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A mean-field-type approximation for the (t–J) model

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Abstract. The equations for a mean-field-type approximation in the (t–J) model are formulated in terms of a diagrammatic technique with Hubbard X-operators. With their help, equations for the order parameters are derived in ferromagnetic and antiferromagnetic phases of a metal. In both cases, two coupled order parameters exist: a magnetization m and a gap Δ in the electron spectrum. They reflect a dual behaviour of a strongly correlated system: it is simultaneously an itinerant and a localized magnet. Formulae for Curie temperature T_C and Néel temperature T_N are derived, from which the different nature of ferromagnetic and antiferromagnetic ordering is explicitly seen. For a simple cubic lattice the electron concentration n dependences of T_C and T_N are numerically calculated. It is shown that T_N rapidly falls with deviation from half-filling, when $n = 1$. Magnetic correlation length l_c varies at low temperature as $\sim (1-n)^{-1/2}$. Such behaviour corresponds to that observed in experiments in copper oxide high-T_C superconductors. The magnetic phase diagram is constructed on the (t/U, n) plane. The equations for the coupled order parameters are solved for $T = 0$ and the dependences of the order parameters m and Δ on n are presented in a wide interval of electron concentrations. They indicate the growing degree of itinerancy with deviation from half-filling. It is shown that the critical concentration n_c for a crossover from itinerant magnetism to magnetism with localized magnetic moments should be a peculiar point where perturbation theory breaks down.

1. Introduction

The (t–J) model can be treated as a limiting case of the Hubbard model with large value of on-site Coulomb repulsion U. When U is much larger than the hopping electron matrix element t ($U \gg t$), states of the system with two electrons of one site can be excluded in the second order of perturbation theory. As a result an effective Hamiltonian appears with antiferromagnetic exchange interaction $J = t^2/U$, and hopping of electrons over the lattice with more than one electron at a site is not allowed. This is just the (t–J) model.

The Hamiltonians of the Hubbard model and the (t–J) model are written in the second quantization representation as

$$\mathcal{H} = t \sum_{\langle ij \rangle} \sum_{\sigma} c_{i\sigma}^{+} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{1.1}$$

for the Hubbard model [1] and

$$\mathcal{H} = t \sum_{\langle ij \rangle} \sum_{\sigma} (1 - n_{i\bar{\sigma}}) c_{i\sigma}^{+} c_{j\sigma} (1 - n_{j\bar{\sigma}}) + J \sum_{\langle ij \rangle} (S_i S_j - \tfrac{1}{4} n_i n_j) \tag{1.2}$$

for the (t–J) model [2]. Here $c_{i\sigma}^{+}$ and $c_{i\sigma}$ are Fermi operators of an electron at site i and spin projection $\sigma = \uparrow, \downarrow$; $n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma}$ is the operator of electron number at site i with spin

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σ; $n_i = n_{i\uparrow} + n_{i\downarrow}$ is the operator of the total number of electrons at site i; and S_i is the spin operator. Factors $(1 - n_{i\bar{\sigma}})$ do not allow a second electron to be at a given site i. These factors create the major difficulties when one works with Hamiltonian (1.2).

The Hubbard and $(t$–$J)$ models are fundamental models for the study of itinerant magnetism in metals. In the case of weak Coulomb interaction ($U \ll t$), the second term in (1.1) can be treated by perturbation theory in terms of the usual Fermi operators. To study different physical properties, one can use standard approximations in many-body theories. Particularly, for many years the random-phase approximation (RPA) result has been known [3]:

$$\chi_{\mathrm{RPA}}(k) = \frac{\chi^0(k)}{1 - U\chi^0(k)} \tag{1.3}$$

where $\chi^0(k)$ is the magnetic susceptibility of the free (band) electrons (k is 4-momentum). This result corresponds to summing up of loop-type diagrams, and

$$\chi^0(k) = -\Pi(k) \tag{1.4}$$

where $\Pi(k)$ is an electron loop with different spins for a particle and a hole. Formula (1.3) is the basis of the itinerant magnetism theory and its generalization, the theory of localized spin fluctuations (see the book by Moriya [4]).

In the case of strong Coulomb repulsion ($U \gg t$), one must apply Hamiltonian (1.2). In [5,6] we suggested expressing it in terms of the variables natural for this case—X-operators—and developed a perturbation theory with these Hubbard operators. The generalized random-phase approximation (GRPA) was suggested and the magnetic susceptibility of the paramagnetic phase was calculated [5]. The result resembles the structure of expression (1.3):

$$\chi_{\mathrm{GRPA}}(k) = \frac{\chi^0(k)}{[1 - \Lambda(k)][1 - Q(k)] + \chi^0(k)[\Phi(k) + J(k)]}. \tag{1.5}$$

However, the bare susceptibility $\chi^0(k)$ contains two contributions:

$$\chi^0(k) = (n_0/2T)\delta_{\omega_k,0} - \Pi(k). \tag{1.6}$$

Here the first term presents the Curie-type susceptibility $\sim 1/T$, *while the second one gives* the Pauli-type susceptibility.

The quantities Π, Λ, Q and Φ represent electron loops with different spins for a particle and a hole. Green lines correspond not to free electrons, as in the RPA case, but to electrons in the 'Hubbard-I' approximation partly taking into account the electron correlations. These quantities correspond to four types of electron loops and they are equal to

$$\begin{pmatrix} \Pi(k) \\ \Lambda(k) \\ Q(k) \\ \Phi(k) \end{pmatrix} = \frac{1}{N}\sum_{k_1} \begin{pmatrix} 1 \\ \varepsilon(k_1) \\ \varepsilon(k_1 - k) \\ \varepsilon(k_1)\varepsilon(k_1 - k) \end{pmatrix} \frac{f(\xi(k_1 - k)) - f(\xi(k_1))}{\mathrm{i}\omega_k + \xi(k_1 - k) - \xi(k_1)} \tag{1.7}$$

where

$$\xi(k) = (1 - \tfrac{1}{2}n)\varepsilon(k) \tag{1.8}$$

is the energy of an electron in the lower Hubbard subband in the limit $U \to \infty$, and $f(x)$ is the Fermi function.

The parameter n_0 in (1.6) changes rapidly with electron concentration n. At zero temperature $n_0 = 0$ when $n < n_c$ and $n_0 = 1$ when $n > n_c$. The critical concentration n_c is determined by the condition: chemical potential is equal to zero at $T = 0$. In our approximation $n_c = 2/3$ [5]. Owing to such behaviour of n_0, formula (1.5) together with (1.6) implies that the system undergoes a crossover at the point $n = n_c$ from itinerant magnetism to magnetism with localized magnetic moments.

For a description of magnetically ordered phases with corresponding set of order parameters, a mean-field-type approximation (MFA) is usually applied. For the $(t–J)$ model with Hamiltonian (1.2), such an approximation is completely non-trivial, and the purpose of the present paper is the formulation of equations corresponding to such an approximation. In section 2 general diagram equations in MFA are suggested, and in section 3 on their basis equations for the order parameters for ferromagnetic and antiferromagnetic phases are derived. Curie T_C and Néel T_N temperatures are calculated numerically from these equations in section 4. Also the magnetic phase diagram on the $(t/U, n)$ plane is constructed. In section 5 the equations for ferromagnetic and antiferromagnetic order parameters for zero temperature are solved numerically and their electron concentration dependence is found for the wide range of n. In section 6 the role of Gaussian fluctuations in the behaviour of the quantity n_0 is discussed in a self-consistent way. It is shown that the critical concentration n_c appears to be a special point, where perturbation theory breaks down. It means that all fluctuations in the system are relevant in the vicinity of n_c. In section 7 the relation to the MFA for the Hubbard model, based on the high-dimensions limit $d \to \infty$, is discussed.

2. Diagram equations for MF approximation in the (t–J) model

The Hamiltonian of the $(t–J)$ model (1.2) is expressed as a quadratic form of the X-operators [5]. It is also convenient to introduce a term with chemical potential μ and external magnetic field H. Then $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{int}$, where

$$\mathcal{H}_0 = \varepsilon_+ \sum_i X_i^{++} + \varepsilon_- \sum_i X_i^{--} \tag{2.1}$$

$$\mathcal{H}_{int} = t \sum_{\langle ij \rangle} \sum_\sigma X_i^{\sigma 0} X_j^{0\sigma} + J \sum_{\langle ij \rangle} (X_i^{-+} X_j^{+-} - X_i^{++} X_j^{--}). \tag{2.2}$$

Here $\varepsilon_\sigma = -\mu - \sigma h/2$ are the energies of on-site states for two spin projections $\sigma = +, -$, and $h = g\mu_B H$.

Let us introduce the electron and spin Matsubara-type Green functions:

$$G_\sigma(i\tau; i'\tau') = -\langle T(\tilde{X}_i^{0\sigma}(\tau)\tilde{X}_{i'}^{\sigma 0}(\tau'))\rangle \tag{2.3}$$

$$D_\perp(i\tau; i'\tau') = -\langle T(\tilde{X}_i^{+-}(\tau)\tilde{X}_{i'}^{-+}(\tau'))\rangle \tag{2.4}$$

with all standard definitions [7]. A perturbation theory in the form of diagrammatic technique with X-operators was described by us in detail [5, 6]. Its elements are fermion G_σ^0 and boson D^0 Green functions denoted by solid lines (with open and filled arrows for spins $\sigma = \uparrow, \downarrow$) and broken lines respectively. The coupling constants t and J are denoted by wavy and dotted lines. The diagrammatic technique includes also cumulants (semi-invariants), which are the statistical averages of diagonal X-operator products. They are

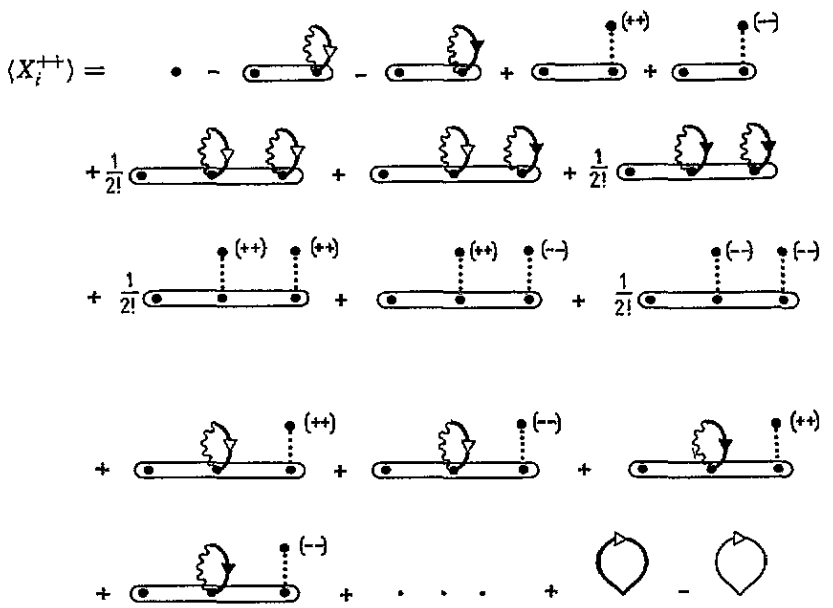
denoted by filled circles (representing these X-operators) placed in an oval. A first-order cumulant is the average $\langle X^{\sigma\sigma}\rangle$ and is denoted by one filled circle without an oval.

When summing up graphical sequences in the technique with X-operators it is necessary to dress not only Green lines but cumulants as well. This is just a peculiarity of the MFA for the $(t$–$J)$ model compared to the usual Fermi-liquid theory. So, we must construct the self-consistent equations for a self-energy part Σ_σ of the fermion Green function G_σ, and for the cumulant $\langle X^{\sigma\sigma}\rangle$. In accordance with the general concept of MFA we have to select graphs for Σ_σ that do not depend on momentum. It is not difficult to see that such graphs are

$\Sigma_\uparrow =$  (2.5)

(incoming and outgoing Green lines $G^0_\uparrow$ are not included due to the determination of $\Sigma_\uparrow$). A similar equation can be written for $\Sigma_\downarrow$ by interchange of the arrows' colour. A thick fermion line in (2.5) corresponds to the dressed Green function $G_\downarrow$, which must be obtained from a self-consistent equation (2.5) and a similar equation for $\Sigma_\downarrow$.

Cumulants in (2.5) represent $1 - \langle X_i^{--}\rangle$ (in the first graph) and $\langle X_i^{--}\rangle$ (in the third graph). They must be found by summing up of graph series for $\langle X_i^{++}\rangle$ and $\langle X_i^{--}\rangle$ with the same graph structures, which determines $\Sigma_\uparrow$ and $\Sigma_\downarrow$. Thus, in MFA the following graphs must be summarized

$\langle X_i^{++}\rangle =$  (2.6)

A similar series must be written for $\langle X_i^{--}\rangle$. In the series (2.6) each external vertex corresponds to X_i^{++}. Notice that just the dressed Green functions enter the series for $\langle X_i^{++}\rangle$ and therefore equations (2.5), (2.6) and similar equations for the other spin projection constitute a system of coupled equations for the four quantities: Σ_σ and $\langle X_i^{\sigma\sigma}\rangle$.

One can see that the infinite graph series (2.6) presents analytically a Taylor expansion for a function with a shifted argument, given by the first term in the series, which means function $\langle X_i^{++}\rangle$ of zero approximation, which at zero value of the external field is

$$\langle X_i^{\sigma\sigma}\rangle_0 = e^x/(1+2e^x) \equiv \tfrac{1}{2}n_0 \tag{2.7}$$

where $x = \mu/T$. The shift of argument in the Taylor expansion (2.6) is determined by the following four graphs of the 'first' approximation. Because of that, an analytical expression corresponding to the infinite series (2.6) can be written quite simply.

3. Equations for the order parameters in ferromagnets and antiferromagnets

Graph equations (2.5) and (2.6) are the basis for writing the equations for the order parameters in ferro- or antiferromagnetic phases. In a ferromagnet the average number of electrons $n_\uparrow$ at a site with spin $\uparrow$ is not equal to $n_\downarrow$, and therefore the self-energy of an electron depends on spin σ. Let us write an expression for the electron Green function in the form

$$G_\sigma(k; i\omega_k) = 1/[i\omega_k - \xi_\sigma(k) - \Delta_\sigma + \mu] \tag{3.1}$$

where

$$\xi_\sigma(k) = (1 - n_{\bar\sigma})\varepsilon(k) \tag{3.2}$$

and

$$\Delta_\sigma = -Jzn_{\bar\sigma} - \frac{1}{N}\sum_k \varepsilon(k) f(\xi_{\bar\sigma}(k) + \Delta_{\bar\sigma}). \tag{3.3}$$

Here $\varepsilon(k) = t\sum_\Delta \exp(ik\cdot\Delta)$ is the band energy of an electron without Coulomb interaction. Factor $(1-n_{\bar\sigma})$ describes correlation narrowing of a band, so $\xi_\sigma(k)$ is electron energy in the 'Hubbard-I' approximation. This approximation corresponds only to the first graph in expression (2.5) for Σ_σ. Two other graphs lead to the frequency-independent correction Δ_σ obeying the self-consistent equation (3.3).

Let us write analytical equations corresponding to the graphical equation (2.6) for $\langle X_i^{\sigma\sigma}\rangle$. Taking into account that the graphical series (2.6) is a Taylor expansion, we present it in the following form:

$$\langle X_i^{\sigma\sigma}\rangle = \frac{e^{x+\lambda_\sigma}}{1+e^{x+\lambda_\uparrow}+e^{x+\lambda_\downarrow}} + \frac{1}{N}\sum_k [f(\xi_\sigma(k)+\Delta_\sigma) - f(\Delta_\sigma)] \tag{3.4}$$

where $\lambda_\sigma = \Delta_\sigma/T$. This expression allows us to write equations for the order parameter m and chemical potential μ. With the help of the identity $n_\sigma = \langle X_i^{\sigma\sigma}\rangle$, we have according to the definitions:

$$m = \langle X_i^{++}\rangle - \langle X_i^{--}\rangle \qquad n = \langle X_i^{++}\rangle + \langle X_i^{--}\rangle. \tag{3.5}$$

Substituting expression (3.4) in these relations we can find explicit equations for m and μ.

One should remember that, in an itinerant ferromagnet, the order parameter should be not only m but also the value of the gap $\Delta = \Delta_\downarrow - \Delta_\uparrow$ in the electron spectrum with different spin projections. With the help of equation (3.3) for Δ_σ and equation (3.5) for m and μ, we come to the system of three coupled equations for order parameters Δ and m and also for chemical potential μ:

$$\Delta = -Jzm + \frac{1}{N}\sum_k \varepsilon(k)\left[f\left(\xi(k) + \frac{\Delta - m\varepsilon(k)}{2}\right) - f\left(\xi(k) - \frac{\Delta - m\varepsilon(k)}{2}\right)\right] \tag{3.6}$$

$$m = n_0\left(\frac{\Delta}{2T}\right)\tanh\left(\frac{\Delta}{2T}\right) + \left[f\left(\frac{\Delta}{2}\right) - f\left(-\frac{\Delta}{2}\right)\right] - \frac{1}{N}\sum_k \left[f\left(\xi(k) + \frac{\Delta - m\varepsilon(k)}{2}\right) - f\left(\xi(k) - \frac{\Delta - m\varepsilon(k)}{2}\right)\right] \tag{3.7}$$

and

$$n = n_0\left(\frac{\Delta}{2T}\right) - \left[f\left(\frac{\Delta}{2}\right) + f\left(-\frac{\Delta}{2}\right)\right] + \frac{1}{N}\sum_k \left[f\left(\xi(k) + \frac{\Delta - m\varepsilon(k)}{2}\right) + f\left(\xi(k) - \frac{\Delta - m\varepsilon(k)}{2}\right)\right]. \tag{3.8}$$

Here $\xi(k) = (1 - n/2)\varepsilon(k)$ is electron energy in the 'Hubbard-I' approximation for a paramagnetic phase.

In a similar way, one can derive equations for the antiferromagnetic phase. An order parameter should be introduced by the relation

$$\langle X_i^{++}\rangle - \langle X_i^{--}\rangle = mp_i \tag{3.9}$$

where $p_i = \exp(\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{R}_i)$, and $\boldsymbol{Q}$ is the wavevector of magnetic structure. If we take

$$\boldsymbol{Q} = (\pi, \pi, \pi)/a \tag{3.10}$$

then factor $p_i = \pm 1$, and one can see that the order parameter m is the magnetization of a sublattice. In such a system the electron Green function $G_\sigma(k)$ is a 2×2 matrix of the following form:

$$G_\sigma(k; \mathrm{i}\omega_k) = \frac{1}{d(k; \mathrm{i}\omega_k)}\begin{pmatrix} \mathrm{i}\omega_k + \mu + \xi(k) & \sigma[-\Delta - \frac{1}{2}m\varepsilon(k)] \\ \sigma[-\Delta + \frac{1}{2}m\varepsilon(k)] & \mathrm{i}\omega_k + \mu - \xi(k)\end{pmatrix} \tag{3.11}$$

where

$$d(k; \mathrm{i}\omega_k) = (\mathrm{i}\omega_k + \mu)^2 - E^2(k)$$

and

$$E(k) = [\xi_A^2(k) + \Delta^2]^{1/2} \qquad \xi_A(k) = [(1 - \tfrac{1}{2}n)^2 - \tfrac{1}{4}m^2]^{1/2}\varepsilon(k). \tag{3.12}$$

The graph equations (2.5) and (2.6) with electron Green function (3.11) lead to the following equations for m, Δ and μ:

$$\Delta = \tfrac{1}{2}Jzm + \tfrac{1}{4}m\frac{1}{N}\sum_{k}\varepsilon^2(k)\frac{f(E(k)) - f(-E(k))}{E(k)} \tag{3.13}$$

$$m = n_0\left(\frac{\Delta}{2T}\right)\tanh\left(\frac{\Delta}{2T}\right) + [f(\Delta) - f(-\Delta)] - \Delta\frac{1}{N}\sum_{k}\frac{f(E(k)) - f(-E(k))}{E(k)} \tag{3.14}$$

and

$$n = n_0\left(\frac{\Delta}{2T}\right) - [f(\Delta) + f(-\Delta)] + \frac{1}{N}\sum_{k}[f(E(k)) + f(-E(k))]. \tag{3.15}$$

In equations (3.6)–(3.8) and (3.13)–(3.15) we introduce a quantity

$$n_0(\lambda) = 2e^{x}\cosh\lambda/(1 + 2e^{x}\cosh\lambda) \tag{3.16}$$

which at $\lambda = 0$ reduces to the expression (2.7) for n_0. The second parameter Δ is the gap in the spectrum of an electron moving in an antiferromagnetic matrix.

The structure of equations (3.6)–(3.8) for a ferromagnet and equations (3.13)–(3.15) for an antiferromagnet are similar. Each equation has two contributions on the right-hand side: one reflects the localized and the other the itinerant character of magnetism in the $(t–J)$ model. The existence of two parameters also reflects the dual behaviour of the system. The parameter m is a local characteristic, being the magnetization of a sublattice, while Δ is a characteristic of the electron spectrum. Notice that, in the entirely localized (Heisenberg) model, only one order parameter m exists, but in the entirely itinerant model (with weak Coulomb repulsion) only parameter Δ exists.

4. Curie and Néel temperatures

Neither of the order parameters m and Δ is primary, but both appear simultaneously. This is easy to see from the linearized equations. Equating to zero the determinant of these equations gives equations for Curie T_C and Néel T_N temperatures. In the case of a ferromagnet the linearization of equations (3.6) and (3.7) leads to the following equation for T_C:

$$[1 - \Lambda(\mathbf{0}, 0)]^2 + [n_0/(2T_C) - \Pi(\mathbf{0}, 0)][\Phi(\mathbf{0}, 0) + Jz] = 0 \tag{4.1}$$

where we introduce the notation

$$\begin{pmatrix}\Pi(\mathbf{0}, 0)\\ \Lambda(0, 0)\\ \Phi(\mathbf{0}, 0)\end{pmatrix} = \frac{1}{T}\frac{1}{N}\sum_{k}\begin{pmatrix}1\\ \varepsilon(k)\\ \varepsilon^2(k)\end{pmatrix}f'(\xi(k)). \tag{4.2}$$

Here a prime means a derivative of the Fermi function with respect to the dimensionless argument. It is not difficult to see that the quantities (4.2) are particular values of the quantities $\Pi(k)$, $\Lambda(k)$ and $\Phi(k)$ at zero frequency and zero wavevector, and $Q(\mathbf{0}, 0) = \Lambda(\mathbf{0}, 0)$.

Equation (4.1) coincides with an equation determining poles of the dynamic magnetic susceptibility of paramagnetic phase at $k = 0$. The coincidence of the stability boundary

of ferromagnetic phase with the stability boundary of paramagnetic phase is the sign of a second-order phase transition. Let us rewrite equation (4.1) in the form:

$$T_C = \frac{n_0}{2} \frac{-\Phi(\mathbf{0},0) - Jz}{[1-\Lambda(\mathbf{0},0)]^2 - \Pi(\mathbf{0},0)[\Phi(\mathbf{0},0) + Jz]}. \tag{4.3}$$

This formula is valid while it gives positive values, and therefore the boundary of the ferromagnetic state is determined by the condition

$$-\Phi(\mathbf{0},0) = Jz. \tag{4.4}$$

Quantities Π, Λ and Φ depend weakly on temperature in the whole temperature interval of electron concentration $0 < n < 1$ except for a narrow vicinity of the point $n = 1$, where they contain a linear term in T. Because of that, on the right-hand side of (4.3) all quantities can be taken at $T = 0$; then (4.3) is an explicit expression for T_C. When $T \to 0$ formula (4.2) reduces to

$$\begin{pmatrix} \Pi(\mathbf{0},0) \\ \Lambda(\mathbf{0},0) \\ \Phi(\mathbf{0},0) \end{pmatrix} = -(1-\tfrac{1}{2}n)^{-1} \begin{pmatrix} 1 \\ \tilde{\mu} \\ \tilde{\mu}^2 \end{pmatrix} \rho_0(\tilde{\mu}) \tag{4.5}$$

where $\rho_0(\varepsilon)$ is the density of states in the bare electron spectrum $\varepsilon(k)$ and $\tilde{\mu} = \mu/(1-\frac{1}{2}n)$. With (4.5), expression (4.3) for T_C can be written in the form:

$$T_C = \frac{n_0}{2} \frac{\tilde{\mu}^2 \rho_0(\tilde{\mu})(1-\frac{1}{2}n)^{-1} - Jz}{1 + (Jz + 2\tilde{\mu})\rho_0(\tilde{\mu})(1-\frac{1}{2}n)^{-1}} \tag{4.6}$$

from which the dependence of T_C on n follows, if the electron concentration dependence of the chemical potential is known. From (4.6) one can see that T_C vanishes because of the factor n_0 when $n < n_c$ and also when $n_F < n < 1$, where concentration n_F is determined by equation (4.4), which can be rewritten in the form

$$(1-\tfrac{1}{2}n)^{-1} \tilde{\mu}^2 \rho_0(\tilde{\mu}) = Jz. \tag{4.7}$$

Therefore ferromagnetism exists in the interval

$$n_c < n < n_F \tag{4.8}$$

where n_F should be close to $n = 1$, because $J \ll t$. At the limit $U \to \infty$, $n_F \to 1$.

In the case of an antiferromagnet, the linearized equations (3.7) and (3.8) lead to the equation for T_N of the following form:

$$1 + [n_0/(2T_N) - \Pi(Q,0)][\Phi(Q,0) - Jz] = 0 \tag{4.9}$$

where quantities $\Pi(Q,0)$ and $\Phi(Q,0)$ were introduced, which reduce at $T \to 0$ to

$$\Pi(Q,0) = \frac{1}{1-n/2} \int_{-\infty}^{\tilde{\mu}} d\varepsilon \, \frac{\rho_0(\varepsilon)}{\varepsilon} \tag{4.10}$$

$$\Phi(Q,0) = -\frac{1}{1-n/2} \int_{-\infty}^{\tilde{\mu}} d\varepsilon \, \varepsilon \rho_0(\varepsilon). \tag{4.11}$$

These quantities are particular values of quantities $\Pi(k)$ and $\Phi(k)$ for zero frequency and $k = Q$, and $\Lambda(Q,0) = Q(Q,0) = 0$. Thus, equation (4.9) coincides with the equation determining the instability boundary of the paramagnetic phase with respect to the appearance of antiferromagnetism. From here it follows that

$$T_N = \frac{n_0}{2}\frac{Jz - \Phi(Q,0)}{1 - \Pi(Q,0)[\Phi(Q,0) - Jz]}. \tag{4.12}$$

As in the case of ferromagnetism in the vicinity of $n = 1$, it is necessary to take into account a linear term in T in the expression for $\Phi(Q,0)$. It corrects formula (4.12) by the numerical factor $(1 + \ln 2)^{-1}$.

Let us compare formulae (4.3) and (4.12) for T_C and T_N. In both cases the denominators are positive values of the order of unity for all n, and therefore

$$\begin{aligned} T_C &\sim n_0[-\Phi(\mathbf{0},0) - Jz] \\ T_N &\sim n_0[Jz - \Phi(Q,0)]. \end{aligned} \tag{4.13}$$

These relations make clear the nature of ferromagnetic and antiferromagnetic ordering in the $(t–J)$ model. It is seen (if we note that $\Phi(\mathbf{0},0) < 0$) that ferromagnetic ordering has kinetic nature and the exchange interaction hinders it. The nature of antiferromagnetic ordering is quite different: it is caused by the exchange interaction, and electron motion only suppresses it.

Thus, relations (4.13) determine the effective ferromagnetic and antiferromagnetic couplings. The factor n_0 means that magnetic ordering occurs only with the appearance of localized magnetic moments. From formula (4.12) one can see that nesting does not play an essential role in the antiferromagnetic ordering, in contrast to the itinerant (Fermi-liquid) model.

Now we present the results of numerical calculations of T_C and T_N for a simple cubic (SC) lattice from formulae (4.3) and (4.12). In figure 1 the quantities Π, Λ and Φ are given as functions of chemical potential. One can see Van Hove points and a logarithmic singularity of $\Pi(Q,0)$. The dependence of chemical potential μ upon n is shown in figure 2. The full curve presents the calculation with equation (3.8) or (3.15) for the paramagnetic phase in the limit $T \to 0$. In both cases the equation for μ reduces to the following:

$$n = n_0 + \frac{2}{N}\sum_k [f(\xi(k)] - f(0)]. \tag{4.14}$$

At $\mu = 0$ the chemical potential has a jump because of the jump in the quantity n_0 from 0 to 1. The physical nature of this jump is connected with the change of electron states when passing the point $\mu = 0$. In it the system undergoes a crossover from itinerant magnetism to magnetism with localized magnetic moments. In the last case an electron spends most of the time at a site and behaves like a localized magnetic moment. At the same time the electron hops from one site to another, being a delocalized object. Thus when $\mu > 0$ an electron exists as a superposition of localized and delocalized states. This leads to two contributions on the right-hand side of equation (4.14). We mentioned already that a step-like behaviour of n_0 is a result of a too simple approximation ignoring fluctuations. Their participation should give somewhat smoothed behaviour of the quantity n_0 and also chemical potential near the point $\mu = 0$.

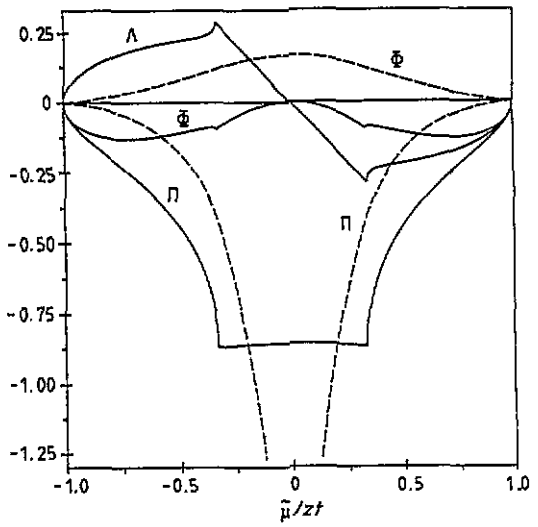


Figure 1. Electron loops as functions of chemical potential for sc lattice ($z = 6$): full curves, $\Phi(0,0)/zt$, $\Lambda(0,0)/zt$, $\Pi(0,0)/zt$; broken curves, $\Phi(Q,0)/zt$, $\Pi(Q,0)/zt$.

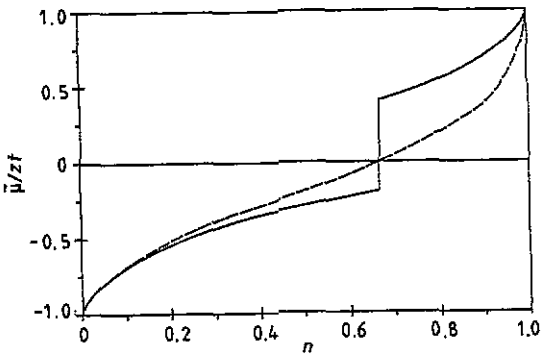


Figure 2. Electron concentration dependence of chemical potential for sc lattice: full curve, μ calculated from equation (4.14); broken curve, μ calculated from equation (4.15).

The broken curve in figure 2 gives the behaviour of chemical potential obtained from an equation very often used in the theories of strongly correlated systems [8–10]:

$$\tfrac{1}{2}n = (1 - \tfrac{1}{2}n)\frac{1}{N}\sum_{k} f(\xi(k)). \tag{4.15}$$

This equation is usually applied when electron states are taken in the 'Hubbard-I' approximation. Such an approximation does not take into account the change of electron states character with a change of electron concentration, and that is why it gives a smooth curve $\mu(n)$. Hereafter when calculating T_C and T_N we shall use equation (4.14) for the chemical potential.

It is obvious that in the dependence of the electron loops on n there will be a jump, which leads to a jump for T_C and T_N at $\mu = 0$, when $n = n_c = 2/3$ (see figure 3). One can

see a sharp decrease of T_N with deviation from half-filling. The changes of curves for T_C and T_N with increase of parameter κ develop in opposite directions, as one would expect from relation (4.13). When κ (exchange interaction) is increasing, T_N is also increasing but T_C is decreasing, and as a result when $\kappa \geqslant 0.15$ the antiferromagnetic state dominates. In the close vicinity of half-filling, ferromagnetism is absent owing to the fast increase of density of states in the electron spectrum near the top of a band. Comparison of curves for T_C and T_N shows that there is a region of overlap of the ferromagnetic and antiferromagnetic states. This overlap is seen better in figure 4, where magnetic phase diagrams are shown for different temperatures. When $T = 0$ the ferromagnetic (F) and antiferromagnetic (A) phases occupy almost the whole part of the $(t/U, n)$ plane with $n > n_c = 2/3$. When $n < n_c$ the paramagnetic phase is realized. Calculations for a square lattice lead to quantitatively close results, which is why we do not present them. Such coincidence is quite natural because the MFA is not sensitive to the space dimension.

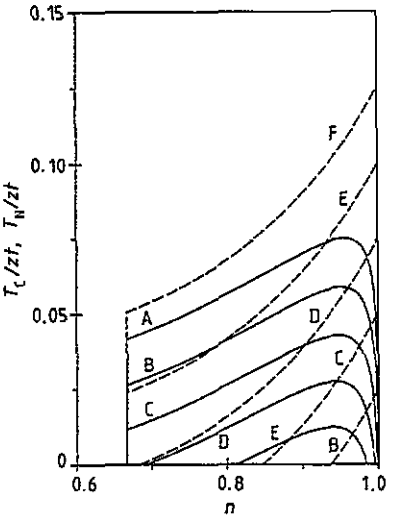


Figure 3. Dependence of Curie (full curves) and Néel (broken curves) temperatures on electron concentration at different values of parameter $\kappa = J/t = t/U$: (A) $\kappa = 0$, (B) $\kappa = 0.05$, (C) $\kappa = 0.10$, (D) $\kappa = 0.15$, (E) $\kappa = 0.20$, (F) $\kappa = 0.25$; μ is determined from equation (4.14).

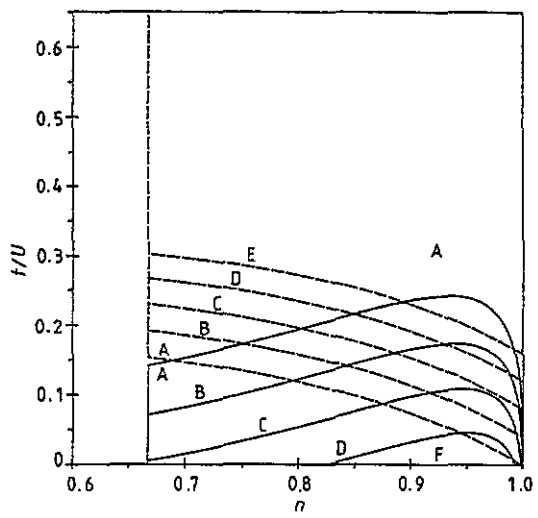


Figure 4. Magnetic phase diagram on the $(t/U, n)$ plane at different temperatures ($\tau = T/zt$): (A) $\tau = 0$, (B) $\tau = 0.02$, (C) $\tau = 0.04$, (D) $\tau = 0.06$, (E) $\tau = 0.08$; μ is determined from equation (4.14).

We presented results based on equation (4.14) for μ. For comparison some results are given in figure 5 when equation (4.15) is used for chemical potential. An essential difference in the results shown in figures 3 and 5 occurs near the critical concentration n_c. Beyond its vicinity the results for T_C and T_N differ only quantitatively. It should be emphasized that equation (4.15) has no serious grounds. In its derivation is used an expression $\langle X_i^{\sigma\sigma} \rangle$ through the electron Green function, based on the algebraic identity $X_i^{\sigma\sigma} = X_i^{\sigma 0} X_i^{0\sigma}$. However, one could use another identity $X_i^{\sigma\sigma} = X_i^{\sigma\pm} X_i^{\pm\sigma}$ and express $\langle X_i^{\sigma\sigma} \rangle$ in terms of the boson Green function. It is possible also to use an arbitrary combination of both identities. With using such an approach, we face ambiguous results for representation of the average number of electrons $n = \langle X_i^{++} \rangle + \langle X_i^{--} \rangle$. Because of that, the direct calculation of $\langle X_i^{\sigma\sigma} \rangle$ through graphical expansion is preferable, as was described in section 2.

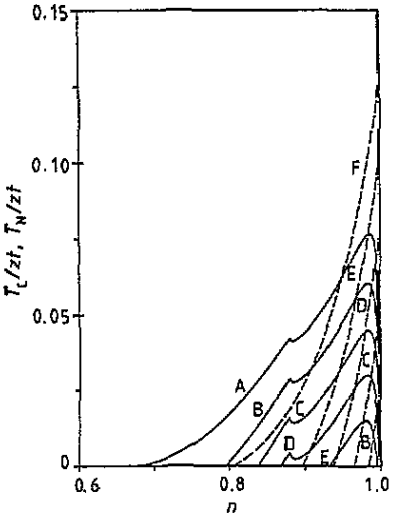


Figure 5. Curie (full curves) and Néel (broken curves) temperatures calculated with the chemical potential determined from equation (4.15) (curves have the same meaning as in figure 3).

5. Behaviour of the order parameters

In this section we present the results of numerical solution of equations for the order parameters at $T = 0$ for the ferromagnetic and antiferromagnetic case. The solutions of equations (3.6)–(3.8) and (3.13)–(3.15) for the SC lattice are given in figures 6 and 7. A linear dependence of curve A in figure 6 means a state of saturated ferromagnetism $m = n$. For a ferromagnet including the exchange interaction, the linear behaviour of m with electron concentration persists in a wide interval of n except for the vicinity of point $n = 1$, where magnetization $m \to 0$ when $n \to 1$. When n deviates from 1, both parameters m and Δ pass through maxima but these maxima lie on different ends of the interval $n_c < n < 1$.

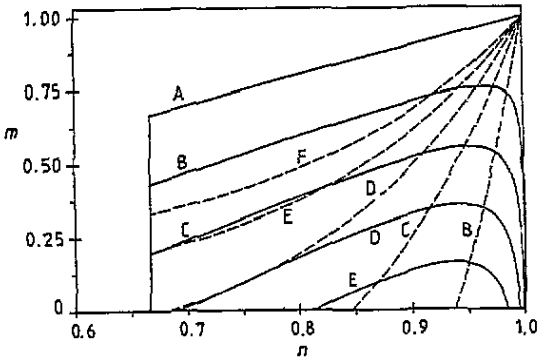


Figure 6. Electron concentration dependence of the order parameter m for ferromagnetic state (full curves) and antiferromagnetic state (broken curves) (curves have the same meaning as in figure 3).

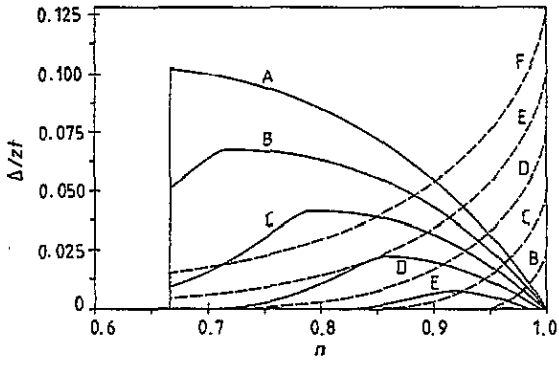


Figure 7. Electron concentration dependence of the order parameter Δ for ferromagnetic state (full curves) and antiferromagnetic state (broken curves) (curves have the same meaning as in figure 3).

As for the antiferromagnet, one can see that at $n = 1$ the order parameter $m = 1$ at any κ, that is the magnetization of a sublattice has the maximal value, while the gap Δ depends on κ and correlates with the value of T_N. It is possible to see this analytically from the analysis of equations (3.13)–(3.15) when $T = 0$ and $n = 1$. They have the form:

$$m = 1 - 2\int_{\mu_0}^{tz} d\varepsilon\, \rho_0(\varepsilon)\frac{\Delta}{(\alpha^2\varepsilon^2 + \Delta^2)^{1/2}} \tag{5.1}$$

$$\Delta = \tfrac{1}{2}\kappa tzm - \tfrac{1}{2}m\int_{\mu_0}^{tz} d\varepsilon\, \rho_0(\varepsilon)\frac{\varepsilon^2}{(\alpha^2\varepsilon^2 + \Delta^2)^{1/2}} \tag{5.2}$$

$$1 = \int_{-tz}^{\mu_0} d\varepsilon\, \rho_0(\varepsilon) \tag{5.3}$$

where

$$\mu_0 = (1/\alpha)(\mu^2 - \Delta^2)^{1/2} \qquad \alpha = \tfrac{1}{2}(1 - m^2)^{1/2}.$$

From equation (5.3) one finds that $\mu_0 = tz$. Then from equations (5.1) and (5.2) it follows that

$$m = 1 \qquad \Delta/tz = \tfrac{1}{2}\kappa. \tag{5.4}$$

Let us return now to formula (4.12) for T_N. When $n = 1$ we have $\Phi(Q, 0) = \Pi(Q, 0) = 0$, $n_0 = 1$, so we get

$$T_N/tz = \tfrac{1}{2}\kappa. \tag{5.5}$$

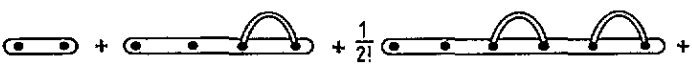
By comparison of (5.4) and (5.5) we find that at half-filling $\Delta = T_N$. However, this equality is approximate, because in equation (4.12) for T_N at $n \simeq 1$ it is necessary to take into account the linear term with respect to T. This decreases the value of T_N by a factor $C \geqslant 1$. Thus, when $n = 1$ the ratio of Δ to T should be

$$\Delta/T_N = C \geqslant 1. \tag{5.6}$$

6. Role of Gaussian fluctuations

Now we discuss the parameter n_0, which describes the crossover from itinerant magnetism to magnetism with localized magnetic moments. The step-like behaviour of n_0 with electron concentration is the result of a rough approximation that ignores the spin and charge fluctuations. Earlier we have made an attempt to take into account the Gaussian fluctuations when calculating n_0, and have shown that they decrease n_0 when $n > n_c$ but do not remove the finite jump of n_0 at the point $n = n_c$ [11]. However, these calculations were not self-consistent, which is why we reproduce them in a self-consistent approach.

Let us consider the paramagnetic phase. The parameter n_0 is expressed through a derivative of a zero-order cumulant $\langle X_i^{++}\rangle - \langle X_i^{--}\rangle$ with respect to the magnetic field. The derivative itself is a first-order cumulant [11]. Consider a series including two-tail elements in all orders of approximation. It can be symbolically represented in the form:



(6.1)

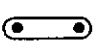
The sum of this series is represented by the following integral [12]:

$$\frac{1}{(\pi\Delta y)^{1/2}}\int_{-\infty}^{\infty} d\eta \exp(-\eta^2/\Delta y)\varphi(x+\eta). \tag{6.2}$$

Here $\varphi(x)$ is a function corresponding to the first term in the series (6.1), and $x = \mu/T$. Parameter η gives a fluctuation change of the parameter x. The magnitude η should be averaged with a Gaussian distribution function with dispersion

$\Delta y =$  (6.3)

Formulae (6.1)–(6.3) have a general character. By choice of a proper cumulant



we obtain the following expression for the magnitude n_0 dressed by the Gaussian spin fluctuations (we denote the dressed magnitude n_0 by $\tilde{n}_0$):

$$\tilde{n}_0 = \frac{1}{(\pi\Delta y)^{1/2}}\int_{-\infty}^{\infty} d\eta \exp(-\eta^2/\Delta y)\frac{2e^x}{1+2e^x\cosh\eta}\frac{1}{\cosh\eta} \tag{6.4}$$

where

$$\Delta y = -\frac{1}{T}\frac{1}{N}\sum_k \frac{\Phi(k,0)+J(k)}{d(k,0)}. \tag{6.5}$$

Here $d(k,0)$ is the denominator of the magnetic susceptibility (1.5) at zero frequency. With use of (4.3) or (4.12) for the temperature of magnetic phase transition T_m, formula (6.5) can be represented in the form:

$$\Delta y = \frac{1}{2n_0}\frac{1}{N}\sum_k \frac{T_m - bk^2}{T - T_m + bk^2}. \tag{6.6}$$

The sum over k goes only over the vicinity of point $k = 0$ for a ferromagnet and $k = Q$ for an antiferromagnet. From (6.6) an estimation for the average quadratic fluctuation can be made:

$$\Delta y = \frac{1}{n_0}\frac{T_C}{4\pi^2 b}a^3 k_0 = \frac{\delta y}{n_0} \tag{6.7}$$

where k_0 is the cut-off wavevector and a is the lattice parameter.

Expression (6.7) has to be substituted in (6.4). If in (6.7) we change the factor n_0 to the dressed factor $\tilde{n}_0$, we arrive at a self-consistent equation, which in the limit $T \ll \mu$ is written in the form:

$$\tilde{n}_0 = \frac{1}{(\pi\delta y)^{1/2}}\int_{-\infty}^{\infty} d\eta \exp(-\eta^2/\delta y)\frac{1}{\cosh^2(\eta/\tilde{n}_0)}. \tag{6.8}$$

The dependence of $\tilde{n}_0$ on δy is presented in figure 8. We see some decrease of $\tilde{n}_0$ with parameter δy. However, since $\delta y \lesssim 1$, the change of $\tilde{n}_0$ is small compared with the value $n_0 = 1$ even in the self-consistent case. Thus the Gaussian fluctuations do not influence much the crossover near the point n_c. At this point obviously all fluctuations are important and perturbation theory breaks down.

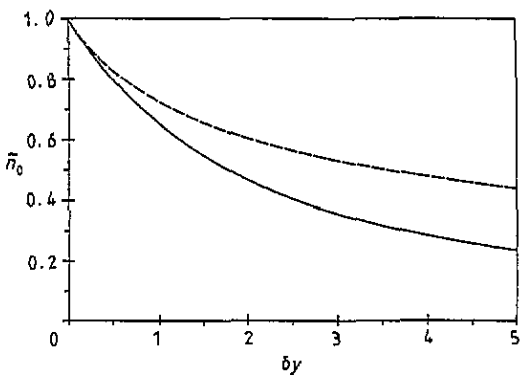


Figure 8. Dependence of $\tilde{n}_0$ on the strength of magnetic Gaussian fluctuations δy: full curve, self-consistent calculations; broken curve, perturbation theory calculations.

7. Conclusions

The main result of this paper is the derivation of mean-field equations for the $(t–J)$ model. Being generally one of the simplest approximations in many-body theories, the MFA for the $(t–J)$ model turned out to be non-trivial because of the very complicated Hamiltonian taking into account the condition of not allowing two electrons to be at one site. Use of the representation of the Hamiltonian through the X-operators allows most effective retention of this condition in any concrete approximation.

Contrary to the usual Fermi systems, where MFA reduces to the formulation of some self-consistent equation for the self-energy part Σ_σ, in the $(t–J)$ model such an equation should

be accompanied by an equation for the average electron number n_σ at a site. However, n_σ is not expressed through the electron Green function but demands the summation of infinite series of diagrams for n_σ. These series, as we could see, converge to a simple analytical form allowing us to write a coupled system of equations for n_σ and Σ_σ.

From the general diagram equations for Σ_σ and n_σ the equations for the order parameters m and Δ follow that describe ferromagnetic and antiferromagnetic phases. The presence of two coupled order parameters appearing simultaneously reflects the dual behaviour of the strongly correlated system being an itinerant and a localized magnet at the same time. It is remarkable that the boundary of magnetically ordered phase stability coincides with the boundary of the paramagnetic phase instability with respect to corresponding magnetic ordering. This implies that a phase transition from paramagnetic phase to ferromagnetic or antiferromagnetic phase is a second-order phase transition. It means that the same connection exists between GRPA and MFA for the $(t$–$J)$ model as between RPA and MFA in the usual Fermi system theory. In both cases the conditions of zero-frequency magnetic susceptibility of paramagnetic phase divergence coincide with the conditions for the magnetic phase transition, which follow from the zero value of the magnetic order parameters determined by MFA.

From our approach, reasonable results follow for the magnetic phase transition description, particularly the electron concentration dependence of T_C and T_N. One circumstance is unsatisfactory: the behaviour of the system near the critical electron concentration n_c, where the system undergoes a crossover from itinerant magnetism to magnetism with localized magnetic moments. This crossover is too sharp with change of n_0 from 0 to 1. As a result of such behaviour of n_0, the chemical potential jumps at the point $n = n_c$, which leads to jumping of curves on the magnetic phase diagram. Certainly such step-like behaviour of n_0 is a result of ignoring the spin and charge fluctuations in the system. However, our analysis has shown that even a self-consistent approach taking into account the Gaussian fluctuations of spins does not eliminate this jump. It is clear that near n_c all strongly interacting fluctuations are important, and at the point n_c perturbation theory breaks down. In this sense, this is a peculiar point as a second-order phase transition point or as a mobility edge in the theory of localization. For this reason in all the presented figures the vicinity of this point should be cut off. Beyond its vicinity the difference in results based on the different equations for chemical potential are not too contradictory. Rigorous calculation of critical concentration n_c, as a point of the crossover, and the behaviour of physical quantities in its vicinity appear to be a challenging theoretical problem.

Another, more solvable but nevertheless rather difficult, problem for the $(t$–$J)$ model is the calculation of the fluctuation (spin-wave) spectrum in a magnetically ordered phase. For its solution it is necessary to calculate the magnetic susceptibility for ferromagnetic and antiferromagnetic phases. Then its poles should give the spin-wave spectrum. For this it is necessary to use equations for magnetic order parameters characterizing the ground state of a magnetically ordered phase. Such equations have been obtained in the present paper, and the dependence of the order parameters upon electron concentration have been calculated numerically. Now the second step should be taken, namely, the calculation of the fluctuation spectrum above this ground state. Such calculations are now in progress.

One of the preliminary results of such study concerns the contraction of MF region for a ferromagnetic state due to instability of spin waves [13]. Particularly, for the case $U = \infty$ a ferromagnetic state becomes unstable already at values n higher than $n_c = 2/3$. Similarly to the case of the weak Coulomb interaction in the strong U limit, quantum fluctuations decrease the tendency of a system to ferromagnetism. Probably we shall have the same

result for an antiferromagnetic state. Thus in the strong U limit a general feature of MFA to overestimate the tendency to magnetic ordering will persist.

Generally the problem of ferromagnetism in the strong U limit is still not resolved yet. The ferromagnetic state, expected from Nagaoka's rigorous result for one hole in a half-filled case [14], turned out not to be thermodynamically stable [15] at finite concentration of holes. However, ferromagnetism was found for several non-cubic lattices in the case of the Hubbard model (see [16] and references therein). Some discussion of the various controversial results about ferromagnetism in the Hubbard and $(t–J)$ models has been presented in our earlier paper [17], but we intend to give an up-to-date discussion of this problem soon in connection with the spin-wave analysis of the $(t–J)$ model [13].

In conclusion, we briefly discuss the status of a mean-field-type approximation approach suggested in the present paper from the point of view of exact solutions for the itinerant strongly correlated models obtained recently from the limit of infinite dimension ($d = \infty$) [18]. 'In this situation the exact solution of a fermionic lattice model in the limit $d \to \infty$ provides an ideal mean-field solution for these models which has all the desired features of a comprehensive MF theory: it is a self-consistent, conserving approximation which is valid for all input parameters and can be systematically improved by taking $1/d$ corrections into account' [19].

According to this statement, the MF theory for the $(t–J)$ model should be based on the limit $d \to \infty$. If we consider the $(t–J)$ model as a limiting case $U \gg t$ of the Hubbard model, the MF theory for the $(t–J)$ model should appear from the Hubbard model in the limit $d \to \infty$. One has to remember, however, that the Hamiltonian of the $(t–J)$ model is derived from the Hamiltonian of the Hubbard model only near half-filling ($1 - n \ll 1$) [20]. To treat the $(t–J)$ model as a fundamental model with independent parameters t and J, the MF theory should be derived directly from the $d \to \infty$ limit of the $(t–J)$ model. Notice that expansion over $1/d$ was applied recently to study a hole in the $(t–J)$ model [21]. Now we know that in the $d \to \infty$ limit the Hubbard model maps onto a single impurity model with appropriate parameters, which can be exactly solvable numerically [22–26].

Our MF-type approximation is not the MF theory in the statistical mechanics sense (similarly the Hartree–Fock approach for a Fermi liquid is not the MF theory in that sense). However, our self-consistent approach is convenient for two reasons: first, it is an analytical one; and, second, it allows easy introduction of order parameters. For the $(t–J)$ model our MF-type approach is valid for the interval of electron concentration $n_c < n < 1$ besides its two edges: the vicinity of the critical concentration n_c and half-filling. Inside of this interval the $(t–J)$ model describes the dual behaviour of a system with both itinerant and localized features.

Acknowledgment

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