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MAGNETISM AND FERROELECTRICITY

Spectral Functions in the Hubbard Model with Half-Filling

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Abstract—Under the assumption of long-range antiferromagnetic order at low temperatures, the spectral functions and the density of states are calculated in the two-dimensional Hubbard model with half-filling in the Hubbard-I approximation. The results are compared with the data obtained using an exact numerical technique, namely, the quantum Monte Carlo method. The influence of hopping to the next-to-nearest neighbor on the formation of the electronic structure is considered. © *2004 MAIK "Nauka/Interperiodica".*

1. The Hubbard model taking into account electron motion in solids along with the electron–electron interaction is one of the basic models in the theory of systems with strong electron correlations (SECs). The point is that this model does reflect important effects characteristic of systems with SECs, even though it is insufficient for describing the properties of specific materials quantitatively [1]. It is interesting to study approximations in the atomic limit, because, as is known, it is simpler to describe such systems by starting with the local approach than with the theory of the Hartree–Fock band limit [2]. In the limit of $t \ll U$, the Hubbard-I approximation yields a simple description of a system in terms of two energy bands separated by a Mott–Hubbard gap [1]. As the ratio t/U increases, this approximation becomes incorrect a priori; however, it is quite applicable to systems with SECs. In a diagram technique based on Hubbard X operators [2, 3], the Hubbard-I solution is a result of the Hartree–Fock approximation. Using the quantum Monte Carlo (QMC) method, one can compare the electronic structure of the Hubbard model obtained in the limit $t \ll U$ in the Hubbard-I approximation and the results of exact numerical calculations (see, e.g., [4, 5]). Such a comparison was performed in [4] to show that, at high temperatures, the spectral functions $A(\mathbf{k}, \omega)$ are sufficiently well described by the Hubbard-I paramagnetic solution. At low temperatures, neither the Hubbard-I paramagnetic solution nor the solution in the form of a spin density wave (SDW) can even approximately reproduce the model electronic structure. It is known that the SDW solution is applicable under conditions of weak electron correlations, when $U \ll W = zt$, but this solution is inapplicable to systems with SECs. In this paper, the spectral functions of the two-dimensional (2D) Hubbard model with half-filling are calculated in the Hubbard-I approximation under the assumption of long-range antiferromagnetic order at low temperatures.

Comparison of our results with the data obtained using the QMC method showed that the spectral functions are in reasonable agreement with the exact numerical calculations, despite the disadvantages of the approximation used. These disadvantages are as follows.

(i) According to the Mermin–Wagner theorem, there is no antiferromagnetic order in a 2D system at finite temperatures; hence, an interplane interaction or certain anisotropy should be assumed. Nevertheless, the approximation used is appropriate, since we compare the results of this study with QMC data for finite systems, for which the above-mentioned theorem is invalid.

(ii) The Hubbard-I approximation does not yield a self-consistent description of the antiferromagnetic state; indeed, there is only a zero solution for the sublattice magnetization m. For this reason, in the limit $t \ll U$ for a system with $n_e = 1$, we construct an effective Heisenberg Hamiltonian with the antiferromagnetic interaction constant $J = 4t^2/U$ and calculate the magnetization self-consistently in the Heisenberg model. At $T = 0$, m decreases from a nominal value due to zero quantum fluctuations and we get $m = 0.3$ under the assumption that the interplane interaction is weak in comparison with the in-plane interaction.

It should be noted that going beyond the mean-field approximation requires consideration of self-energy one-loop diagrams [2, 3]. In the magnetically ordered phase, the largest contribution comes from diagrams describing spin-wave excitations. The main effect of spin excitations consists in a renormalization of the occupation numbers. According to [6], we define the occupation numbers as

$$\begin{aligned} n_{f,\sigma} + n_{f,\bar{\sigma}} &= n_e, \\ n_{f,\sigma} - n_{f,\bar{\sigma}} &= 2m = (1 - 2n_{sf}). \end{aligned} \tag{1}$$

where $2n_{sf}$ is the magnon concentration and $n_{f,\sigma}$ is the number of electrons at a site with a specified spin projection. Thus, the introduction of the nonzero magnetization of sublattices corresponds to consideration of the first significant correction to the mean-field approximation.

2. The Hubbard model Hamiltonian can be written as

$$\hat{H} - \mu\hat{N}_e = \sum_{f,\sigma}\left[(\varepsilon - \mu)n_{f,\sigma} + \frac{1}{2}Un_{f,\sigma}n_{f,\bar{\sigma}}\right] + \sum_{f,g,\sigma}(t_{f,g}a^+_{f,\sigma}a_{g,\sigma} + \text{H.c.}), \quad (2)$$

where $a^+_{f,\sigma}$ ($a_{f,\sigma}$) is the creation (annihilation) operator of an electron at site f with spin $\sigma = \pm 1/2$, $n_{f\sigma} = a^+_{f\sigma}a_{f\sigma}$, ε is the one-electron energy in the crystal field, μ is the chemical potential, U is the intra-atomic repulsion matrix element, and $t_{f,g}$ is the hopping integral between sites f and g in the nearest neighbor approximation.

In what follows, we analyze a simple spatially inhomogeneous solution to the above Hamiltonian for a 2D square lattice with antiferromagnetic ordering of the spins (the antiferromagnetic order near half-filling is caused by kinetic superexchange in the system). In the case of two sublattices, the Green's function [7] is written as

$$G(\mathbf{k},\omega) = \frac{1}{N}\begin{pmatrix} \sum_{f,f'}\exp\{i\mathbf{k}(\mathbf{f}-\mathbf{f}')\}\langle\langle a_f|a^+_{f'}\rangle\rangle & \sum_{f,g}\exp\{i\mathbf{k}(g-\mathbf{f})\}\langle\langle a_g|a^+_f\rangle\rangle \\ \sum_{f,g}\exp\{i\mathbf{k}(\mathbf{f}-\mathbf{g})\}\langle\langle a_f|a^+_g\rangle\rangle & \sum_{g,g'}\exp\{i\mathbf{k}(\mathbf{g}-\mathbf{g}')\}\langle\langle a_g|a^+_{g'}\rangle\rangle \end{pmatrix}. \quad (3)$$

Analytical expressions for the Green's functions are derived in the Hubbard-I approximation, which corresponds to the following uncoupling of averages [1]:

$$\langle\langle a_{f+h,\sigma}n_{f,\bar{\sigma}}|a^+_{f',\sigma}\rangle\rangle \longrightarrow \langle n_{f,\bar{\sigma}}\rangle\langle\langle a_{f+h,\sigma}|a^+_{f',\sigma}\rangle\rangle. \quad (4)$$

In the atomic limit, it is more convenient to use the representation of Hubbard operators, with which the conventional Fermi operators are related through the linear combination

$$a^+_{f,\sigma} = X^{\sigma,0}_f + 2\sigma X^{2,\bar{\sigma}}_f, \quad a_{f,\sigma} = X^{0,\sigma}_f + 2\sigma X^{\bar{\sigma},2}_f. \quad (5)$$

Therefore, the Green's functions can be written in the new representation (A, B are intersublattice indices) as

$$G^u_{AA} = \langle\langle X^{\bar{\sigma},2}_A|X^{2,\bar{\sigma}}_A\rangle\rangle = F^{\bar{\sigma},2}_A((E-\varepsilon_1)^2[\nu + F^{\bar{\sigma},2}_B t(\mathbf{k})] - F^{0,\sigma}_A t^2(\mathbf{k})(E-\varepsilon_1 - F^{0,\sigma}_B U))/\prod_{i=1}^{4}(E-E_i),$$

$$G^u_{AB} = \langle\langle X^{\bar{\sigma},2}_A|X^{2,\bar{\sigma}}_B\rangle\rangle = F^{\bar{\sigma},2}_B((E-\varepsilon_1)^2[\nu + F^{\bar{\sigma},2}_A t(\mathbf{k})] - F^{0,\sigma}_B t^2(\mathbf{k})(E-\varepsilon_1 - F^{\bar{\sigma},2}_A U))/\prod_{i=1}^{4}(E-E_i),$$

$$G^l_{AA} = \langle\langle X^{0,\sigma}_A|X^{\sigma,0}_A\rangle\rangle = F^{0,\sigma}_A((E-\varepsilon_1)[\nu^2 - F^{\bar{\sigma},2}_A F^{\bar{\sigma},2}_B t^2(\mathbf{k})] + F^{0,\sigma}_B t(\mathbf{k})[\nu^2 - F^{\bar{\sigma},2}_A t(\mathbf{k})\nu])/\prod_{i=1}^{4}(E-E_i),$$

$$G^l_{AB} = \langle\langle X^{0,\sigma}_B|X^{\sigma,0}_A\rangle\rangle = F^{0,\sigma}_B((E-\varepsilon_1)[\nu^2 - F^{\bar{\sigma},2}_A F^{\bar{\sigma},2}_B t^2(\mathbf{k})] + F^{0,\sigma}_A t(\mathbf{k})[\nu^2 - F^{\bar{\sigma},2}_B t(\mathbf{k})\nu])/\prod_{i=1}^{4}(E-E_i), \quad (6)$$

where $F^{0,\sigma}_A = \langle X^{0,0}_A + X^{\sigma,\sigma}_A\rangle$ and $F^{\bar{\sigma},2}_A = \langle X^{2,2}_A + X^{\bar{\sigma},\bar{\sigma}}_A\rangle$ are the filling factors, $\varepsilon_1 = (\varepsilon - \mu)$, $\nu = (E - \varepsilon_1 - U)$, and superscripts l and u correspond to the lower and upper Hubbard bands, respectively.

We restrict the analysis to the half-filling region, where the chemical potential is described by the well-known expression $\mu = \varepsilon + U/2$ [8], which is valid for any temperature and all values of the model parameters. In this case, the equation defining the spectrum of quasiparticles in the 2D antiferromagnetic lattice has the analytical solution

$$E^{l,u}_{\pm} = \pm\frac{1}{2}(t^2(\mathbf{k}) \pm \sqrt{t^4(\mathbf{k}) + 4U^2t^2(\mathbf{k})n_{f,\sigma}n_{f,\bar{\sigma}} - 2\varepsilon_1(\varepsilon_1 + U)})^{1/2}. \quad (7)$$

Since the Brillouin zone becomes twice as small in the antiferromagnetic phase, each Hubbard subband in the paraelectric phase is split into two. If the bands obtained had been ordinary one-electron bands with a

number of states per atom equal to unity, the total number of states would have been equal to four. However, these bands correspond to quasiparticles with a fractional spectral weight, which can be explicitly calculated using the QMC method. In our calculations, the spectral weight is defined by the filling factor $F_g^{m,n} = \langle X_g^{m,m} + X_g^{n,n} \rangle$.

It is noteworthy that the quasiparticle spectrum (7) can be rewritten using the well-known solution for the paramagnetic phase. In this case, it turns out that the dispersion in the antiferromagnetic state has a form similar to that for SDWs,

$$E_{\pm}^{l,u} = \pm\sqrt{(\xi^{\pm})^2 + \Delta^2}, \tag{8}$$

where $\Delta = Um$ is the gap parameter, $m = (1/2)(n_{f,\sigma} - n_{f,\bar{\sigma}})$ is the sublattice magnetization, $\varepsilon_{\mathbf{k}}^{\pm}$ is the dispersion of the upper and lower Hubbard bands in the paramagnetic phase with the renormalized Coulomb repulsion parameter $\tilde{U} = U\sqrt{1-4m^2}$, and

$$\xi_{\mathbf{k}}^{\pm} = \frac{1}{2}(t(\mathbf{k}) \pm \sqrt{t^2(\mathbf{k}) + \tilde{U}^2}). \tag{9}$$

If the magnetization is zero, the obtained bands exactly correspond to the upper and lower Hubbard bands in the paraelectric phase. In the one-electron SDW state, the quasiparticle dispersion is described by a formula similar to Eq. (9), with $\xi^{\pm}$ being the dispersion of free electrons.

Now, we consider the full spectral function of the system, which is the sum of the imaginary parts of the Green's functions in Eq. (6),

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi}\mathrm{Sp}(\mathrm{Im}\,G(\mathbf{k}, \omega)) = -\frac{1}{\pi}\mathrm{Im}(G_{AA}^{l}(\mathbf{k}, \omega) + G_{BB}^{l}(\mathbf{k}, \omega) + G_{AA}^{''}(\mathbf{k}, \omega) + G_{BB}^{''}(\mathbf{k}, \omega)) \tag{10}$$

and the one-electron density of states,

$$N(\omega) = \frac{1}{N}\sum_{\mathbf{k}} A(\mathbf{k}, \omega). \tag{11}$$

The approximation used does not contain information on the spectral linewidths (the spectral density contains delta functions). To compare our results with the numerical QMC data, we approximate the delta functions by a Lorentzian with the most appropriate parameter δ. This renormalization of the width and weight of the quasiparticle spectral lines corresponds to the introduction of a certain nonzero imaginary part of the self-energy $\Sigma(\mathbf{k}, \omega)$. We note that there is no one-to-one correspondence between the parameter δ and temperature; however, this parameter tends to zero as the temperature decreases. Despite the fact that the Mermin–Wagner theorem forbids the existence of antiferromagnetic

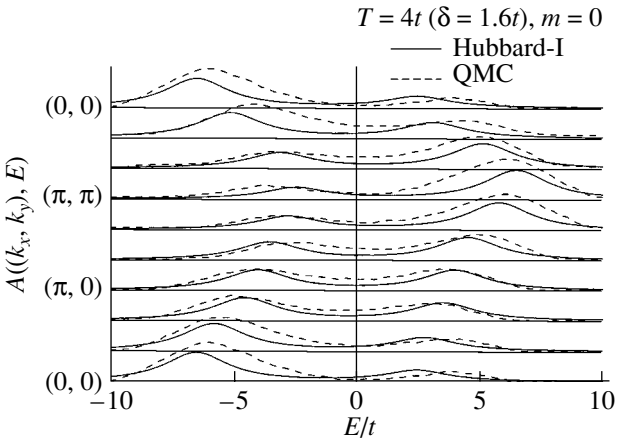

Fig. 1. Spectral functions of the Hubbard model at high temperatures $T = 4t$ (Hubbard-I and QMC [4] calculations).

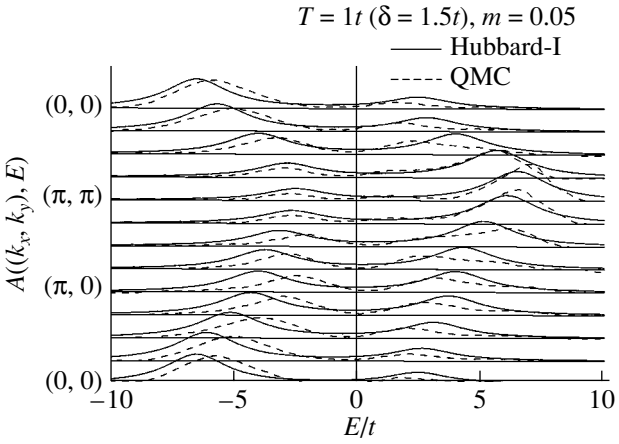

Fig. 2. Spectral functions of the Hubbard model at high temperatures $T = 1t$ (Hubbard-I and QMC [4] calculations).

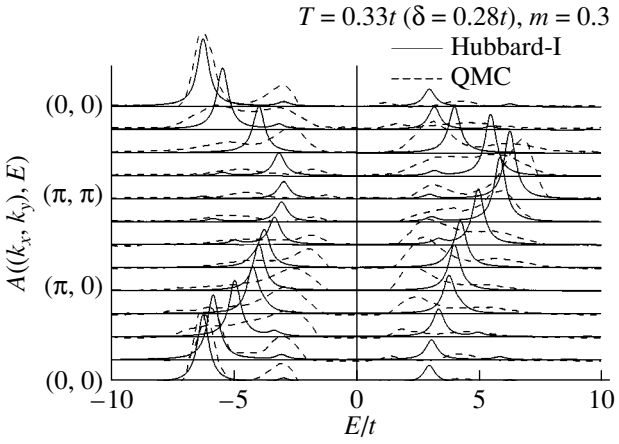

Fig. 3. Spectral functions of the Hubbard model at intermediate temperatures $T = 0.33t$ (Hubbard-I and QMC [4] calculations).

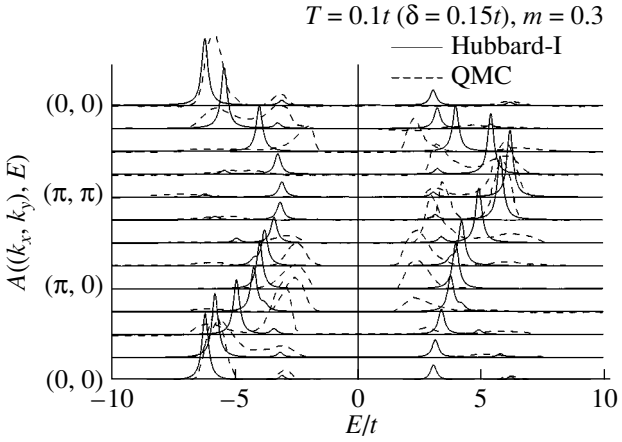

Fig. 4. Spectral functions of the Hubbard model at low temperatures $T = 0.1t$ (Hubbard-I and QMC [4] calculations).

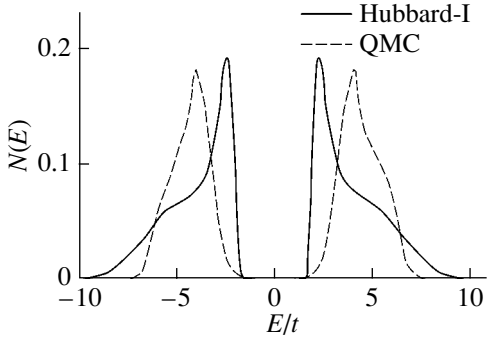

Fig. 5. Density of states in the Hubbard model with half-filling (Hubbard-I and QMC [5] calculations).

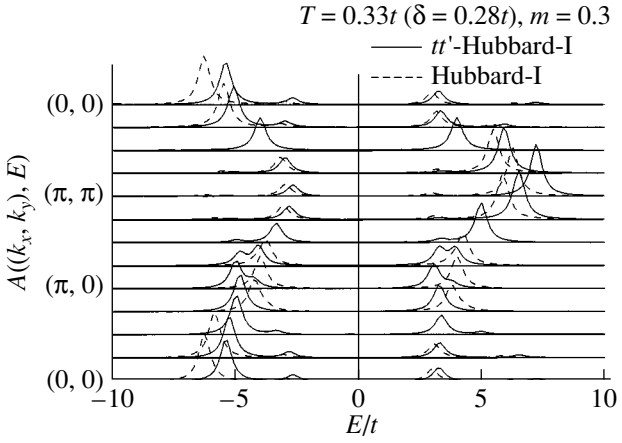

Fig. 6. Spectral functions of the Hubbard model (Hubbard-I and *tt*'-Hubbard-I, $t'/t = 0.3$).

order in 2D systems at finite temperatures, it is generally assumed that the system is "effectively ordered" if the spin correlation length becomes comparable to the system size.

Figures 1–5 show the determined spectral functions and the density of states, as well as the results of exact numerical QMC calculations from [4, 5]. In this case, the following values of the system parameters were used: $U = 8t$, $\varepsilon - \mu + U/2 = 0$, and $t(\mathbf{k}) = -2t(\cos k_x + \cos k_y)$. We assume that the sublattice magnetization parameter m is equal to 0.3 in the low-temperature range.

At high temperatures (Figs. 1, 2), the Hubbard-I approximation reproduces the position and weight of the spectral peaks corresponding to the upper and lower Hubbard bands to sufficient accuracy. This is explained by the fact that the spin correlation effects (disregarded in this approximation) become insignificant above the Néel temperature.

At $T = 1.00t$, QMC calculations [4] indicate very weak satellites for an unoccupied state at the $\mathbf{k} = (0, 0)$ point and for an occupied state at the $\mathbf{k} = (\pi, \pi)$ point. These satellites correspond to the calculated bands E_+^u and E_-^l with a very small spectral weight. Of course, long-range antiferromagnetic ordering does not exist in the system at such temperatures; however, we think that there is a short-range magnetic order, which gives rise to weak satellites in the function $E(\mathbf{k})$.

At intermediate and low temperatures (Figs. 3, 4), each Hubbard band in the paramagnetic state is split into two subbands $E_{1,2}^{l,u}$. In this case, one of the subbands has the largest spectral weight, while the other appears as a weak satellite. A nontrivial result obtained using the QMC method and the Hubbard-I approximation is the spectral weight redistribution between strong and weak peaks. The tendencies toward redistribution of the spectral weight in our calculations and the QMC calculations are retained. In some regions of the Brillouin zone [near $\mathbf{k} = (0, 0)$ and $\mathbf{k} = (\pi, \pi)$], reasonable agreement is observed in the shape and position of the peaks in $A(\mathbf{k}, \omega)$. However, the QMC and Hubbard-1 data significantly differ in other $\mathbf{k}$-space regions [$\mathbf{k} = (\pi/2, \pi/2)$and $\mathbf{k} = (\pi, 0)$].

The one-electron density of states (Fig. 5) at low temperatures has two peaks corresponding to the occupied (l) and unoccupied (u) Hubbard bands. The weak satellites in the spectral density give rise to shoulders on both peaks. Our results and the QMC data from [6] are in qualitative agreement.

We also considered the influence of the next-to-nearest neighbor on the formation of the electronic structure. The Hamiltonian of the *tt*' model includes hopping on a sublattice described by the term $\sum_{f, f' \in A, \sigma}(t'_{f, f'} a^+_{f, \sigma} a_{g, \sigma} + \text{H.c.})$. In the simplest case, the $\mathbf{k}$ dependence of the parameter t' is described by the formula $t'(\mathbf{k}) = 4t' \cos k_x \cos k_y$. The spectral functions of the Hubbard model, corresponding to the Hubbard-I antiferromagnetic solution, are shown in Fig. 6 for the ratio $t'/t \approx 0.3$. A comparison of the solutions shows that

the most significant effect is the formation of additional quasiparticle states at points $(\pi, 0)$ and $(\pi, \pi/4)$ of the Brillouin zone. At the $(\pi, 0)$ point, these states appear as small satellites located near the main peak. The position of the additional peaks is controlled by spin fluctuations and the parameter t'. When the magnon concentration $2n_{sf}$ is zero and $t' = 0$, there are two dispersionless levels in the electronic structure, which lie above the valence band top and below the conduction band bottom.

3. Thus, it was shown that the spectral function at low temperatures, determined using the Hubbard model in the Hubbard-I approximation, as well as that obtained using exact numerical QMC calculations, consists of four peaks corresponding to antiferromagnetic Hubbard subbands. The approximation used retains the basic tendencies toward redistribution of the spectral weight; however, quantitative disagreement is observed in some regions of the **k** space. The density of states in the Hubbard-I solution agrees with the QMC calculations. A significant effect resulting from the inclusion of the next-to-nearest neighbor leads in calculating the electronic structure is the formation of additional quasiparticle states at certain points of the Brillouin zone.

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