange multiplier $\lambda^{(2)}_{l\sigma}$, defined in (5). Their difference is displayed in Fig. 6 in units of J and as a function of U. One should note that the effective field difference $\Delta\lambda_l \equiv (\lambda^{(2)}_{l\downarrow} - \lambda^{(2)}_{l\uparrow})/J$ is of the order of U. It is this effective field, which in conjunction with the Hund rule interaction stabilizes ferromagnetism in a wide range of the band filling for $n < 2$.

4. Effective *s–d (s–f)* model

From the discussion above a clear division into the localized and itinerant electrons emerges for $1 < n < 2$, when the interaction is strong enough. This division is achieved via a phase transition in which $\sum_{l\sigma} n_{il\sigma}$ electrons per site decomposes into p localized and $n_{i\sigma}$ itinerant particles. We provide now a simple analytic argument and show that in the partially localized situation the model represented by Hamiltonian (2) reduces to an effective $s{-}d$ $(s{-}f)$ model with a proper form of kinetic exchange interactions. The argument is valid for an arbitrary p, but for the present model with the orbital degeneracy $(d = 2)$ $p = 1$.

In order to deal with the interaction terms, in the situation with the localized--itinerant mixture, we use the following identities involving the interaction term in (2):

$$\sum_l \hat{n}_{il\uparrow}\hat{n}_{il\downarrow} = \frac{1}{2}\sum_{l\sigma}\hat{n}_{il\sigma} - \frac{2}{3}\sum_l \boldsymbol{S}^2_{il\uparrow}, \tag{18}$$

$$\sum_{l\neq l';\sigma\sigma'} \hat{n}_{il\sigma}\hat{n}_{il'\sigma'} = \left(\sum_{l\sigma}\hat{n}_{il}\right)^2 - 2\sum_l \hat{n}_{il\uparrow}\hat{n}_{il\downarrow} - \sum_{l\sigma}\hat{n}_{il\sigma}, \tag{19}$$

and

$$\sum_{l\neq l'} \boldsymbol{S}_{il}\cdot\boldsymbol{S}_{il'} = \left(\sum_{l}\boldsymbol{S}_{il\uparrow}\right)^2 - \sum_{l}\boldsymbol{S}^2_{il\uparrow}. \tag{20}$$

Next, we make the decomposition $\sum_l \boldsymbol{S}_{il} = \boldsymbol{S}_i + \boldsymbol{s}_i$, with $\boldsymbol{S}_i^2 = \frac{\boldsymbol{p}}{2}(\frac{\boldsymbol{p}}{2}+\boldsymbol{1})$. This means that we have subdivided the total spin into the conserved (localized) and the itinerant parts. Employing this rule, taking into account also that $\sum_l n_{il\sigma} = p + n_{i\sigma}$, and projecting out the double occupancies in the localized Mott state, one obtains up to a constant

$$\mathcal{H} = \sum_{ij\sigma} t_{ij1} a^\dagger_{i\sigma} a_{j\sigma} - 2J\sum_i \boldsymbol{S}_i\cdot\boldsymbol{s}_i + \sum_i U\hat{n}_{i1\uparrow}\hat{n}_{i1\downarrow} + \mathcal{H}_{\rm ex}, \tag{21}$$

where t_{ij1} is the larger of the two hopping integrals. The hopping in the narrower band vanishes at the localization threshold because we have then $n_{i2\uparrow}+n_{i2\downarrow}=1$ and therefore, $a^\dagger_{i2\sigma}a_{j2\sigma} = a^\dagger_{i2\sigma}(1-\hat{n}_{i2\bar{\sigma}})a_{j2\sigma}(1-\hat{n}_{j2\bar{\sigma}}) = 0$. Also, $\mathcal{H}_{\rm ex}$ contains the kinetic exchange interaction in the localized states (band 2). It has the following form [14]:

$$\mathcal{H}_{\rm ex} = \sum_{\langle i,j\rangle}\left(\frac{t^2_{ij2}}{U} + \frac{t^2_{ij2}}{U+J}\right)\left(\boldsymbol{S}_i\cdot\boldsymbol{S}_j - \frac{1}{4}\right). \tag{22}$$

Obviously, this simple form of the effective Hamiltonian is still orbital-dependent, since only a part of the electrons (that in a narrower band) localizes. It has the form of $s{-}d$ ($s{-}f$) Hamiltonian with the Hubbard interaction among the remaining itinerant electrons. Actually, in the case $n = 1.9$, shown in Fig. 6, the double occupancy $d_1^2 \to 0$, when electrons in the narrower band localize. In that situation, the itinerant electrons become also strongly correlated, i.e. represented by the effective Hamiltonian with the projected out double occupancies also for the itinerant states, namely

$$\mathcal{H} = t_1\sum_{\langle ij\rangle\sigma} a^\dagger_{i1\sigma}(1-\hat{n}_{i1\bar{\sigma}})a_{j1\sigma}(1-\hat{n}_{j1\bar{\sigma}}) - 2J\sum_i \boldsymbol{S}_i\cdot\boldsymbol{s}_i + \mathcal{H}'_{\rm ex}, \tag{23}$$

where $\mathcal{H}'_{\rm ex}$ has now a more complicated structure, which will not be discussed in detail here.

One should note that in this regime the natural limit is to be $|t_2| \approx J$, in which the $s{-}d$ exchange may become comparable to the kinetic exchange, since the strong *double exchange* interaction sets in [15]. This may lead to ferromagnetism well beyond $n = 1$ situation, but this topic should be analyzed separately.

5. Conclusions

The mixed (localized+itinerant) nature of the correlated quantum--mechanically indistinguishable electrons has been discussed for the case of a doubly degenerate narrow band. It is connected with the assumed difference in band width, $W_1 \neq W_2$. The breakdown of the particle indistinguishability is accomplished through a phase transition. This indistinguishability breakdown takes the extreme form in the limit of PL, where $m_{2\uparrow} = m_{2\downarrow} = \infty$ and $m_{1\uparrow} \neq m_{1\downarrow} < \infty$.

The two transitions shown in Fig. 1 (top part) for the case of the half-filled band can be tested by applying the pressure in the case of appropriate Mott insulating system. Also, the properties obtained here should be tested further on a model involving realistic orbitals, including the orbital ordering, as well as the antiferromagnetism. The most stringent test for the existence of PL state should come from the situation involving the hybridized orbitals. The inclusion of the hybridization (i.e. of the hopping $t_{ij}^{ll'}$ with $l \neq l'$) would allow us to study the intermediate situation between the heavy fermion limit ($t_2 = 0, t^{12} \neq 0$, with atomic degeneracy lifted) and the present situation (with $t_2 \neq 0, t^{12} = 0$). Also, the situation in an anisotropic system modeled by, e.g., doubly degenerate band of e_{g} type should be considered in detail.

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