https://doi.org/10.3176/phys.math.1994.3.06
Proc. Estonian Acad. Sci. Phys. Math., 1994, **43**, 3, 193–197

TEMPERATURE DEPENDENCE OF THE ENERGY SPECTRUM OF THE TWO-DIMENSIONAL *t-J* MODEL

Oleg SHVAIKOVSKY and Aleksei SHERMAN

Eesti Teaduste Akadeemia Füüsika Instituut (Institute of Physics, Estonian Academy of Sciences), Riia 142, EE-2400 Tartu, Eesti (Estonia)

Presented by V. Hizhnyakov

Received July 4, 1994; accepted July 8,1994

KAHEDIMENSIOONILISE *t-J* MUDELI ENERGEETILISE SPEKTRI SÕLTUVUS TEMPERATUURIST. Oleg ŠVAIKOVSKI, Aleksei ŠERMAN

ТЕМПЕРАТУРНАЯ ЗАВИСИМОСТЬ ЭНЕРГЕТИЧЕСКОГО СПЕКТРА ДВУМЕРНОЙ *t-J*-МОДЕЛИ. Олег ШВАЙКОВСКИЙ, Алексей ШЕРМАН

Abstract. A motion of a hole in a two-dimensional antiferromagnet is considered in the framework of the *t-J* model. A temperature dependence of the lowest energy band is calculated for the range $T/t \leq 0.1$ where T and t are the temperature and the hopping constant, respectively. For the exchange constant $J = J_c \approx 0.52t$ the lowest energy is shown to be degenerate along the boundaries of the magnetic Brillouin zone. For $J < J_c$ the lowest energy is achieved in the points $\mathbf{q} = (\pm\pi/2, \pm\pi/2)$ while for larger J, in the points $(\pm\pi,0)$, $(0,\pm\pi)$ of the Brillouin zone. The critical value is independent on T. A perceptible dependence of the quasiparticle energy on T is observed for $T \geqslant 0.3\,J$

Key words: strongly correlated electron systems, *t-J* model.

Effects of electron correlations have been a subject of an intense study starting from the discovery of high-T_c superconductivity [1]. Already at the early stage of the investigations it was supposed [2] that the carrier transport in CuO_2 planes of high-T_c cuprate superconductors may be described by the two-dimensional Hubbard model [3] or the related *t-J* model [4].

The energy spectrum of the *t-J* model has been considered by different methods in a number of papers (see, e.g., [5–7]). In the case of strong correlations, $J \ll t$, where J and t are the exchange and hopping constants, respectively, it has been shown that the spectrum contains well-defined quasiparticle bands and the hole-magnon continuum of scattering states. These results were obtained in the limit of zero temperature. In the present paper we consider a temperature dependence of the lowest energy band. For this purpose we use the modified Lanczos algorithm [8] which gives the regular way for calculating correlation and Green's functions with averaging over the canonical ensemble. Besides, we consider some peculiarities in the dependence of the lowest energy on J/t.

For low temperatures and small hole concentrations the CuO_2 planes of cuprate superconductors are known to be antiferromagnetically ordered. In spite of the destruction of the long-range order for temperatures larger than the Néel temperature and for larger concentrations, considerable antiferromagnetic correlations are retained even in this case [9]. This gives grounds to use the spin-wave approximation for the description of CuO_2 planes. The two-dimensional *t-J* Hamiltonian in this approximation can be written in the form [7]

$$\mathcal{H} = \varepsilon \sum_{\mathbf{k}} h^{\dagger}_{\mathbf{k}} h_{\mathbf{k}} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} b^{\dagger}_{\mathbf{k}} b_{\mathbf{k}} + \sum_{\mathbf{kk'}} (g_{\mathbf{kk'}} h^{\dagger}_{\mathbf{k}} h_{\mathbf{k}-\mathbf{k'}} b_{\mathbf{k'}} + H.c.), \qquad (1)$$

where $h^{\dagger}_{\mathbf{k}}$ is the creation operator of a hole with the wave vector $\mathbf{k}$ in one of two classical Néel states, $b^{\dagger}_{\mathbf{k}}$ is the boson creation operator of spin waves which in the site representation can be considered as the spin-flip operator. In Eq. (1), $\omega_{\mathbf{k}} = 2J\sqrt{1-\gamma^2_{\mathbf{k}}}$ is the magnon frequency with $\gamma_{\mathbf{k}} = [\cos(k_x a) + \cos(k_y a)]/2$ and a is the lattice constant which is taken as the unit of length. The interaction constant $g_{\mathbf{kk'}} = -4t(\gamma_{\mathbf{k}-\mathbf{k'}} u_{\mathbf{k'}} + \gamma_{\mathbf{k}} v_{\mathbf{k'}})/\sqrt{N}$ comprises the number of sites N, $u_{\mathbf{k}} = \cosh(\alpha_{\mathbf{k}})$, $v_{\mathbf{k}} = -\sinh(\alpha_{\mathbf{k}})$, and $\alpha_{\mathbf{k}} = \ln[(1+\gamma_{\mathbf{k}})/(1-\gamma_{\mathbf{k}})]/4$, and ε is the energy of hole formation.

To find the temperature dependence of the energy spectrum we calculate the following correlation function:

$$R(z) = \int_0^{\infty} e^{-zt} R(t)\,dt, \qquad (2)$$

where $R(t) = \langle h_{\mathbf{q}}(t)\, h^{\dagger}_{\mathbf{q}} \rangle$, $h_{\mathbf{q}}(t) = \exp(i\mathcal{H}t)\, h_{\mathbf{q}} \exp(-i\mathcal{H}t)$ and the angle brackets denote the averaging over the canonical ensemble. Poles of $R(z)$ determine energies and dampings of elementary excitations at a given temperature.

Correlation function (2) can be represented in the form of the continued fraction

$$R(z) = \cfrac{1}{z + iE_0 + \cfrac{V_1^2}{z + iE_1 + \cfrac{V_2^2}{z + iE_2 + \cfrac{V_3^2}{\dots}}}}, \tag{3}$$

where the elements of the continued fraction E_i and V_i are recursively calculated from the modified Lanczos algorithm [8]

$$E_n = -\langle [\mathcal{H}, A_n], A_n^\dagger \rangle, \; A'_{n+1} = [\mathcal{H}, A_n] + E_n A_n - V_n A_{n-1},$$
$$V_0 = 0, \; V_{n+1}^2 = \langle A'_{n+1} (A'_{n+1})^\dagger \rangle, \; A_{n+1} = A'_{n+1}/V_{n+1}, \tag{4}$$

with the initial operator $A_0 = h_{\mathbf{q}}$.

We restrict ourselves to the first two steps of this procedure that can be estimated to be appropriate for $J/t \geqslant 0.1$. The obtained elements of the continued fraction read

$$E_0 = \varepsilon, \quad V_1^2 = \sum_{\mathbf{k}} g_{\mathbf{qk}}^2 (1 + n_{\mathbf{k}}) + \sum_{\mathbf{k}} g_{\mathbf{q+k,k}}^2 n_{\mathbf{k}},$$
$$E_1 = \varepsilon + \frac{1}{V_1^2} \left[\sum_{\mathbf{k}} \omega_{\mathbf{k}} g_{\mathbf{qk}}^2 (1 + n_{\mathbf{k}}) + \sum_{\mathbf{k}} \omega_{\mathbf{k}} g_{\mathbf{q+k,k}}^2 n_{\mathbf{k}} \right], \tag{5}$$

where $n_{\mathbf{k}} = [\exp(\omega_{\mathbf{k}}/T) - 1]^{-1}$ is the boson occupation number, T is the temperature in energy units. Substituting elements (5) into Eq. (3) and picking the lowest pole we obtain an approximate lowest energy band of the model considered for given J/t and T/t.

The ranges $0.05 \leq J/t \leq 1$ and $0 \leq T/t \leq 0.1$ were used for the calculations. It is worth noting that for the typical representative of high-T_c cuprate superconductors, the La_2CuO_4 crystal, the value of J/t is supposed to lie in the range from 0.1 to 0.3 [10]. ε, a change of which gives an unessential total shift of the spectrum, was set to be equal to $10t$.

The general shape of the lowest band $E_{\mathbf{q}}$ is shown in Fig. 1 for $T = 0$, $J/t = 0.1$ and $J/t = 0.8$. In agreement with the previously obtained results [5–7] for the former value of J/t the band minima are positioned in the points $\mathbf{q} = (\pm\pi/2, \pm\pi/2)$ of the Brillouin zone. For the latter value of J/t the minima are shifted to the points $\mathbf{q} = (0, \pm\pi), (\pm\pi, 0)$. This transformation of the band is more clearly seen in Fig. 2 from which the critical value of the transformation, $J_c \approx 0.52t$, can be extracted. In the considered temperature range J_c is independent on T. It should be noted that for $J = J_c$ the lowest energy is degenerate along the boundaries of the magnetic

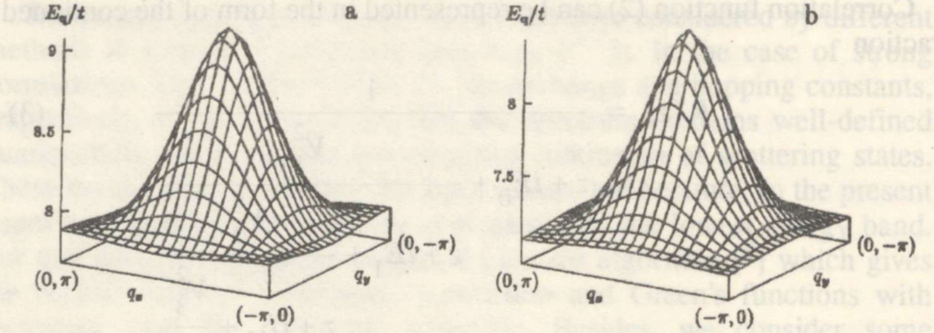

Fig. 1. The lowest band in the magnetic Brillouin zone for $T = 0$ and for $J/t = 0.1$ (*a*) and $J/t = 0.8$ (*b*).

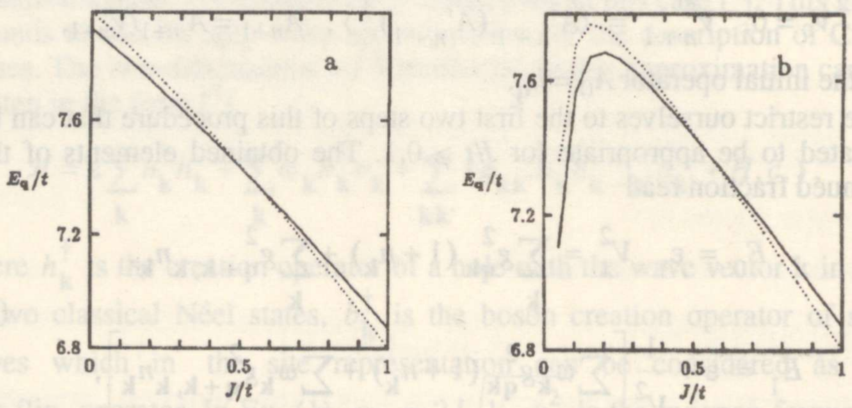

Fig. 2. The band energy E_q versus J/t in the points q = ($\pi/2$, $\pi/2$) (solid line) and q = $(0,\pi)$ (dotted line) for $T = 0$ (*a*) and $T = 0.1$ (*b*).

Fig. 3. The dependence of E_q on J/t and T/t in the points q = (0,0) (*a*) and q = ($\pi/2$, $\pi/2$) (*b*).

Brillouin zone (this zone corresponds to a lattice with a doubled period arising due to the antiferromagnetic ordering).

The dependence of $E_{\mathbf{q}}$ on T/t and J/t is shown in Fig. 3 for wave vectors corresponding to the top and bottom of the band. As follows from the figure and Eq. (5), the pronounced dependence of the quasiparticle energy on temperature is observed for $T \geqslant 0.3J$. For parameters of La_2CuO_4 [10] this corresponds to temperatures starting from 300 K. For lower temperatures the dependence is determined by low-frequency phonons rather than by magnons.

REFERENCES

1. Bednorz, J. G. and Mueller, K. A. Z. Phys. B, **64**, 189 (1988).
2. Anderson, P. W. Science, **235**, 1196 (1987).
3. Hubbard, J. Proc. R. Soc. A, **276**, 238 (1963).
4. Hirsch, J. E. Phys. Rev. Lett., **54**, 1317 (1985).
5. Schmitt-Rink, S., Varma, C. M. and Ruckenstein, A. E. Phys. Rev. Lett., **60**, 2793 (1988); Marsiglio, F., Ruckenstein, A. E., Schmitt-Rink, S. and Varma, C. M. Phys. Rev. B, **43**, 10882 (1991).
6. Bonča, J., Prelovšek, P. and Sega, I. Phys. Rev. B, 39 (1989) 7074; Fehske, H., Waas, V., Röder, H. and Büttner, H. Phys. Rev. B, **44**, 8473 (1991).
7. Sherman, A. V. Physica C, **171**, 395 (1990); Sabczynski, J., Schreiber, M. and Sherman, A. Phys. Rev. B, **48**, 543 (1993).
8. Sherman, A. V. J.Phys. A, **20**, 569 (1987); Phys. status solidi (b), **145**, 319 (1988).
9. Keimer, B., Belk, N., Birgeneau, R. G., Cassanho, A., Chen, C. Y., Greven, M., Kastner, M. A., Aharony, A., Endoh, Y., Erwin, R. W. and Shirane, G. Phys. Rev. B, **46**, 14034 (1992).
10. McMahan, A. K., Annet, J. F. and Martin, R. M. Phys. Rev. B, **42**, 6828 (1990).