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Spin waves in a Hubbard antiferromagnet

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Abstract. The Hubbard model of an itinerant antiferromagnet (in particular, a Mott insulator) is considered. Starting from the generalised Hartree–Fock approximation, an expansion in the fluctuating part of the Coulomb interaction is developed. The magnon spectrum, corrections to the electron spectrum, the amplitude of the local moment and the total energy are calculated in the spin-wave region for arbitrary values of the Hubbard parameter U. A comparison with corresponding results within the framework of the s–d exchange model is carried out.

1. Introduction

The problem of describing itinerant magnets with strong Mott–Hubbard correlations is still being extensively investigated. Modern band theory (spin-density functional approach, usually using the local approximation) is apparently insufficient to solve it (see recent band calculations of transition metal oxides by Terakura *et al* (1984) and the discussion by Anderson (1988)). On the other hand, Hubbard's approach enables one to obtain easily the splitting in the paramagnetic region. However, this theory leads to serious difficulties in the treatment of the antiferromagnetic (AFM) ground state of the Mott insulator. In particular, the AFM cannot be obained self-consistently within the Hubbard-I (1963) approximation, and the corresponding electron spectrum contains four sub-bands (see, e.g., Khomsky 1970). A variational description of the AFM state and Mott transition within the generalised Hartree–Fock approximation was considered by Katsnelson and Irkhin (1984).

In the present paper we provide a more accurate treatment of the AFM state in the Hubbard model at low temperatures (in the spin-wave region). Using the generalised Hartree–Fock approximation as the zero-order approximation, we develop an expansion in the fluctuating part of the Coulomb interaction. This approach is a kind of perturbation theory in the inverse nearest-neighbour number $1/z$. (Formally, each order in $1/z$ corresponds to a summation over a wavevector.) In § 2 we discuss the zero-order approximation and calculate the spin-wave spectrum. The results obtained are valid for arbitrary U's; they describe both the limit of large U's (Anderson superexchange) and the RKKY limit. In § 3 we obtain electron spectrum corrections due to electron–magnon interactions. In § 4 we calculate the number of doubles (i.e., the local moment on a site) and the corresponding contribution to the ground-state energy. In the Appendix we consider the same problems for the case of the s–d exchange model and demonstrate that the models have similar properties.

2. Calculation of the spin-wave spectrum

We proceed with the Hubbard Hamiltonian

$$H = \sum_{k\sigma} t_k c^+_{k\sigma} c_{k\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} . \tag{1}$$

In an antiferromagnet with the magnetic structure corresponding to the wavevector $\boldsymbol{\kappa}$, AFM ordering leads to splitting of the conduction band into two Slater sub-bands described by new electron creation operators,

$$\begin{aligned} \alpha^+_k &= A_k c^+_{k+\kappa/2\uparrow} + B_k c^+_{k-\kappa/2\downarrow} \\ \beta^+_k &= A_k c^+_{k-\kappa/2\downarrow} - B_k c^+_{k+\kappa/2\uparrow} \qquad A^2_k + B^2_k = 1. \end{aligned} \tag{2}$$

Within the generalised Hartree–Fock approximation, the AFM ground state of the Mott–Hubbard insulator is given by the trial function

$$|\psi\rangle = \prod_k \alpha^+_k |0\rangle \tag{3}$$

so that the lower Slater sub-band is completely filled and the upper one is empty. As for metallic states with partly filled Slater sub-bands, we have

$$|\psi^{(1)}_{\mathrm{met}}\rangle = \prod_{k<k_{\mathrm{F}}} \alpha^+_k |0\rangle \tag{4}$$

$$|\psi^{(2)}_{\mathrm{met}}\rangle = \prod_{k<k_{\mathrm{F}}} \beta^+_k \prod_k \alpha^+_k |0\rangle. \tag{5}$$

The function (3) does not conserve the total spin z-projection and is therefore not quite satisfactory. This problem was discussed by Katsnelson and Irkhin (1984) who considered another trial function, which described an exciton condensate and was an eigenfunction of the operator S^z (see also Vonsovsky *et al* 1986). Using the exciton approach, we can investigate corrections to the Hartree–Fock zero approximation, e.g., spin-wave excitations (for a comparison see the consideration of the Heisenberg model by Irkhin and Katsnelson 1986). However, we shall exploit, for simplicity, the standard transformation (2) which introduces anomalous averages $\langle c^+_{k\uparrow} c_{k-\kappa\downarrow} \rangle$.

Diagonalising the Hamiltonian (1) with the use of (2) we obtain two quasi-particle bands with the energies

$$\mathscr{E}_{k\alpha} = \theta_k - \mathscr{E}_k \qquad \mathscr{E}_{k\beta} = \theta_k + \mathscr{E}_k . \tag{6}$$

Here we introduce the notations

$$\mathscr{E}_k = (\tau^2_k + U^2 \bar{S}^2)^{1/2}$$

$$\theta_k = \tfrac{1}{2}(t_{k+\kappa/2} + t_{k-\kappa/2}) \qquad \tau_k = \tfrac{1}{2}(t_{k+\kappa/2} - t_{k-\kappa/2})$$

$$\bar{S} = \sum_k \langle c^+_{k\uparrow} c_{k-\kappa\downarrow} \rangle = \sum_k A_k B_k (n_{k\alpha} - n_{k\beta})$$

$$n_{k\alpha} = \langle \alpha^+_k \alpha_k \rangle = f(\mathscr{E}_{k\alpha}) \qquad n_{k\beta} = \langle \beta^+_k \beta_k \rangle = f(\mathscr{E}_{k\beta})$$

where $f(E)$ is the Fermi function. The quantity $2U\bar{S}$ is the direct energy gap. For A_k, B_k, $\bar{S}$ we obtain the equations

$$A_k^2 = \tfrac{1}{2}(1 - \tau_k/\mathscr{E}_k) \qquad B_k^2 = \tfrac{1}{2}(1 + \tau_k/\mathscr{E}_k) \tag{7}$$

$$1 = \frac{U}{2}\sum_k \frac{n_{k\alpha} - n_{k\beta}}{(\tau_k^2 + U^2\bar{S}^2)^{1/2}}. \tag{8}$$

To consider properly the spin degrees of freedom, it is suitable to the local coordinate system by introducing the electron operators

$$d_{k\sigma}^+ = (1/\sqrt{2})(c_{k+\kappa/2\uparrow}^+ + \sigma c_{k-\kappa/2\downarrow}^+) \qquad \sigma = \uparrow, \downarrow\ (\pm). \tag{9}$$

Then the Hamiltonian (1) takes the form

$$H = \sum_{k\sigma}(\theta_k d_{k\sigma}^+ d_{k\sigma} + \tau_k d_{k\sigma}^+ d_{k-\sigma}) + U\left(\sum_k d_{k\downarrow}^+ d_{k\downarrow} - \sum_q S_{-q}^- S_q^+\right)$$

where S_q^i is the Fourier transform of spin-density operators,

$$S_q^\sigma = \sum_k d_{k\sigma}^+ d_{k+q,-\sigma}, \qquad S_q^z = \tfrac{1}{2}\sum_{k\sigma} \sigma d_{k\sigma}^+ d_{k+q\sigma}$$

($\langle S_0^z \rangle = \bar{S}$ is the sub-lattice magnetisation).

The magnon spectrum is determined by the poles of the commutator retarded spin Green functions

$$G^\sigma(q\omega) = \langle\langle S_q^\sigma | S_{-q}^- \rangle\rangle_\omega.$$

The corresponding equation of motion reads

$$\omega G^+(q\omega) = 2\bar{S} + \sum_k \langle\langle(\theta_{k+q} - \theta_k)d_{k\uparrow}^+ d_{k+q\downarrow} + \tau_{k+q} d_{k\uparrow}^+ d_{k+q\uparrow} - \tau_k d_{k\downarrow}^+ d_{k+q\downarrow} | S_{-q}^- \rangle\rangle_\omega. \tag{10}$$

Expressing the operators $d_{k\sigma}^+$ in terms of α_k^+, β_k^+, using (2) and representing the Hamiltonian in the form

$$H = \sum_k (\mathscr{E}_{k\alpha}\alpha_k^+\alpha_k + \mathscr{E}_{k\beta}\beta_k^+\beta_k) + H_{\text{int}} \tag{11}$$

we can construct a perturbation theory with respect to the fluctuating part of the Coulomb interaction

$$H_{\text{int}} = -U\Delta\sum_q S_{-q}^- S_q^+$$

(Δ means that the Hartree–Fock decouplings must be excluded when treating H_{int}). To first order, we may carry out decouplings of the type

$$\Delta\langle\langle \alpha_k^+ \alpha_{k+p} S_{q-p}^\sigma | S_{-q}^- \rangle\rangle \simeq n_{k\alpha}\delta_{p0} G^\sigma(q\omega).$$

Then we obtain the system

$$\begin{aligned}[]
[\omega - \mathscr{C}(q\omega)]G^+(q\omega) &= 2\bar{S} + \mathscr{E}(q\omega) + \mathscr{D}(q\omega)G^-(q\omega) \\
[\omega + \mathscr{C}(q, -\omega)]G^-(q\omega) &= \mathscr{F}(q\omega) + \mathscr{D}(q, -\omega)G^+(q\omega)
\end{aligned} \tag{12}$$

where the functions $\mathscr{C}, \mathscr{D}, \mathscr{E}, \mathscr{F}$ are linear combinations of the expressions

$$(n_{ki} - n_{k+qj})/(\omega + \mathscr{E}_{ki} - \mathscr{E}_{k+qj}) \qquad (i, j = \alpha, \beta).$$

The magnon spectrum is given by

$$\omega_q^2 = \mathscr{C}^2(\boldsymbol{q}0) - \mathscr{D}^2(\boldsymbol{q}0). \tag{13}$$

On substituting the values of the coefficients A_k, B_k, a little manipulation yields

$$\omega_q^2 = \frac{U^4\bar{S}^2}{4}\left\{\sum_k\left[\frac{2}{\mathscr{E}_k}(n_{k\alpha}-n_{k\beta}) + \left(1-\frac{U^2\bar{S}^2}{\mathscr{E}_k\mathscr{E}_{k+q}}\right)\right.\right.$$
$$\left.\left.\times\left(\frac{n_{k\alpha}-n_{k+q\alpha}}{\mathscr{E}_{k\alpha}-\mathscr{E}_{k+q\alpha}} + \frac{n_{k\beta}-n_{k+q\beta}}{\mathscr{E}_{k\beta}-\mathscr{E}_{k+q\beta}}\right) + 2\left(1+\frac{U^2\bar{S}^2}{\mathscr{E}_k\mathscr{E}_{k+q}}\right)\frac{n_{k\alpha}-n_{k+q\beta}}{\mathscr{E}_{k\alpha}-\mathscr{E}_{k+q\beta}}\right]\right\}^2$$
$$-\frac{U^4\bar{S}^2}{4}\left[\sum_k\frac{\tau_k}{\mathscr{E}_k}\frac{\tau_{k+q}}{\mathscr{E}_{k+q}}\left(\frac{n_{k\alpha}-n_{k+q\alpha}}{\mathscr{E}_{k\alpha}-\mathscr{E}_{k+q\alpha}} + \frac{n_{k\beta}-n_{k+q\beta}}{\mathscr{E}_{k\beta}-\mathscr{E}_{k+q\beta}} - 2\frac{n_{k\alpha}-n_{k+q\beta}}{\mathscr{E}_{k\alpha}-\mathscr{E}_{k+q\beta}}\right)\right]^2. \tag{14}$$

First, we consider the narrow-band case, where $|t_k| \ll U$. For the half-filled band we get ($\bar{S} \simeq 1/2$)

$$\omega_q^2 = \tfrac{1}{2}(J_\kappa - J_q)(2J_\kappa - J_{\kappa+q} - J_{\kappa-q}) \tag{15}$$

$$J_q = -(2/U)\sum_k t_k t_{k+q}. \tag{16}$$

Expression (15) has a form typical for the Heisenberg exchange, J_q being Fourier transforms of the exchange parameters. Thus we obtain a generalisation of the corresponding result of Anderson's (1963) superexchange theory, derived in the nearest-neighbour approximation, where $J_{ij} = -2t_{ij}^2/U$.

Now we discuss the case where $U \to \infty$ and the upper sub-band is partly filled (the function (5), $n_{k\alpha} = 1$, $n_{k\beta} = n_k \equiv f(\theta_k)$), so that the current carriers induce a non-Heisenbergian double-exchange interaction. We have

$$\omega_q^2 = \left[J_\kappa^{\mathrm{H}} - J_q^{\mathrm{H}} + \sum_k\left((\theta_{k+q}-\theta_k)n_k + \tau_k(\tau_{k+q}+\tau_k)\frac{n_{k+q}-n_k}{\theta_{k+q}-\theta_k}\right)\right]$$
$$\times\left[\tfrac{1}{2}(2J_\kappa^{\mathrm{H}} - J_{\kappa+q}^{\mathrm{H}} - J_{\kappa-q}^{\mathrm{H}}) + \sum_k\left((\theta_{k+q}-\theta_k)n_k\right.\right.$$
$$\left.\left.-\tau_k(\tau_{k+q}-\tau_k)\frac{n_{k+q}-n_k}{\theta_{k+q}-\theta_k}\right)\right]. \tag{17}$$

We retain here the Heisenbergian exchange J_q^{H} (say, the superexchange (16), or another exchange interaction added to the Hamiltonian), which is needed to stabilise the AFM ground state. This expression coincides with that obtained within the s–d exchange model using the Hubbard (1965) X-operators (Irkhin and Katsnelson 1988c). For the s–d exchange parameter $|I| \to \infty$, the latter model is equivalent to the Hubbard model in the quasi-classical limit where spin $S \gg 1$ (Nagaev 1983), and also for $S = \frac{1}{2}$ (with the replacement $t_k \to t_k/2, I < 0$). For finite U and I both models have similar properties (see below and especially the Appendix). Because of the imaginary parts of the denominators in (17), spin waves acquire at $T = 0$ a large damping, which has only a formal smallness ($\gamma_q/\omega_q = \text{const} \sim 1/z, q \to 0$).

In the broad-band limit $U \ll W$ (W is the band width), we expand expression (14) in U. We have ($f_k = f(t_k)$)

$$\omega_q^2 = 2\bar{S}^2(J_{\kappa 0} - J_{q0})(2J_{\kappa 0} - J_{\kappa+q,0} - J_{\kappa-q,0}) \tag{18}$$

$$J_{p\omega} = J_p^{\mathrm{H}} + J_{p\omega}^{\mathrm{RKKY}} \qquad J_{p\omega}^{\mathrm{RKKY}} = U^2\sum_k\frac{f_k - f_{k+p}}{\omega + t_{k+p} - t_k}. \tag{19}$$

This result coincides with that of the RKKY perturbation theory, in which I is replaced by U (Irkhin and Katsnelson 1988a). Thus, a RKKY-type exchange takes place also in the Hubbard model. Note that our approach yields an explicit expression for the magnon spectrum, unlike the RPA approach due to Young (1975) and Kuzmin and Ovchinnikov (1977).

Expression (18) enables one to calculate the magnon damping $\gamma = -\mathrm{Im}\omega$ if we make the replacement $J_{p0} \rightarrow J_{p,\omega+i0}$. At small q and $T = 0$, γ_q/ω_q is a constant of order U^2/W^2. It is worthwhile to mention that the damping is absent in the case of an insulator ($n_{k\alpha} = 1$, $n_{k\beta} = 0$), since only transitions between the sub-bands α and β make a contribution and $\mathrm{Im}\omega \neq 0$ at

$$\omega > \min(\mathscr{E}_{k\beta} - \mathscr{E}_{k+q\alpha}) = \delta \tag{20}$$

with $\delta \simeq U^2\bar{S}^2/W$ ($U\bar{S} \ll W$) being the indirect energy gap.

3. The electron spectrum

Now we treat the electron spectrum. In the zero-order approximation we have

$$\langle\langle d_{k\uparrow}|d^{+}_{k\uparrow}\rangle\rangle_E = \frac{1}{2}\left(\frac{(A_k + B_k)^2}{E - \mathscr{E}_{k\alpha}} + \frac{(A_k - B_k)^2}{E - \mathscr{E}_{k\beta}}\right) \tag{21}$$

$$\langle\langle d_{k\downarrow}|d^{+}_{k\uparrow}\rangle\rangle_E = \frac{1}{2}\left(\frac{A_k^2 - B_k^2}{E - \mathscr{E}_{k\alpha}} - \frac{A_k^2 - B_k^2}{E - \mathscr{E}_{k\beta}}\right) \tag{22}$$

so that the anticommutator electron Green functions have a two-pole structure. To find corrections due to spin fluctuations, we pass to the operators α_k, β_k and write equations of motion, e.g.

$$(E - \mathscr{E}_{k\alpha})\langle\langle \alpha_k|d^{+}_{k\uparrow}\rangle\rangle_E = L^{+}_k/\sqrt{2} - (U/2)\sum_q \Delta\langle\langle L^{+}_k(L^{-}_{k+q}\alpha_{k+q} - L^{+}_{k+q}\beta_{k+q})S^{-}_{-q}$$
$$+ L^{-}_k S^{+}_{-q}(L^{+}_{k+q}\alpha_{k+q} + L^{-}_{k+q}\beta_{k+q})|d^{+}_{k\uparrow}\rangle\rangle_E \qquad (L^{\mp}_k = A_k \pm B_k). \tag{23}$$

When calculating the Green functions, which arise, we may carry out to first-order the decouplings

$$\Delta\langle\langle S^{i}_{-q}S^{j}_{p}d_{k+q-p,\sigma}|d^{+}_{k\uparrow}\rangle\rangle_E \simeq \delta_{qp}\chi^{ij}_q\langle\langle d_{k\sigma}|d^{+}_{k\uparrow}\rangle\rangle_E \qquad \chi^{ij}_q \equiv \langle S^{i}_{-q}S^{j}_q\rangle,$$

and substitute (21) and (22). Then, according to the Dyson equation, the first-order corrections to the one-electron energies E_{ki} are determined by the coefficients of the singular factor $(E - \mathscr{E}_{ki})^{-2}$ after substituting $E \rightarrow \mathscr{E}_{ki}$. A similar procedure was used by Irkhin and Katsnelson (1988c) to investigate the electron spectrum in a ferromagnet with Hubbard sub-bands. We have

$$E_{k\alpha,\beta} = \theta_k \mp (\tau_k^2 + U^2\bar{S}^2)^{1/2} + \frac{U^2}{2}\sum_q\left[\chi^{-+}_q\left(\frac{1 - U^2\bar{S}^2/\mathscr{E}_k\mathscr{E}_{k+q}}{\mathscr{E}_{k\alpha,\beta} - \mathscr{E}_{k+q\alpha,\beta}} - \frac{1 + U^2\bar{S}^2/\mathscr{E}_k\mathscr{E}_{k+q}}{\mathscr{E}_{k\alpha,\beta} - \mathscr{E}_{k+q\beta,\alpha}}\right)\right.$$
$$+ \chi^{--}_q\frac{\tau_k\tau_{k+q}}{\mathscr{E}_k\mathscr{E}_{k+q}}\left(\frac{1}{\mathscr{E}_{k\alpha,\beta} - \mathscr{E}_{k+q\alpha,\beta}} - \frac{1}{\mathscr{E}_{k\alpha,\beta} - \mathscr{E}_{k+q\beta,\alpha}}\right)$$
$$\mp U\bar{S}^2\left((\mathscr{E}_k^{-1} - \mathscr{E}_{k+q}^{-1})\frac{1 - 2n_{k+q\alpha,\beta}}{\mathscr{E}_{k\alpha,\beta} - \mathscr{E}_{k+q\alpha,\beta}}\right.$$

$$+ (\mathscr{E}_k^{-1} + \mathscr{E}_{k+q}^{-1}) \frac{1 - 2n_{k+q\beta,\alpha}}{\mathscr{E}_{k\alpha,\beta} - \mathscr{E}_{k+q\beta,\alpha}}\bigg)\bigg]. \tag{24}$$

To calculate the spin correlation functions χ_q^{ij} in the spin-wave region, we carry out a canonical transformation to magnon operators

$$S_q^+ = (2\bar{S})^{1/2}(u_q b_q - v_q b_{-q}^+) \qquad u_q^2 - v_q^2 = 1 \tag{25}$$

$$[b_q, H] \simeq \omega_q b_q \qquad \langle b_q^+ b_q \rangle = N_q = N(\omega_q) \tag{26}$$

$$\chi_q^{-+} = 2\bar{S}[(u_q^2 + v_q^2)N_q + v_q^2] \qquad \chi_q^{--} = -2\bar{S}u_q v_q(1 + 2N_q) \tag{27}$$

where $N(\omega)$ is the Bose function. As follows from (12), (25) and (26), the coefficients u_q, v_q obey the system

$$\begin{aligned} &(u_q^2 + v_q^2)\mathscr{E}(\boldsymbol{q}0) - 2u_q v_q \mathscr{D}(\boldsymbol{q}0) = 0 \\ &- 2u_q v_q \mathscr{E}(\boldsymbol{q}0) + (u_q^2 + v_q^2)\mathscr{D}(\boldsymbol{q}0) = 0 \end{aligned} \tag{28}$$

so that

$$u_q^2 = \tfrac{1}{2}(\mathscr{E}(\boldsymbol{q}0)/\omega_q + 1) \qquad v_q^2 = \tfrac{1}{2}(\mathscr{E}(\boldsymbol{q}0)/\omega_q - 1). \tag{29}$$

Consider the temperature dependence of the electron spectrum due to magnons. One has to take into account the contribution to the sub-lattice magnetisation in the second term of (24),

$$\delta\bar{S} = -\frac{1}{2\bar{S}}\sum_q \langle S_{-q}^- S_q^+ \rangle = -\sum_q [(u_q^2 + v_q^2)N_q + v_q^2]. \tag{30}$$

We obtain

$$\begin{aligned} \delta E_{k\alpha,\beta}(T) = U^2\bar{S}\sum_q N_q \bigg[&(u_q^2 + v_q^2)\left(\frac{1 - U^2\bar{S}^2/\mathscr{E}_k\mathscr{E}_{k+q}}{\mathscr{E}_{k\alpha,\beta} - \mathscr{E}_{k+q\alpha,\beta}} + \frac{1 + U^2\bar{S}^2/\mathscr{E}_k\mathscr{E}_{k+q}}{\mathscr{E}_{k\alpha,\beta} - \mathscr{E}_{k+q\beta,\alpha}}\right) \\ &-2u_q v_q \frac{\tau_k}{\mathscr{E}_k}\frac{\tau_{k+q}}{\mathscr{E}_{k+q}}\left(\frac{1}{\mathscr{E}_{k\alpha,\beta} - \mathscr{E}_{k+q\alpha,\beta}} - \frac{1 + U^2\bar{S}^2/\mathscr{E}_k\mathscr{E}_{k+q}}{\mathscr{E}_{k\alpha,\beta} - \mathscr{E}_{k+q\beta,\alpha}}\right) \\ &\pm (u_q^2 + v_q^2)\mathscr{E}_k^{-1}\bigg] \propto (T/T_{\mathrm{N}})^2. \end{aligned} \tag{31}$$

Using (31) and (14), it is easy to prove the relation

$$\delta E_{ki}/\delta N_q = \delta\omega_q/\delta n_{ki} = \delta^2\langle H \rangle/\delta N_q \delta n_{ki} \tag{32}$$

(see also § 4).

It should be noted that, unlike the case of a ferromagnet (see, e.g., Irkhin and Katsnelson 1988c), the vanishing of the magnon frequency at $q \to 0$ does not result in a weakening of the temperature dependence of the electron spectrum as compared with that of the sub-lattice magnetisation. This is due to non-linearity of the magnon spectrum in the electron occupation numbers. It is interesting that our perturbation theory yields finite corrections to the electron spectrum (as well as to the magnon frequency, see equation (17)) in the limit $U \to \infty$. For an almost half-filled band we get

$$E_{k\alpha,\beta} = \theta_k \mp \frac{U}{2} + \sum_q \left((\theta_{k+q} - \theta_k)\chi_q^{-+} - \chi_q^{+-} \frac{\tau_k^2 + \tau_{k+q}^2}{\theta_{k+q} - \theta_k} - \tfrac{1}{2}\chi_q^{--} \frac{\tau_k \tau_{k+q}}{\theta_{k+q} - \theta_k} - \tfrac{1}{2} \frac{\tau_{k+q}^2 - \tau_k^2}{\theta_{k+q} - \theta_k} \right). \tag{33}$$

This result is in agreement with that following from the equations obtained by Irkhin (1986) within the narrow-band s–d model using the many-electron Hubbard (1965) operators. (However, the present method does not enable one to consider the case where $\theta_k \equiv 0$, i.e., simple lattices in the nearest-neighbour approximation). On the other hand, at finite U (or I) the results of these two approaches are different since Hubbard I-type approximations give four sub-bands in a magnetically ordered state. The broad-band case, where $U \ll W$, is discussed in the Appendix.

4. The number of doubles, local moment and total energy

Finally, we investigate the spin-wave contribution to the total energy. To this end, we calculate the mean number of doubly occupied sites (doubles) N_2. This quantity is related to the mean square of the local moment by

$$\langle S_i^2 \rangle = \tfrac{3}{4}(n - 2N_2) \tag{34}$$

with n the number of electrons per site. Allowing for the spectral representation, we have

$$N_2 = \langle n_{i\uparrow} n_{i\downarrow} \rangle = \langle d_{i\uparrow}^+ S_i^+ d_{i\downarrow} \rangle = -\frac{1}{\pi} \sum_{kq} \int \mathrm{d}E\, f(E)\, \mathrm{Im}\, \langle\langle d_{k\uparrow} | d_{k+q\downarrow}^+ S_q^+ \rangle\rangle_E. \tag{35}$$

Proceeding as in previous sections, we derive

$$N_2 = \langle d_{i\uparrow}^+ d_{i\uparrow} \rangle \langle d_{i\downarrow}^+ d_{i\downarrow} \rangle + \frac{U}{2} \sum_{kq} \left\{ \chi_q^{-+} \left[\left(\frac{1 - P_k P_{k+q}}{\mathscr{E}_{k\alpha} - \mathscr{E}_{k+q\alpha}} + \frac{1 + P_k P_{k+q}}{\mathscr{E}_{k\alpha} - \mathscr{E}_{k+q\beta}} \right) n_{k\alpha} + \left(\frac{1 - P_k P_{k+q}}{\mathscr{E}_{k\beta} - \mathscr{E}_{k+q\beta}} + \frac{1 + P_k P_{k+q}}{\mathscr{E}_{k\beta} - \mathscr{E}_{k+q\alpha}} \right) n_{k\beta} \right] \right.$$
$$\left. + \chi_q^{--} \frac{\tau_k \tau_{k+q}}{\mathscr{E}_k \mathscr{E}_{k+q}} \left[\left(\frac{1}{\mathscr{E}_{k\alpha} - \mathscr{E}_{k+q\alpha}} - \frac{1}{\mathscr{E}_{k\alpha} - \mathscr{E}_{k+q\beta}} \right) n_{k\alpha} + \left(\frac{1}{\mathscr{E}_{k\beta} - \mathscr{E}_{k+q\beta}} - \frac{1}{\mathscr{E}_{k\beta} - \mathscr{E}_{k+q\alpha}} \right) n_{k\beta} \right] \right\}$$
$$+ U\bar{S} \sum_{kq} \left((1 + P_k)(1 - P_{k+q}) n_{k+q\alpha} \frac{n_{k\alpha} - n_{k+q\alpha}}{\mathscr{E}_{k\alpha} - \mathscr{E}_{k+q\alpha}} + (1 + P_k)(1 + P_{k+q}) n_{k+q\beta} \frac{n_{k\alpha} - n_{k+q\beta}}{\mathscr{E}_{k\alpha} - \mathscr{E}_{k+q\beta}} + (1 - P_k)(1 - P_{k+q}) n_{k+q\alpha} \frac{n_{k\beta} - n_{k+q\alpha}}{\mathscr{E}_{k\beta} - \mathscr{E}_{k+q\alpha}} \right.$$

$$+ (1 - P_k)(1 + P_{k+q}) n_{k+q\beta} \frac{n_{k\beta} - n_{k+q\beta}}{\mathscr{E}_{k\beta} - \mathscr{E}_{k+q\beta}}\Big) \tag{36}$$

with $P_k = U\bar{S}/\mathscr{E}_k$.

The first term in (36) corresponds to the zeroth order in $1/z$ (Hartree–Fock approximation). It may be rewritten as

$$(N_2)_{\mathrm{HF}} = \tfrac{1}{4}(n^2 - 4\bar{S}^2) \tag{37}$$

which coincides with the result by Katsnelson and Irkhin (1984). Taking into account the correction (30) in (37) and transverse spin-fluctuation contributions (other terms in (36)) we obtain the spin-wave contribution to the number of doubles

$$\begin{aligned} \delta\langle n_{i\uparrow} n_{i\downarrow}\rangle &= (1/U)\delta\langle H\rangle_{\mathrm{sw}} = -(3/U)\delta F_{\mathrm{sw}} = (1/U)\sum_q \omega_q N_q \propto (T/T_{\mathrm{N}})^4 \\ \delta N_2(T) &= \partial\delta F_{\mathrm{sw}}/\partial U < 0 \end{aligned} \tag{38}$$

where δF_{sw} is the corresponding correction to the free energy. It enables one to calculate spin-wave contributions to various thermodynamic properties (e.g., elastic moduli). Integration gives

$$\delta\langle H\rangle_{\mathrm{sw}} = (\pi^2/30)\, v_0\, (1/c_1^3 + 1/c_2^3)\, T^4 \tag{39}$$

where v_0 is the lattice cell volume, the magnon velocities are defined by

$$\omega_q = c_1 q \qquad \omega_{\kappa - q} = c_2 q \quad (q \to 0).$$

Now we consider the ground state energy of the Mott insulator ($n = 1$) in the case of large U. The Hartree–Fock contribution has the form (cf. Katsnelson and Irkhin 1984)

$$E_{\mathrm{HF}} = \sum_{k\sigma} t_k \langle c^+_{k\sigma} c_{k\sigma}\rangle_{\mathrm{HF}} + (U/4)(1 - 4\bar{S}^2_{\mathrm{HF}}) = -(1/U)\sum_k \tau_k^2 = -(1/4)(J_\kappa - J_0) \tag{40}$$

where the effective exchange parameters J_q are given by (16). For simple lattices in the nearest-neighbour approximation

$$E_{\mathrm{HF}} = -zt^2/U. \tag{41}$$

Calculating the spin-wave contribution yields

$$\delta\langle E\rangle_{\mathrm{sw}} = \sum_q \omega_q (N_q + \tfrac{1}{2}) - \tfrac{1}{2} J_\kappa. \tag{42}$$

The zero-point contribution reads

$$\delta E_{\mathrm{sw}} = \tfrac{1}{2}\sum_q (J_\kappa - J_q)^{1/2}\,[J_\kappa - \tfrac{1}{2}(J_{\kappa+q} + J_{\kappa-q})]^{1/2} - \tfrac{1}{2}J_\kappa. \tag{43}$$

This correction is similar to that obtained by Anderson (1952) for the Heisenberg model and is of the order of $1/z$. For a d-dimensional cubic lattice ($z = 2d$) we have

$$\delta E_{\mathrm{sw}} = -\tfrac{1}{2}J_\kappa\left[1 - \frac{1}{d}\sum_{i=1}^{d}\sum_q (1 - \cos q_i a)^{1/2}\right] \simeq -\frac{J_\kappa}{4z} = -\frac{t^2}{2U} \qquad (z \gg 1). \tag{44}$$

For $d = 3$,

$$\delta E_{\mathrm{sw}} = -0.097 J_\kappa/2 = -0.58 t^2/U \tag{45}$$

(Anderson 1952). In the one-dimensional case ($d = 1$)

$$\delta E_{sw} = (J_\kappa/2)(2/\pi - 1) = -0.73t^2/U. \quad (46)$$

The result for the total energy,

$$E = E_{HF} + E_{sw} = -2.73t^2/U,$$

is in excellent agreement with the exact result by Lieb and Wu (1968) in the limit under consideration,

$$E = -(4\ln 2)\,t^2/U = -2.77t^2/U.$$

Appendix: Comparison with the s–d exchange model

Consider the Hamiltonian of the s–d model for an antiferromagnet (cf. Irkhin and Katsnelson 1988a)

$$H = \sum_k t_k c^+_{k\sigma} c_{k\sigma} + H_d + H_{sd} \quad (47)$$

$$H_{sd} = -I\sum_{kq} [S^z_q(c^+_{k+q\uparrow}c_{k-\kappa\downarrow} + c^+_{k-\kappa\downarrow}c_{k-q\uparrow}) + S^x_q(c^+_{k+q\uparrow}c_{k\uparrow} - c^+_{k+q\downarrow}c_{k\downarrow})$$
$$+ iS^y_q(c^+_{k+q\uparrow}c_{k-\kappa\downarrow} - c^+_{k-\kappa\downarrow}c_{k-q\uparrow})] \quad (48)$$

where H_d is the Heisenberg Hamiltonian of the localised spin system, S^i_q are the Fourier components of the spin operators in the local coordinate system, I is the s–d exchange parameter. If we pass to the local coordinate system also for electron operators (equation (9)) we obtain

$$H_{sd} = -I\sum_i [S^z_i(d^+_{i\uparrow}d_{i\uparrow} - d^+_{i\downarrow}d_{i\downarrow}) + S^+_i d^+_{i\downarrow}d_{i\uparrow} + S^-_i d^+_{i\uparrow}d_{i\downarrow}]. \quad (49)$$

In the Hartree–Fock approximation, the electron spectrum is given by

$$\mathscr{E}_{k\alpha,\beta} = \theta_k \mp (\tau^2_k + I^2\langle S^z\rangle^2)^{1/2} \quad (50)$$

with $\langle S^z\rangle \simeq S$ the sub-lattice magnetisation. Writing the equation of motion for the spin Green function, we get

$$\left(\omega - I\sum_k \langle d^+_{k\uparrow}d_{k\uparrow} - d^+_{k\downarrow}d_{k\downarrow}\rangle\right)\langle\langle S^+_q|S^-_{-q}\rangle\rangle_\omega = 2S\left[1 - I\sum_k \langle\langle d^+_{k\uparrow}d_{k+q\downarrow}|S^-_{-q}\rangle\rangle_\omega\right]. \quad (51)$$

On passing, as in (2), from the operators $d_{k\sigma}$ to the operators α_k, β_k, which correspond to the new sub-bands (50), and calculating the Green function on the right-hand side of (51), we derive an expression for the magnon spectrum. This expression turns out to coincide with (14) with the replacement $U \to I$, $\bar{S} \to S$.

The same replacement takes place for the electron spectrum (24) (of course, in the second term, $\bar{S} \to \langle S^z\rangle$). Specifically, in the limit where $|I| \to \infty$, we obtain

$$E_{k\alpha} = -I\langle S^z\rangle - I\sum_q (N_q + n_{k+q\beta}) = -I(S + n_\beta) \quad (52)$$

$$E_{k\beta} = I(S + 1 - n_\alpha). \quad (53)$$

Note that our Hartree–Fock-type approximation yields correct 'atomic' values $E = \pm IS$, $\pm I(S+1)$ for the integers n_α, n_β.

In the case of small I (or U) it is more convenient to use the Hamiltonian in the form (48). Then we obtain in the second order for the magnon spectrum the RKKY result (18) and (19). Calculating in the same way the electron spectrum (see also Irkhin and Katsnelson 1988b), we obtain

$$\frac{\delta \omega_q}{\delta f_k} = \frac{1}{2}\left(\frac{\delta E_k^{\uparrow}}{\delta N_q} + \frac{\delta E_k^{\downarrow}}{\delta N_q}\right) \tag{54}$$

$$\frac{\delta E_k^{\uparrow,\downarrow}}{\delta N_q} = 2I^2 S\left[\frac{(u_q - v_q)^2}{t_k - t_{k+q}} + \frac{(u_q + v_q)^2}{t_k - t_{k\mp\kappa+q}} - 2\frac{u_q^2 + v_q^2}{t_k - t_{k\mp\kappa}}\right]. \tag{55}$$

The third term in the square brackets, which is due to the sub-lattice magnetisation decreasing with T, leads to an increase in the band bottom ($t_k = t_{\min}$). However, the contribution of the transverse spin fluctuations (two first terms) is of opposite sign and may prevail. So, in the case where $\theta_k \equiv 0, J_q \propto t_q$ (simple lattices in the nearest-neighbour approximation) the latter contribution is two times larger (Irkhin 1986).

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