Density-of-states picture and stability of ferromagnetism in the highly correlated Hubbard model

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The problem of stability of saturated and nonsaturated ferromagnetism in the Hubbard model is considered in terms of the one-particle Green's functions. Approximations by Edwards and Hertz and some versions of the self-consistent approximations based on the $1/z$ expansion are considered. The account of longitudinal fluctuations turns out to be essential for description of the nonsaturated state. The corresponding pictures of density of states are obtained. "Kondo" density-of-states singularities owing to spin-flip processes are analyzed. The critical electron concentrations for instabilities of saturated ferromagnetism and paramagnetic state are calculated for various lattices. Drawbacks of various approximations are discussed. A comparison with the results of previous works is performed.

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I. INTRODUCTION

The problem of ferromagnetic ordering in narrow energy bands has been extensively discussed. Despite the large number of publications on the topic, the magnetism of highly correlated electronic systems described by the Hubbard model[1] remains at the center of attention.[2–11] Physically, in this case, the picture of magnetism is characterized by the existence of local magnetic moments and differs substantially from the Stoner picture of a weak itinerant magnetism.[12]

According to Nagaoka,[13] in the limit of infinite Hubbard repulsion the ground state for simple lattices is a saturated ferromagnetic state for a low density δ of charge carriers (doubles or holes in an almost half-filled band). In particular, Nagaoka rigorously proved the existence of a saturated ferromagnetic state for a single hole at $U\rightarrow\infty$ and found the instability of the spin-wave spectrum in the case with increasing δ and decreasing U.

Roth[14] applied a variational principle to this problem and obtained two critical concentrations. The first one δ_c corresponds to the instability of the saturated ferromagnetic state, and the second one δ_c', to the transition from the nonsaturated ferromagnetic into the paramagnetic state. For the simple cubic (sc) lattice, the values $\delta_c=0.37$ and $\delta_c'=0.64$ were obtained. Next, the region of stability of the saturated ferromagnetic was investigated within various approximations in numerous works (see, e.g., Refs. 16–30).

An interpolational approach to description of magnetic ordering in narrow bands, which yields saturated ferromagnetism for small δ and nonsaturated ferromagnetism for large δ, was developed in Refs. 31 and 32 on the basis of dynamic magnetic susceptibility treatment. However, the critical concentrations themselves were not determined.

Using high-temperature expansions in early papers[5,6,23,33,34] yielded nonstable results concerning the stability of ferromagnetism because of poor accuracy connected with slow convergence.[19] However, according to recent results,[5,6] ferromagnetism also occurs near $\delta=0.3$.

It should be noted that the hole concentration $\delta=1/3$ corresponds to the sign change of the chemical potential in the Hubbard-I approximation[1] in the case of a symmetric conduction band and instability of the paramagnetic state can occur at this point in some simple approximations.[2] The same critical values are obtained in the modern DMFT calculations for the hypercubic lattice.[10,15]

Experimental data on $Fe_{1-x}Co_xS_2$,[16] a system with strong correlations, give large values of δ_c (saturation ferromagnetism is preserved up to conduction electron concentrations $n=1-\delta$ of order 0.2), but degeneracy effects in the conduction band appear to be important in this system.

The approaches mentioned do not analyze as a rule in detail the structure of the one-particle excitation spectrum in the ferromagnetic phase of the Hubbard model. The simplest "Hubbard-I" result[1] for the electron spectrum corresponds to the zeroth order in the inverse nearest-neighbor number $1/z$. This is a kind of "mean-field" approximation in the electron transfer (however, it does not coincide with the limit of infinite space dimensionality treated in DMFT). The Hubbard-I approximation is quite nonsatisfactory at describing ferromagnetism (in particular, ferromagnetic solutions are absent, except for peculiar models of bare density of states).

A consistent calculation of the one-particle Green's functions in the case of small δ (almost half-filled band) and low temperatures was performed in Refs. 35 and 36. The results demonstrated an important role of nonquasiparticle (incoherent) states in the density-of-states picture. Expressions for the one-particle Green's functions in a more wide region of δ and T were obtained in Ref. 37.

A physically transparent mechanism of instability of saturated ferromagnetic state was treated in detail in the works by Edwards and Hertz.[18] This mechanism is connected with occurrence of spin-polaron states above the Fermi level of the charge carriers.

In this paper, the stability of the saturated ferromagnetic state as the charge carrier concentration is raised is studied using the one-particle Green's functions of first order in $1/z$ and corresponding self-consistent approximations. This approach makes it possible to construct a rather simple and physically transparent picture of the density of states in a saturated Hubbard ferromagnet. At the same time, the problem of description of nonsaturated state is much more difficult, but our approach turns out to be successful too.

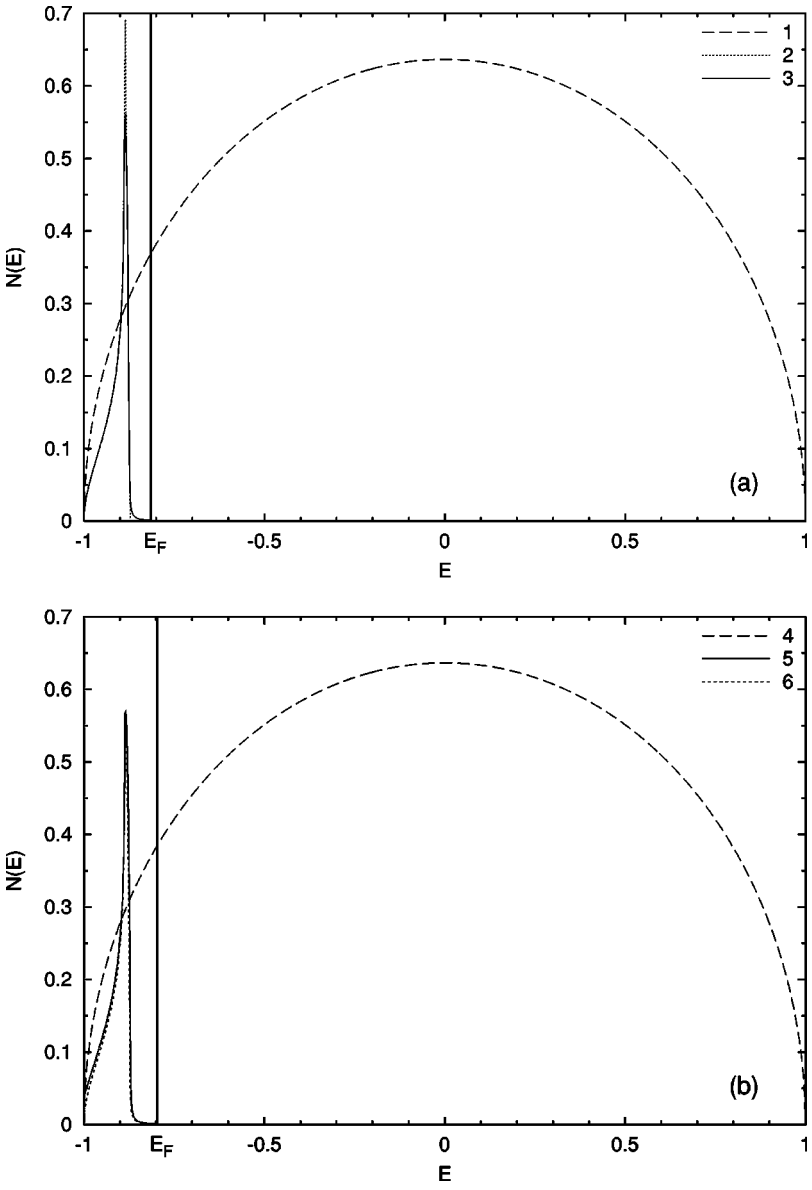

FIG. 1. Density of states for the bare semielliptic DOS at concentration of carriers current $\delta = 0.02$. (a) Lines 1 ($\sigma=\uparrow$) and 2 ($\sigma=\downarrow$) correspond to the non-self-consistent approximation (9); lines 1 ($\sigma=\uparrow$) and 3 ($\sigma=\downarrow$) to the non-self-consistent approximation with account of spin dynamics (20); (b) lines 4 ($\sigma=\uparrow$) and 5 ($\sigma=\downarrow$) correspond to the self-consistent approximation (17), and lines 4 ($\sigma=\uparrow$) and 6 ($\sigma=\downarrow$) to the Edwards-Hertz approximation (24).

II. CALCULATION OF THE ONE-PARTICLE GREEN'S FUNCTIONS

We shall use the Hamiltonian for the Hubbard model in the limit of infinitely strong Coulomb repulsion in the many-electron X-operator representation[38,39]

$$H = \sum_{\mathbf{k}\sigma} t_{\mathbf{k}} X^{0\sigma}_{-\mathbf{k}} X^{\sigma 0}_{\mathbf{k}}, \tag{1}$$

where $t_{\mathbf{k}}$ is the band energy and $X^{\alpha\beta}_{\mathbf{k}}$ is the Fourier transform of the Hubbard operators $X^{\alpha\beta}_i = |i\alpha\rangle\langle i\beta|$ [0 denotes holes and $\sigma = \pm(\uparrow,\downarrow)$ denotes singly occupied states].

It should be noted that in this problem of infinitely strong Coulomb interaction, a number of difficulties arise in connection with the non-Fermi excitation statistics. These difficulties occur both in the diagram technique[2] and in the equations-of-motion method.[40] In particular, it has been found[40] that in the expansion with respect to $1/z$ the analytic properties of the retarded Green's functions were violated for the paramagnetic state.

We use the method of the Zubarev double-time retarded Green's functions. The Green's function for operators A and B

$$\langle\langle A|B\rangle\rangle^{\pm}_E = \int_{-\infty}^{0} dt e^{iEt} \langle [e^{iHt} A e^{-iHt}, B]_{\pm}\rangle, \quad \mathrm{Im}\, E > 0 \tag{2}$$

satisfies the equation of motion

$$E\langle\langle A|B\rangle\rangle^{\pm}_E = \langle [A,B]_{\pm}\rangle + \langle\langle [A,\mathcal{H}]|B\rangle\rangle^{\pm}_E. \tag{3}$$

We write down the equation for the anticommutator Green's functions

$$G_{\mathbf{k}\sigma}(E) = \langle\langle X^{\sigma 0}_{\mathbf{k}} | X^{0\sigma}_{-\mathbf{k}}\rangle\rangle_E, \quad \mathrm{Im}\, E > 0 \tag{4}$$

to obtain

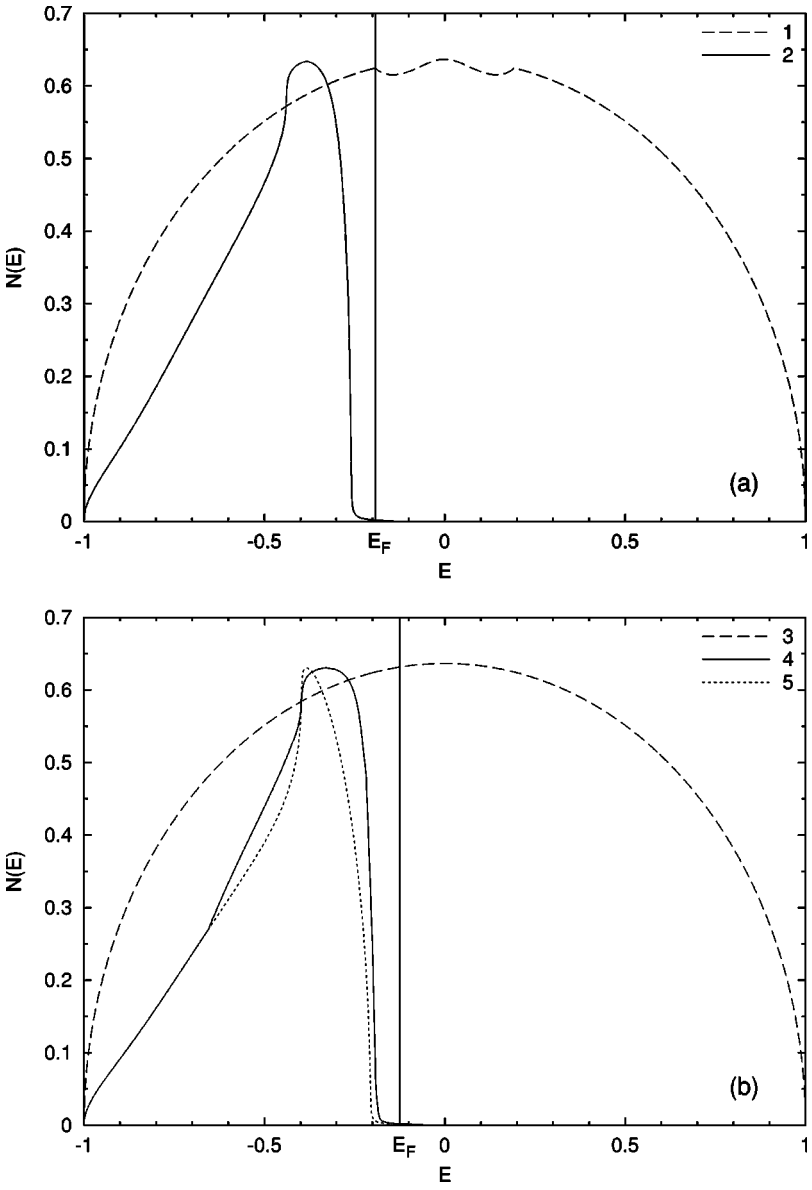

FIG. 2. Density of states for the bare semielliptic DOS at $\delta=0.20$. (a) Lines 1 ($\sigma=\uparrow$) and 2 ($\sigma=\downarrow$) correspond to the non-self-consistent approximation with spin dynamics (12); (b) lines 3 ($\sigma=\uparrow$) and 4 ($\sigma=\downarrow$) correspond to the self-consistent approximation (17), and lines 3 ($\sigma=\uparrow$) and 5 ($\sigma=\downarrow$) to the Edwards-Hertz approximation (24).

$$(E - t_{\mathbf{k}\sigma})G_{\mathbf{k}\sigma}(E) = (n_0 + n_\sigma) + \Gamma_{\mathbf{k}\sigma}(E), \tag{5}$$

where

$$t_{\mathbf{k}\sigma} = t_{\mathbf{k}}(n_0 + n_\sigma), \quad n_\alpha = \langle X_i^{\alpha\alpha}\rangle, \quad \alpha = 0, \sigma,$$

$$\Gamma_{\mathbf{k}\sigma}(E) = \sum_{\mathbf{q}} t_{\mathbf{k}-\mathbf{q}}\langle\langle X_{\mathbf{q}}^{\sigma-\sigma}X_{\mathbf{k}-\mathbf{q}}^{-\sigma 0} + \delta(X_{\mathbf{q}}^{00} + X_{\mathbf{q}}^{\sigma\sigma})X_{\mathbf{k}-\mathbf{q}}^{\sigma 0}|X_{-\mathbf{k}}^{0\sigma}\rangle\rangle_E,$$

with $\delta A = A - \langle A\rangle$. Decoupling the sequence of equations of motion at the first stage corresponds to the zeroth order in $1/z$ and is known as the Hubbard-I approximation. The corresponding Green's function may be represented in the form

$$G_{\mathbf{k}\sigma}^0(E) = [F_\sigma^0(E) - t_{\mathbf{k}}]^{-1}, \quad F_\sigma^0(E) = \frac{E}{n_0 + n_\sigma}. \tag{6}$$

When taking into account fluctuations we obtain

$$G_{\mathbf{k}\sigma}(E) = G_{\mathbf{k}\sigma}^0(E)\left(1 + \frac{\Gamma_{\mathbf{k}\sigma}(E)}{n_0 + n_\sigma}\right).$$

Following Ref. 37, we perform decoupling at the next stage to derive

$$\begin{aligned}(E - t_{\mathbf{k}-\mathbf{q}-\sigma} - \sigma\omega_{\mathbf{q}})\langle\langle X_{\mathbf{q}}^{\sigma-\sigma}X_{\mathbf{k}-\mathbf{q}}^{-\sigma 0}|X_{-\mathbf{k}}^{0\sigma}\rangle\rangle_E \\ = \chi_{\mathbf{q}}^{\sigma-\sigma} + n_{\mathbf{k}-\mathbf{q}-\sigma} + [t_{\mathbf{k}}\chi_{\mathbf{q}}^{\sigma-\sigma} - (t_{\mathbf{k}-\mathbf{q}} - t_{\mathbf{k}})n_{\mathbf{k}-\mathbf{q}-\sigma}] \\ \times\langle\langle X_{\mathbf{k}}^{\sigma 0}|X_{-\mathbf{k}}^{0\sigma}\rangle\rangle_E,\end{aligned} \tag{7}$$

$$\begin{aligned}(E - t_{\mathbf{k}-\mathbf{q}\sigma})\langle\langle \delta(X_{\mathbf{q}}^{00} + X_{\mathbf{q}}^{\sigma\sigma})X_{\mathbf{k}-\mathbf{q}}^{\sigma 0}|X_{-\mathbf{k}}^{0\sigma}\rangle\rangle_E \\ = \chi_{\mathbf{q}}^{-\sigma-\sigma}(1 + t_{\mathbf{k}}\langle\langle X_{\mathbf{k}}^{\sigma 0}|X_{-\mathbf{k}}^{0\sigma}\rangle\rangle_E),\end{aligned} \tag{8}$$

where

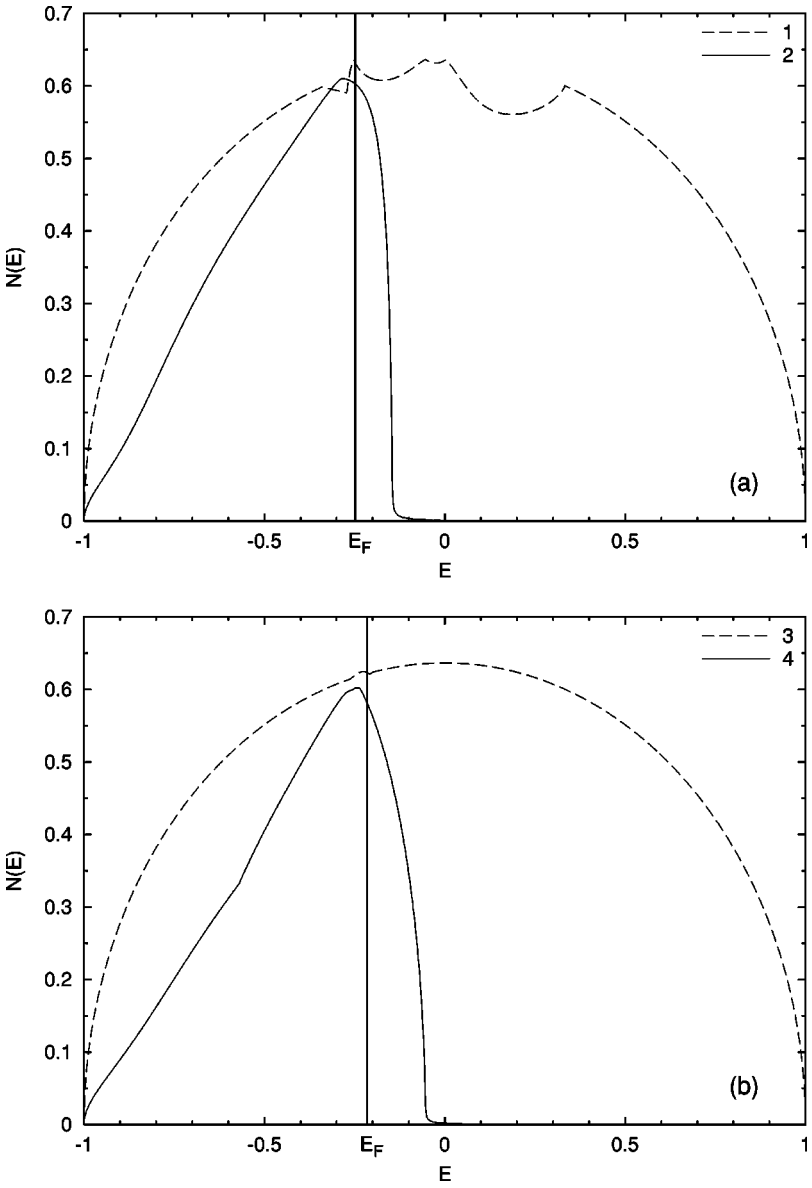

FIG. 3. Density of states for the bare semielliptic DOS at $\delta=0.35$. (a) Lines 1 ($\sigma=\uparrow$) and 2 ($\sigma=\downarrow$) correspond to the non-self-consistent approximation with spin dynamics (12); (b) lines 3 ($\sigma=\uparrow$) and 4 ($\sigma=\downarrow$) correspond to the self-consistent approximation (17).

$$\chi_{\mathbf{q}}^{\sigma-\sigma}=\langle S_{\mathbf{q}}^{\sigma}S_{-\mathbf{q}}^{-\sigma}\rangle=\langle X_{\mathbf{q}}^{\sigma-\sigma}X_{-\mathbf{q}}^{-\sigma\sigma}\rangle,$$

$$\chi_{\mathbf{q}}^{-\sigma-\sigma}=\langle\delta(X_{\mathbf{q}}^{00}+X_{\mathbf{q}}^{\sigma\sigma})\delta(X_{-\mathbf{q}}^{00}+X_{-\mathbf{q}}^{\sigma\sigma})\rangle=\langle\delta X_{\mathbf{q}}^{-\sigma-\sigma}\delta X_{-\mathbf{q}}^{-\sigma-\sigma}\rangle,$$

are the correlation function for spin and charge densities

$$n_{\mathbf{k}\sigma}=\langle X_{-\mathbf{k}}^{0\sigma}X_{\mathbf{k}}^{\sigma 0}\rangle.$$

Main spin fluctuations in the large-U limit under consideration (where local moments are well defined) are standard spin waves. The magnon frequencies $\omega_{\mathbf{q}}$ in Eq. (7) are required to cut the logarithmic "Kondo" divergences which are connected with the Fermi functions.

We write down the Green's function in the locator form

$$G_{\mathbf{k}\sigma}(E)=[F_{\mathbf{k}\sigma}(E)-t_{\mathbf{k}}]^{-1},\quad F_{\mathbf{k}\sigma}(E)=\frac{b_{\mathbf{k}\sigma}(E)}{a_{\mathbf{k}\sigma}(E)}. \tag{9}$$

For the Green's function (9) we have

$$a_{\mathbf{k}\sigma}(E)=n_0+n_\sigma+\sum_{\mathbf{q}}t_{\mathbf{k}-\mathbf{q}}(\chi_{\mathbf{q}}^{\sigma-\sigma}+n_{\mathbf{k}-\mathbf{q}-\sigma})G_{\mathbf{k}-\mathbf{q}-\sigma}^{0}(E-\sigma\omega_{\mathbf{q}})+\sum_{\mathbf{q}}t_{\mathbf{k}-\mathbf{q}}\chi_{\mathbf{q}}^{-\sigma-\sigma}G_{\mathbf{k}-\mathbf{q}\sigma}^{0}(E), \tag{10}$$

$$b_{\mathbf{k}\sigma}(E)=E+\sum_{\mathbf{q}}t_{\mathbf{k}-\mathbf{q}}^{2}n_{\mathbf{k}-\mathbf{q}-\sigma}G_{\mathbf{k}-\mathbf{q}-\sigma}^{0}(E-\sigma\omega_{\mathbf{q}}). \tag{11}$$

To simplify our equations, we use the long-wavelength dispersion law $\omega_{\mathbf{q}}=Dq^2$ (D is the spin-wave stiffness constant), introduce the magnon spectral function $K_{\mathbf{q}}(\omega)$ and average this in $\mathbf{q}$,

$$K_{\mathbf{q}}(\omega)=\delta(\omega-\omega_{\mathbf{q}})\rightarrow\overline{K}(\omega)=\sum_{\mathbf{q}}K_{\mathbf{q}}(\omega).$$

This approximation is sufficient to obtain qualitatively valid results. Indeed, this approximation (which is in the spirit of the large-d or large-z expansion) correctly reproduces the

TABLE I. Values of critical concentrations δ_c and δ_c' for rectangular (ra) and semielliptic (se) bare density of state, square, simple cubic (sc), bcc, fcc lattices. I, VII are the non-self-consistent approximations (9), II is Edwards-Hertz approximation (24), III, VIII are the self-consistent approximations (with fluctuations) (17), IV corresponds to results of Ref. 3, V, IX to results of work Ref. 45, VI to the result of Ref. 29 (variant of calculation RES0, for fcc lattices instability not discovered).

DOS	δ_c						δ_c'		
	I	II	III	IV	V	VI	VII	VIII	IX
ra	0.276	0.284	0.301				0.468	0.488	
se	0.258	0.266	0.290				0.458	0.477	
square	0.244	0.252	0.275	0.49		0.4045	0.449	0.461	
sc	0.233	0.237	0.261	0.32	<0.32	0.237	0.427	0.447	0.66
bcc	0.217	0.221	0.247	0.32	<0.32	0.239	0.414	0.432	0.48
fcc	0.210	0.217	0.241	0.62			0.409	0.427	0.38

low-frequency behavior of spin fluctuations which is important for the electronic structure near the Fermi level. Following Ref. 13 we have taken the value $D=0.7\delta|t|$. It should be noted that the choice of D weakly influences the critical concentration. We also neglect the $\mathbf{q}$ dependence of transverse and longitudinal spin correlation functions by taking the values averaged over the Brillouin zone to obtain

$$\chi_{\mathbf{q}}^{\sigma-\sigma}=n_\sigma, \quad \chi_{\mathbf{q}}^{-\sigma-\sigma}=n_{-\sigma}(1-n_{-\sigma}).$$

Then $a(E)$ and $b(E)$ do not depend on $\mathbf{k}$ and can be expressed in terms of the bare electron density of states $N_0(E)$,

$$G_{\mathbf{k}\sigma}(E)=[F_\sigma(E)-t_{\mathbf{k}}]^{-1}, \quad F_\sigma(E)=\frac{b_\sigma(E)}{a_\sigma(E)}, \tag{12}$$

$$a_\sigma(E)=n_0+n_\sigma+\int \overline{K}(\omega)\sum_{\mathbf{q}} t_{\mathbf{q}}(n_\sigma+n_{\mathbf{q}-\sigma})G^0_{\mathbf{q}-\sigma}(E-\sigma\omega)d\omega + \sum_{\mathbf{q}} t_{\mathbf{q}}n_{-\sigma}(1-n_{-\sigma})G^0_{\mathbf{q}\sigma}(E), \tag{13}$$

$$b_\sigma(E)=E+\int \overline{K}(\omega)\sum_{\mathbf{q}} t_{\mathbf{q}}^2 n_{\mathbf{q}-\sigma}G^0_{\mathbf{q}-\sigma}(E-\sigma\omega)d\omega, \tag{14}$$

$$G^0_{\mathbf{q}-\sigma}(E-\sigma\omega)\to G^0_{-\sigma}(E-\sigma\omega,t)=[F_\sigma(E-\sigma\omega)-t]^{-1},$$

$$F_\sigma(E)=\frac{E}{n_0+n_{-\sigma}},$$

$$a_\sigma(E)=n_0+n_\sigma+\int \overline{K}(\omega)\int N_0(t)t(n_\sigma+f_{-\sigma}(t))G^0_{-\sigma}(E-\sigma\omega,t) \times d\omega dt+\int N_0(t)tn_{-\sigma}(1-n_{-\sigma})G^0_\sigma(E,t)dt,$$

$$b_\sigma(E)=E+\int \overline{K}(\omega)\int N_0(t)t^2 f_{-\sigma}(t)G^0_{-\sigma}(E-\sigma\omega,t)d\omega dt,$$

where $f_\sigma(t_{\mathbf{q}})=n_{\mathbf{q}\sigma}$, $N_0(t)=\Sigma_{\mathbf{k}}\delta(t-t_{\mathbf{k}})$ is the bare density of states. The exact quasiparticle density of states is given by

$$N_\sigma(E)=-\frac{1}{\pi}\mathrm{Im}\sum_{\mathbf{k}} G_{\mathbf{k}\sigma}(E)=-\frac{1}{\pi}\mathrm{Im}\int_{-\infty}^{+\infty} G_\sigma(E,t)N_0(t)dt. \tag{15}$$

Now we write down the self-consistent approximation replacing the bare locator $F^0_\sigma(E)$ by the exact locator $F_\sigma(E)$ in Eqs. (13) and (14), i.e.,

$$G^0_{\mathbf{k}\sigma}(E)\to G_{\mathbf{k}\sigma}(E). \tag{16}$$

In such an approach, large electron damping is present which smears the "Kondo" peak, so that including magnon frequencies does not qualitatively change the picture, but may be important for quantitative results. We obtain

$$G_{\mathbf{k}\sigma}(E)=[F_\sigma(E)-t_{\mathbf{k}}]^{-1}, \quad F_\sigma(E)=\frac{B_\sigma(E)}{A_\sigma(E)}, \tag{17}$$

$$A_\sigma(E)=n_0+n_\sigma+\frac{1}{n_0+n_{-\sigma}}\int \overline{K}(\omega)\sum_{\mathbf{q}} t_{\mathbf{q}}(n_\sigma+n_{\mathbf{q}-\sigma})G_{\mathbf{q}-\sigma}(E - \sigma\omega)d\omega+\frac{1}{n_0+n_\sigma}\sum_{\mathbf{q}} t_{\mathbf{q}}n_{-\sigma}(1-n_{-\sigma})G_{\mathbf{q}\sigma}(E), \tag{18}$$

$$B_\sigma(E)=E+\frac{1}{n_0+n_{-\sigma}}\int \overline{K}(\omega)\sum_{\mathbf{q}} t_{\mathbf{q}}^2 n_{\mathbf{q}-\sigma}G_{\mathbf{q}-\sigma}(E-\sigma\omega)d\omega, \tag{19}$$

$$A_\sigma(E)=n_0+n_\sigma+\frac{1}{n_0+n_{-\sigma}}\int \overline{K}(\omega)\int N_0(t)t[n_\sigma+f_{-\sigma}(t)] \times G_{-\sigma}(E-\sigma\omega,t)dtd\omega+\frac{1}{n_0+n_\sigma}\int N_0(t)tn_{-\sigma}(1-n_{-\sigma}) \times G_\sigma(E,t)dt,$$

$$B_\sigma(E)=E+\frac{1}{n_0+n_{-\sigma}}\int N_0(t)t^2 f_{-\sigma}(t)G_{-\sigma}(E-\sigma\omega,t)dtd\omega.$$

It should be noted that another self-consistent approximation used in Ref. 40 leads to not quite satisfactory results because

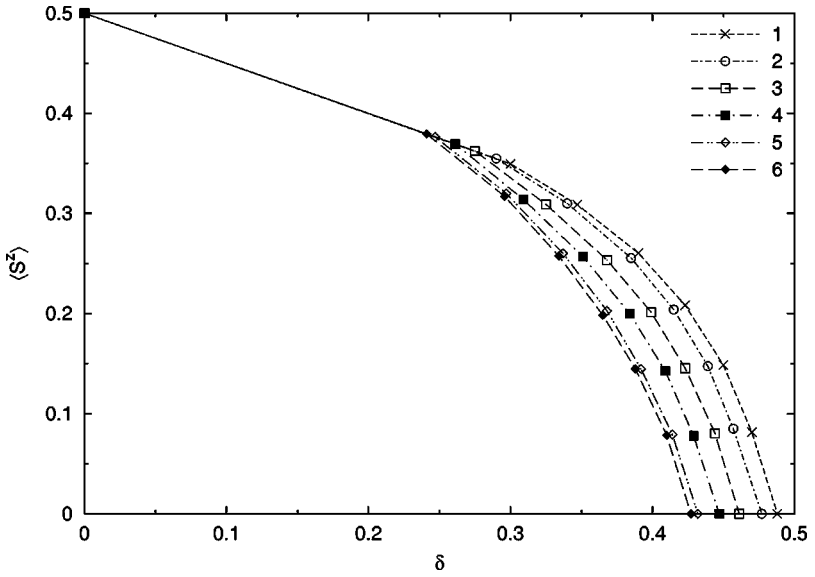

FIG. 4. The dependence of the magnetization $\langle S^z \rangle$ on δ for a number of bare DOS's. Line 1 corresponds to rectangular DOS, line 2 to semielliptic DOS, lines 3, 4, 5, 6 to square, simple cubic (sc), bcc, and fcc latices, respectively.

of the violation of the normalization condition for the density of states. As our calculations demonstrate, such a difficulty also exists for the approximation (12), but the violation is numerically small for $\delta < \delta_c$ (about 2%); note that introducing longitudinal fluctuations considerably improves the results in comparison with Ref. 41. At the same time, the approximation (17) with the locator structure of the Green's function does not violate the analytical properties.

The chemical potential μ is determined by the number of holes. By using the spectral representation for the Green's function (4) this is calculated as

$$\delta \equiv n_0 = \langle X^{00} \rangle = \langle X_i^{0\sigma} X_i^{\sigma 0} \rangle = \sum_{\mathbf{k}} \langle X_{\mathbf{k}}^{0\sigma} X_{-\mathbf{k}}^{\sigma 0} \rangle$$

$$= -\frac{1}{\pi} \mathrm{Im} \sum_{\mathbf{k}} \int_{-\infty}^{+\infty} G_{\mathbf{k}\sigma}(E) f(E) dE, \tag{20}$$

where $f(E)$ is the Fermi function. It is important that the Hubbard-I approximation is hardly satisfactory in the narrow-band ferromagnetism problem since it is difficult to formulate a reasonable criterion of magnetic ordering by direct use of the expressions for one-electron Green's functions such as Eq. (6). Unlike the decoupling scheme by Hubbard,[1] the many-electron X-operator approach clarifies the causes of this failure. In particular, one can see that the approximation (6) violates the kinematical requirements since it is impossible to satisfy the relation (20) at $\langle S^z \rangle \neq 0$ for both spin projections σ. Indeed, the quasiparticle pole for $\sigma = \downarrow$, corresponding to a narrowed band and lying above the Fermi level of the holes, does not provide an adequate description of the energy spectrum and leads to the appearance of finite $n_\downarrow$, i.e., the saturation ferromagnetism cannot be properly treated. However, the situation changes provided we use expressions containing first-order $1/z$ corrections. Unlike the Hubbard-I approximation, the value of μ turns out to be weakly dependent on σ for the approximation (12) and independent of σ for the the approximation (17).

The magnetization is determined from the equation

$$\langle S^z \rangle = \frac{1}{2} \sum_{\sigma} \sigma n_\sigma, \tag{21}$$

with

$$n_\sigma = \sum_{\mathbf{k}} \langle X_{-\mathbf{k}}^{\sigma 0} X_{\mathbf{k}}^{0\sigma} \rangle = \int_{-\infty}^{+\infty} N_\sigma(E)[1 - f(E)] dE.$$

In the leading approximation in $1/z$ for the one-particle occupation numbers, it is necessary to use the Hubbard-I approximation, i.e.,

$$n_{\mathbf{k}\sigma} = (n_0 + n_\sigma) f(t_{\mathbf{k}\sigma}),$$

but the chemical potential should be already chosen from the Green's function (9). As opposed to Eq. (6), the Green's functions (9) contain terms with resolvents and have branch cuts which describe nonquasiparticle (incoherent) contributions to the density of states. It is the latter which ensure qualitative agreement with the sum rule (20) for $\sigma = \downarrow$. At the same time, there are no poles of the Green's function for this projection of the spin for small δ above the Fermi level, i.e., the saturated ferromagnetic state is preserved.

The full density of states can be also represented in terms of the exact resolvent $R_\sigma(E) = \Sigma_{\mathbf{k}} G_{\mathbf{k}\sigma}(E)$ as

$$N_\sigma(E) = -\frac{1}{\pi} \mathrm{Im}\, R_\sigma(E).$$

This quantity satisfies the equation

$$R_\sigma(E) = R_0\{F_\sigma(E)\}, \quad R_0(E) = \sum_{\mathbf{k}} \frac{1}{E - t_{\mathbf{k}}} = \int N_0(t) \frac{1}{E - t} dt.$$

In the case of a saturated ferromagnetic state, the Green's function (9) takes the form

$$G_{\mathbf{k}\uparrow}(E)=\left(E\Big/\left[1+\sum_{\mathbf{q}}\frac{t_{\mathbf{q}}(1-n_0)}{E-t_{\mathbf{q}}n_0}\right]-t_{\mathbf{k}}\right)^{-1}, \quad (22)$$

$$G_{\mathbf{k}\downarrow}(E)=E\sum_{\mathbf{q}}\frac{n_{\mathbf{k}-\mathbf{q}}}{E-t_{\mathbf{k}-\mathbf{q}}+\omega_{\mathbf{q}}}\left(E\left[1-n_0+\sum_{\mathbf{q}}\frac{(E-t_{\mathbf{k}})n_{\mathbf{k}-\mathbf{q}}}{E-t_{\mathbf{k}-\mathbf{q}}+\omega_{\mathbf{q}}}\right]-\sum_{\mathbf{q}}t_{\mathbf{k}-\mathbf{q}}n_{\mathbf{k}-\mathbf{q}}\right)^{-1}, \quad (23)$$

where $n_{\mathbf{k}}=f(t_{\mathbf{k}})$. Note that, as opposed to the one-electron approach,[18] the Green's function $G_{\mathbf{k}\uparrow}(E)$ does not reduce to the free electron Green's function even in the saturated ferromagnetic state, since fluctuations in the hole occupation number contribute to it. Neglecting the resolvent in Eq. (22) and the last term in the denominator of Eq. (23), we obtain a somewhat different form of the Green's function in terms of the electron self-energy

$$G_{\mathbf{k}\uparrow}(E)=\frac{1}{E-t_{\mathbf{k}}}, \quad G_{\mathbf{k}\downarrow}(E)=\frac{1}{E-t_{\mathbf{k}}-\Sigma_{\mathbf{k}\downarrow}(E)},$$

$$\Sigma_{\mathbf{k}\downarrow}(E)=-(1-n_0)\left(\sum_{\mathbf{q}}\frac{n_{\mathbf{k}-\mathbf{q}}}{E-t_{\mathbf{k}-\mathbf{q}}+\omega_{\mathbf{q}}}\right)^{-1}. \quad (24)$$

This result corresponds to the Edwards-Hertz approximation in the limit $U\to\infty$. Of course, these expressions work only in the saturated ferromagnetic state. The results (24) can also be obtained by using the expansion in the electron and magnon occupation numbers.[42]

III. RESULTS OF CALCULATIONS AND DISCUSSION

The $1/z$ corrections lead to a nontrivial structure of the total quasiparticle density of states. In the non-self-consistent approach the integral with the Fermi functions yields, similar to the Kondo problem, the logarithmic singularity

$$\sum_{\mathbf{q}}\frac{f(t_{\mathbf{k}+\mathbf{q}})}{E-t_{\mathbf{k}+\mathbf{q}}}\simeq-\ln|E-E_F|N(E_F).$$

For very low δ a significant logarithmic singularity exists only in the imaginary part of the Green's function, which corresponds to a finite jump in the density of states.[35,36] However, when δ increases, it is necessary to take into account the resolvents in both the numerator and denominator of the Green's function, so that the real and imaginary parts are "mixed" and a logarithmic singularity appears in the density of states. When the magnon frequencies are included in the denominators of Eqs. (13) and (14), the singularity is spread out over the interval $\omega_{\max}$ and the peak is smoothed out. In the self-consistent approximations (18) and (19) the form of $N_{\downarrow}(E)$ approaches the bare density of states and the peak is completely smeared, even neglecting spin dynamics (Fig. 1), so that the latter plays no crucial role, although it shifts the peak below the Fermi level somewhat.

Near the critical concentration the peak in approximation (9) (but not in the Edwards-Hertz approximation) is again smeared (Fig. 2), but this spreading out is no longer noticeable for $\delta=0.15$. In the nonsaturated state a spin-polaron pole occurs, so that quasiparticle states with $\sigma=\downarrow$ occur above the Fermi level with

$$n_{\downarrow}=\int dEf(E)N_{\downarrow}(E).$$

The corresponding DOS picture is shown in Fig. 3.

The critical concentrations δ_c for the loss of stability of saturated ferromagnetism, as calculated in the different approximations considered, are listed in Table I for a number of bare densities of states. In the case of fcc lattices (where the bare density of states is asymmetric and has a logarithmic divergence on one edge) we have chosen the sign of the transfer integral for which the saturated ferromagnetism is stable at low δ.[13] Note that it is necessary to use an equation for the chemical potential (20) that is derived from the complete Green's functions (17). (Using the Hubbard-I approximation here leads to a drop in δ_c of the order of 0.1.)

It is clear from Table I that the results are fairly stable and do not depend too strongly on the form of the approximation. In particular, self-consistency changes them little, leading to a slight reduction in δ_c. The dependence on spin dynamics (magnon spectrum), even in the non-self-consistent approximation, is weaker (the critical concentration only varies in the third decimal place). At the same time, spin dynamics is important for the description of the states near the Fermi level. Results of the Edwards-Hertz approximation (24) lie between those of the self-consistent approximation (17) of the non-self-consistent approximation (9). Unfortunately, in Ref. 18 only a crude estimate of δ_c was made by using the quadratic dispersion relation for the hole spectrum which yielded $\delta_c=0.16$. This approximation is not sufficient for quantitative calculations, as one can see from Table I.

Unlike most other analytical approaches, our results for the one-particle Green's describe the formation of nonsaturated ferromagnetism too. It is important that the account of longitudinal spin fluctuations (which were neglected in Ref. 41) turns out to be important for obtaining the nonsaturated solution and calculating the second critical concentration δ_c'.

The dependence of the saturation magnetization on the concentration of charge carriers for various bare DOS's is shown in Fig. 4. One can see that this dependence deviates from the linear one $\langle S^z\rangle=(1-n)/2$ for $\delta>\delta_c$.

Let us perform a comparison of our results with other calculations. Generally, most calculations for a number of lattices yield a value of δ_c which is close to 0.3 (although the small value $\delta_c=0.045$ was obtained in Ref. 22 for sc lattice by a diagram approach, the close approach of Ref. 25 yields much larger values, e.g., $\delta_c=0.25$ for the quadratic lattice). At the same time, for the critical concentrations δ_c' the interval of values is broader and varies from 0.38 to 0.64. Our calculations yield δ_c' values which are considerably smaller than the results of the spin-wave approximation.[14]

An improved Gutzwiller method[27] yields $\delta_c=0.33$ for the sc lattice, and using the t/U expansion[23] yields $\delta_c=0.27$. For the quadratic lattice the result of the variational approach[8] is $\delta_c=0.251$, and the result of Ref. 43 is $\delta_c'=0.38$. The density matrix renormalization group approach[9] leads to the

value $\delta_c = 0.22$ and the rough estimate $\delta_c' \simeq 0.40$. The quantum Monte Carlo (QMC) method for the density matrix in Ref. 9 gives $\delta_c = 0.22$ and the rough evaluation $\delta_c' \approx 0.40$. The QMC in the two dimensional (2D) case[44] gives $\delta_c' \approx 0.40$. A self-consistent spin density approximation (SDA)[45] leads to the results for simple cubic and bcc lattices $\delta_c < 0.32$; the values of δ_c' for the cubic lattices are given in Table I.

The values we have obtained can be compared with those in the limit of an infinite-dimension space (it should be expected that our method of expanding in powers of $1/z$ is somewhat similar to this approximation), for which the values $\delta_c' = 0.42$ (Ref. 27) and $\delta_c' = 0.33$ (Refs. 10 and 15) have been obtained. Our self-consistent calculations give $\delta_c = 0.20$, $\delta_c' = 0.42$. A more detailed comparison can be made for the DOS shape including the formation of the Kondo peaks at the Fermi level. The picture of nonsaturated ferromagnetism at finite (although large) U considered in the paper by Zitzler *et al.*[15] (see Fig. 9) corresponds to the second critical concentration $\delta_c' = 0.15$ (which is small in comparison to the infinite-U value $\delta_c' = 0.33$) and a very small first critical concentration δ_c. Therefore the DOS peaks at the Fermi level are well pronounced even near δ_c'. At small δ (below δ_c) our picture is similar to that by Zitzler *et al.*, demonstrating unrenormalized spin-up DOS and a sharp Kondo peak in the spin-down DOS. At the same time, in our infinite-U case the peaks near large δ_c' are already almost fully smeared (especially in the self-consistent approximation, which probably overestimates the damping). As for Ref. 10, the calculations were made at small doping and finite temperatures. As noted by the authors (see discussion after Fig. 4), the results are similar to those in the paramagnetic phase. In such a case, our approach also yields sharp Kondo peaks at the Fermi level for both spin projections (Ref. 46).

With our approach it is possible to reproduce the dependence of δ_c on the space dimensionality and the form of the bare density of states. Recently, δ_c has been obtained for a large number of lattices.[3,29] These results are also given in Table I for comparison. It can be seen that in some cases our results agree better with a number of other calculations, especially for a square lattice. We note in this connection that a variational method has been used[4] to obtain a rigorous estimate $\delta_c < 0.29$ for a square lattice. Therefore, our results can be regarded to be fairly reliable, even quantitatively.

To conclude, we have obtained the density-of-states pictures in a Hubbard ferromagnet with account of the "Kondo" scattering and spin-polaron contributions. Our approach yielded a rather simple interpolational description of saturated and nonsaturated ferromagnetism. One can expect that the results obtained will be useful for a qualitative understanding of the ferromagnetism formation in narrow bands.

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