

Energy spectrum of the two-dimensional Hubbard model with infinite repulsion

Yu. V. Mikhaïlova

State Research Institute of Heat-Power Instrument Manufacture, 129085 Moscow, Russia

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In the Hubbard model with infinite repulsion, the energy spectrum and wave functions are studied for an $N \times N$ cluster in a system with one hole and one flipped spin. The calculation is made for given values of the total quasimomentum α of the system. A system of four nonlinear algebraic equations for determining the energy levels of the system is obtained. The analysis is restricted to the simplest case $\alpha_x = \alpha_y = (0, \pi)$. For these states, the energy levels are situated between the free-quasiparticle levels ε_k . The states with spin $S = S_{\max} - 1$ are situated above the Nagaoka level $\varepsilon = -4t$; however, the difference Δ between the energy of the ground state with spin $S = S_{\max} - 1$ and the Nagaoka level is microscopic. It is to be emphasized that this applies both to states with quasimomentum $(0, 0)$ and to states with quasimomentum (π, π) . In the macroscopic limit, the level distribution density for both $\alpha_x = \alpha_y = 0$ and $\alpha_x = \alpha_y = \pi$ is identical to the density of single-particle excitations of a spinless Fermi gas. The solution obtained is used to calculate the level shift when a finite Hubbard interaction is turned on. It is shown that the critical level U_c of the Hubbard energy below which the Nagaoka ferromagnetic state is not the ground state has macroscopic order. © 1996 American Institute of Physics. [S1063-7761(96)02203-X]

1. INTRODUCTION

Since the discovery of high-temperature superconductivity, there has been increased interest in the Hubbard model as the simplest model that describes the properties of high- T_c superconducting compounds. The Hubbard model, which was originally introduced to explain ferromagnetism, has attracted interest as a limiting case of a model corresponding to the description of high-temperature superconductors. The large value of the Coulomb repulsion U per site compared with the hopping energy t gives grounds for believing that the case $U = \infty$ can be regarded as a zeroth approximation to the real model. However, as yet comparatively few theoretical or numerical results have been obtained.

Given the lack of a small parameter in this problem, only one rigorous result is so far known: Nagaoka's theorem on the ground state with one hole.¹ For a two-dimensional square lattice in three cases—1) a free boundary, 2) an even number of sites along each direction, 3) $t > 0$ —it follows from Nagaoka's proof that the ground state has maximum spin. At low hole concentration in the gas approximation for a cubic lattice, an expression was obtained in Ref. 1 for the ground-state energy of a system with one flipped spin at finite U , and from this expression it follows that the ground state has maximum spin at a concentration of holes lower than a certain limiting value. This result cannot be directly extended to the two-dimensional case, since the integral expressions employed by Nagaoka diverge in the two-dimensional case. Since it is precisely the two-dimensional model that is interesting for the majority of high-temperature superconducting compounds, it is necessary to consider the two-dimensional case in more detail.

In this paper, we study the energy spectrum and wave functions in the Hubbard model with infinite repulsion for an $N \times N$ cluster in a system with one hole and one flipped spin.

Calculations are made for given values of the total quasimomentum α of the system. We obtain a system of four nonlinear algebraic equations that determines the energy levels of the system. In this paper, the analysis is restricted to the simplest case: $\alpha_x = \alpha_y = (0, \pi)$.

It follows from our calculation that the energy levels are situated between neighboring levels of the free quasiparticles on the interval $[-4t, 4t]$. The states with spin $S = S_{\max} - 1$ are situated above the Nagaoka level $\varepsilon = -4t$, but the difference Δ between the energies of the ground state with spin $S = S_{\max} - 1$ and the Nagaoka state is microscopic. We emphasize that this applies to states with all values of α . Thus, for states with quasimomentum $(0, 0)$

$$\frac{\Delta}{4t} = \frac{2\pi^2}{M} + \frac{\ln M}{4\pi^2 M^2},$$

and for states with quasimomentum (π, π)

$$\frac{\Delta}{4t} = \frac{2\pi^2}{M} - \frac{\ln M}{8\pi^2 M^2}, \quad M = N^2.$$

We use our solution to calculate the level shift when a finite Hubbard interaction is turned on. We determine the critical level of the Hubbard energy U_c below which the Nagaoka ferromagnetic state is not the ground state. We show that U_c/t has macroscopic order of magnitude (order N^2); this agrees with numerical cluster calculations of Ref. 2.

2. BASIC EQUATIONS

Suppose we have a rectangular $N_x \times N_y$ lattice. We denote by $M = N_x \cdot N_y$ the number of sites, by \hat{a}_i^+ (\hat{a}_i) the creation (annihilation) operator at site i of a particle with spin up, and by \hat{b}_i^+ (\hat{b}_i) the creation (annihilation) operator at site i of a particle with spin down. We assume that the system possesses translational invariance, and we consider

states with given quasimomentum $\alpha = (\alpha_x, \alpha_y)$, $\alpha_x = (2\pi/N_x)i_x$, $i_x = 0, 1, \dots, N_x - 1$, $\alpha_y = (2\pi/N_y)i_y$, $i_y = 0, 1, \dots, N_y - 1$.

For such states, we can give a complete orthogonal set:

$$\begin{aligned} \Phi_i = & \{1 + \exp(i\alpha_x)\hat{K}_x + \exp(2i\alpha_x)\hat{K}_x^2 + \dots \\ & + \exp[(N_x - 1)i\alpha_x]\hat{K}_x^{N_x - 1}\} \{1 + \exp(i\alpha_y)\hat{K}_y \\ & + \exp(2i\alpha_y)\hat{K}_y^2 + \dots + \exp[(N_y - 1)i\alpha_y]\hat{K}_y^{N_y - 1}\} \hat{a}_i \Phi_0, \end{aligned}$$

where \hat{K}_x (\hat{K}_y) is the translation operator through one site along x (y), and $\Phi_0 = \hat{b}_1^+ \hat{a}_2^+ \dots \hat{a}_M^+ | \dots \rangle$, $| \dots \rangle$ is the empty state. The function Φ_i is a translationally invariant state with fixed distance between the hole and the flipped spin (which is equal to the distance between the first site and site i). The translation operators \hat{K}_x (\hat{K}_y) are defined as follows: $\hat{K}_x \Phi_i = \exp(-i\alpha_x) \Phi_i$; $\hat{K}_y \Phi_i = \exp(-i\alpha_y) \Phi_i$.

As basis functions, we take

$$\Phi^{(k)} = \sum_{j \neq 1} \Phi_j \exp(ikr_j), \quad (1)$$

the set $\mathbf{k} = (k_x, k_y)$ being identical to the set of quasimomenta $\alpha = (\alpha_x, \alpha_y)$ except for the case $k_x = k_y = 0$. The vector \mathbf{k} can be interpreted as the momentum of a hole in the system in which the flipped spin is at rest.

Thus, an obvious requirement is satisfied: for given quasimomentum α , we have $M - 1$ independent functions $\Phi^{(k)}$. We note some helpful relations:

$$\sum_{\mathbf{k}} \Phi^{(k)} = - \sum_{i \neq 1} \Phi_i, \quad (2)$$

$$\Phi_i = \frac{1}{M} \sum_{\mathbf{k}} [\exp(-ikr_j) - 1] \Phi^{(k)},$$

where the sum over \mathbf{k} is taken over the $M - 1$ functions.

The energy spectrum λ is found by solving the Schrödinger equation

$$\hat{H}\Psi = \lambda\Psi, \quad (3)$$

where $\hat{H} = H_0$ is the Hubbard Hamiltonian for $U = \infty$:

$$\hat{H}_0 = t \sum_{i,j,\sigma} ' \hat{a}_{i\sigma}^+ \hat{a}_{j\sigma} (1 - \hat{a}_{i\bar{\sigma}}^+ \hat{a}_{i\bar{\sigma}}) (1 - \hat{a}_{j\bar{\sigma}}^+ \hat{a}_{j\bar{\sigma}}) \quad (4)$$

or

$$\hat{H}_0 = t \sum_{i,j,\sigma} ' \hat{X}_i^{\sigma 0} \hat{X}_j^{0\sigma}, \quad (5)$$

where $\hat{X}^{\sigma 0}$ ($\hat{X}^{0\sigma}$) are Hubbard operators. The summation in (4) and (5) is over nearest neighbors.

We seek the wave function Ψ in the form of an expansion with respect to the set $\Phi^{(k)}$:

$$\Psi = \sum_{\mathbf{k}} c_{\mathbf{k}} \Phi^{(k)}. \quad (6)$$

After the substitution of (6) in (3), we obtain for the coefficients

$$\begin{aligned} c_{\mathbf{k}} = & \frac{\exp(-ik_x) - 1}{\lambda + \varepsilon_{\mathbf{k}}} \Psi_1 + \frac{\exp(ik_x) - 1}{\lambda + \varepsilon_{\mathbf{k}}} \Psi_2 \\ & + \frac{\exp(-ik_y) - 1}{\lambda + \varepsilon_{\mathbf{k}}} \Psi_3 + \frac{\exp(ik_y) - 1}{\lambda + \varepsilon_{\mathbf{k}}} \Psi_4. \end{aligned} \quad (7)$$

Here $\varepsilon_{\mathbf{k}}$ is the energy of a free quasiparticle:

$$\varepsilon_{\mathbf{k}} = 2t(\cos k_x + \cos k_y), \quad (8)$$

and the constants Ψ_i are

$$\Psi_1 = \frac{1}{M} \sum_{\mathbf{k}} c_{\mathbf{k}} [1 - \exp(-ik_x + i\alpha_x)], \quad (9)$$

$$\Psi_2 = \frac{1}{M} \sum_{\mathbf{k}} c_{\mathbf{k}} [1 - \exp(ik_x - i\alpha_x)], \quad (10)$$

$$\Psi_3 = \frac{1}{M} \sum_{\mathbf{k}} c_{\mathbf{k}} [1 - \exp(-ik_y + i\alpha_y)], \quad (11)$$

$$\Psi_4 = \frac{1}{M} \sum_{\mathbf{k}} c_{\mathbf{k}} [1 - \exp(ik_y - i\alpha_y)]. \quad (12)$$

Thus, the nontrivial solutions of Eq. (3) can be divided into two classes. In the first class we have solutions with $\Psi_1 = \Psi_2 = \Psi_3 = \Psi_4 = 0$, and in the second, solutions with a nonvanishing set of Ψ_i .

As can be seen from (7), solutions of the first type have the form

$$c_{\mathbf{k}} = A_{\mathbf{k}} \delta_{\varepsilon_{\mathbf{k}}, \varepsilon_{\bar{\mathbf{k}}}}, \quad \lambda = -\varepsilon_{\bar{\mathbf{k}}}. \quad (13)$$

At the same time, there always exists the solution

$$c_{\mathbf{k}} = A_{\mathbf{k}} \delta_{\varepsilon_{\mathbf{k}}, \varepsilon_{\bar{\alpha}}}, \quad \lambda = -\varepsilon_{\bar{\alpha}}, \quad (14)$$

which corresponds to the state with maximum possible spin, as follows from the symmetry of the corresponding wave function (6). Solutions different from (14) and of the type (13) exist only if the level $\varepsilon_{\bar{\mathbf{k}}}$ is degenerate. It is natural to pose the question of the minimum degeneracy at which such solutions appear. A simple calculation shows that for degeneracy 2 there are no such solutions. Because of the presence of the natural degeneracy associated with the substitution $\mathbf{k} \rightarrow -\mathbf{k}$, the level degeneracy is always even. Therefore, the next degeneracy will be 4. Degeneracy 4 is achieved for an $N_x \times N_y$ cluster with $N_x \neq N_y$ for the states (k_x, k_y) , $(k_x, -k_y)$, $(-k_x, k_y)$, $(-k_x, -k_y)$ and for $N_x = N_y$ for the states (k_x, k_x) , $(k_x, -k_x)$, $(-k_x, k_x)$, $(-k_x, -k_x)$. In both cases, a necessary condition for the existence of solutions of the type (13) is

$$\alpha_x = (0, \pi) \text{ or } \alpha_y = (0, \pi). \quad (15)$$

Therefore, if the degeneracy of the level of the free quasiparticles is L , it is reduced to $L - 3$ if the condition (15) is satisfied and to $L - 4$ if the condition (15) is not satisfied.

In what follows, we shall restrict ourselves to the case of an equal even number of cells in each direction, i.e., $N_x = N_y = 2N$.

For what follows, it is more convenient to use the variables $y_1 = \Phi_1 + \Phi_2$, $y_2 = -i(\Phi_1 - \Phi_2)$, $z_1 = \Phi_3 + \Phi_4$,

$z_2 = -i(\Phi_3 - \Phi_4)$, $c_k^+ = c_k + c_{-k}$, $c_k^- = c_k - c_{-k}$. Then Eqs. (7) and (9)–(12) can be rewritten in the form

$$c_k^+ = \frac{2(\cos k_x - 1)}{\lambda + \varepsilon_k} y_1 + \frac{2(\cos k_y - 1)}{\lambda + \varepsilon_k} z_1, \quad (7')$$

$$c_k^- = \frac{2 \sin k_x}{\lambda + \varepsilon_k} y_2 + \frac{2 \sin k_y}{\lambda + \varepsilon_k} z_2, \quad (8')$$

$$y_1 = \frac{1}{M} \sum_{\mathbf{k}} [c_k^+(1 - \cos k_x \cos \alpha_x) - c_k^- \sin k_x \sin \alpha_x], \quad (9')$$

$$y_2 = \frac{1}{M} \sum_{\mathbf{k}} [-c_k^+ \cos k_x \sin \alpha_x + c_k^- \sin k_x \cos \alpha_x], \quad (10')$$

$$z_1 = \frac{1}{M} \sum_{\mathbf{k}} [c_k^+(1 - \cos k_y \cos \alpha_y) - c_k^- \sin k_y \sin \alpha_y], \quad (11')$$

$$z_2 = \frac{1}{M} \sum_{\mathbf{k}} [-c_k^+ \cos k_y \sin \alpha_y + c_k^- \sin k_y \cos \alpha_y]. \quad (12')$$

Substituting the expressions (7') for c_k^\pm in (9')–(12'), we obtain self-consistency equations in the form

$$[2\Gamma_1(1 + \cos \alpha_x) - \Gamma_2 \cos \alpha_x - 1]y_1 + [2\Gamma_1(1 - \cos \alpha_x) - \Gamma_3 \cos \alpha_x]z_1 + y_2\Gamma_2 \sin \alpha_x = 0, \\ -(\Gamma_2 - 2\Gamma_1)y_1 \sin \alpha_x - (1 + \Gamma_2 \cos \alpha_x)y_2 - (\Gamma_3 + 2\Gamma_1)z_1 \sin \alpha_x = 0, \quad (16)$$

$$[2\Gamma_1(1 + \cos \alpha_y) - \Gamma_2 \cos \alpha_y - 1]z_1 + [2\Gamma_1(1 - \cos \alpha_y) - \Gamma_3 \cos \alpha_y]y_1 + z_2\Gamma_2 \sin \alpha_y = 0, \\ (\Gamma_2 - 2\Gamma_1)z_1 \sin \alpha_y - (1 + \Gamma_2 \cos \alpha_y)z_2 - (\Gamma_3 + 2\Gamma_1)y_1 \sin \alpha_y = 0.$$

In Eqs. (16), we denote by Γ_i the quantities

$$\Gamma_1 = \frac{1}{M} \sum_{\mathbf{k}} \frac{\cos k_x - 1}{\lambda + \varepsilon_k}, \quad \Gamma_2 = \frac{2}{M} \sum_{\mathbf{k}} \frac{\cos^2 k_x - 1}{\lambda + \varepsilon_k}, \\ \Gamma_3 = \frac{2}{M} \sum_{\mathbf{k}} \frac{(\cos k_x - 1)(\cos k_y - 1)}{\lambda + \varepsilon_k}. \quad (17)$$

The quantities Γ_i usually appear in the study of Hubbard systems with given hole concentration. It is interesting to note that summation over one of the components of the vector \mathbf{k} can be performed for all values of λ (the corresponding calculations are given in Appendix A). This makes it possible to simplify the calculations, especially in computer calculations of cluster systems. In the one-dimensional case, the summation can be done completely, and this naturally simplifies the problem.

The condition of solvability of Eqs. (16) is the vanishing of a determinant, which can be expressed as follows:

$$A(\alpha_x)A(\alpha_y) - B(\alpha_x)B(\alpha_y) = 0, \quad (18)$$

where

$$A(\alpha) = -\Gamma_2^2 - 1 + 2\Gamma_1\Gamma_2(1 + \cos \alpha) + 2\Gamma_1(1 + \cos \alpha) - 2\Gamma_2 \cos \alpha, \\ B(\alpha) = 2\Gamma_1\Gamma_2(\cos \alpha - 1) + 2\Gamma_1(1 - \cos \alpha) - \Gamma_3 \cos \alpha - \Gamma_2\Gamma_3. \quad (19)$$

The solutions of Eq. (15) have the following property:

$$\lambda(\alpha_x, \alpha_y) = -\lambda(\pi + \alpha_x, \pi + \alpha_y). \quad (20)$$

The proof of the relation (20) is given in Appendix B. In addition, it is obvious that

$$\lambda(\alpha_x, \alpha_y) = \lambda(\pm \alpha_x, \pm \alpha_y), \quad \lambda(\alpha_x, \alpha_y) = \lambda(\alpha_y, \alpha_x). \quad (21)$$

Equations (20) and (21) make it possible when determining the energy spectrum to consider just the region of quasi-momentum values $\pi/2 > \alpha_x > 0$, $\pi > \alpha_y > 0$.

Note also that for $\alpha_x = \alpha_y = \alpha$ Eq. (18) decouples into the two equations

$$A(\alpha) = \pm B(\alpha). \quad (22)$$

3. ENERGY SPECTRUM

In accordance with Nagaoka's theorem, for a system with one hole and with $U = \infty$ the state with $\alpha_x = \alpha_y = 0$ and the maximum possible spin $S = (M - 1)/2$ has the lowest energy. In this paper, we consider in more detail the energy spectrum for values of the quasimomentum $\alpha_x = \alpha_y = 0$ and $\alpha_x = \alpha_y = \pi$.

As follows from Eqs. (20) and (21), the energy spectrum of states with $\alpha_x = \alpha_y = \pi$ can be determined from the states with $\alpha_x = \alpha_y = 0$. As an illustration of this proposition, we give in this paper a parallel description of these two cases. As follows from what is given below, the equations for determining the spectrum correspond to the symmetry (20), (21), and the minimum of the energy of the states with $\alpha_x = \alpha_y = 0$ corresponds to the maximum energy for the states with $\alpha_x = \alpha_y = \pi$.

In the case considered, each of Eqs. (19) decouples further into two equations, and this makes it possible to simplify the calculation of the energy spectrum.

For $\alpha_x = \alpha_y = 0$ Eqs. (22) decouple into the four following equations:

$$\frac{2t}{M} \sum_{\mathbf{k}} \frac{\sin^2 k_x}{\lambda + \varepsilon_k} = 1 \quad (\text{two equations}), \quad (23)$$

$$\frac{1}{M} \sum_{\mathbf{k}} \frac{\lambda + 4t}{\lambda + \varepsilon_k} = 1, \quad (24)$$

$$\frac{t}{M} \sum_{\mathbf{k}} \frac{(\cos k_x - \cos k_y)^2}{\lambda + \varepsilon_k} = -1. \quad (25)$$

In this case, it follows from (14) that there is also a solution with vanishing Ψ_i :

$$\lambda + 4t = 0. \quad (26)$$

For $\alpha_x = \alpha_y = \pi$, we have the following four equations:

$$\frac{2t}{M} \sum_{\mathbf{k}} \frac{\sin^2 k_x}{\lambda + \varepsilon_{\mathbf{k}}} = -1 \quad (\text{two equations}), \quad (27)$$

$$\frac{1}{M} \sum_{\mathbf{k}} \frac{\lambda - 4t}{\lambda + \varepsilon_{\mathbf{k}}} = 1, \quad (28)$$

$$\frac{t}{M} \sum_{\mathbf{k}} \frac{(\cos k_x - \cos k_y)^2}{\lambda + \varepsilon_{\mathbf{k}}} = -1. \quad (29)$$

In this case, it follows from (14) that there is also a solution with vanishing Ψ_i :

$$\lambda - 4t = 0. \quad (30)$$

As we have already noted, the solutions of Eqs. (14), i.e., the values $\lambda = -4t$ for $\alpha_x = \alpha_y = 0$ and $\lambda = 4t$ for $\alpha_x = \alpha_y = \pi$, correspond to the state with the maximum possible spin. The remaining values of the energy determined by Eqs. (23)–(25) and (27)–(29) correspond to the spectrum with spin smaller by one unit.

Each of Eqs. (23), (25), (27), and (29) has a number of roots equal to the number of different values of $\varepsilon_{\mathbf{k}}$. Equations (24) and (28) have two fewer roots. In the $N \times N$ lattice, the free quasiparticles have a natural degeneracy associated with sign reversal of k_x or k_y and also replacement of x by y . For definiteness, we shall in what follows consider lattices with even number of sites in each direction ($N = 2k$). For such a lattice, the free quasiparticles with quasimomenta $(0,0)$ and (π,π) are nondegenerate; those with quasimomenta $(0,k_x)$, $(k_x,0)$, $(0,k_y)$, $(k_y,0)$ ($k_x \neq 0$, $k_y \neq 0$), and with quasimomenta (π,k_x) , (k_x,π) , $(0,k_y)$, (k_y,π) , $(k_x \neq \pi$, $k_y \neq \pi)$ have degeneracy equal to four (the total number of such levels without allowance for degeneracy is $N/2 - 1$); those with quasimomenta $(0,\pi)$, $(\pi,0)$ are doubly degenerate; the quasiparticles with quasimomenta (k,k) for $k \neq 0$ and $k \neq \pi$ have degeneracy four (the total number of such levels without allowance for degeneracy is $N/2 - 1$); the quasiparticles with quasimomenta (k_x,k_y) for $k_x \neq k_y$ have degeneracy eight [the total number of such levels without allowance for degeneracy is $(N/2 - 1)(N/2 - 1)/2$].

Therefore, Eqs. (23) and (27) each have $(N/2 - 1)N/4$ roots, Eqs. (24) and (28) each have $N^2/8 + 3N/4 - 1$ roots, and Eqs. (25) and (29) each have $(N/2 - 1)(N/4 - 1)$ roots. All these roots are nondegenerate. In total, the number of states for spin $S = S_{\max} - 1$ must be $N^2 - 2$. As follows from the expressions (7)–(12), the remaining energy levels coincide with quasiparticle levels having degeneracy greater than 2; for the fourfold degenerate states, the degeneracy is reduced by one, and for the eightfold degenerate states by four. These solutions are valid for all $\Phi_i = 0$.

As follows from Eqs. (23)–(29), the energy levels are situated between neighboring quasiparticle levels on the interval $[-4t, 4t]$. The states with spin $S = S_{\max} - 1$ are situated above the Nagaoka level $\varepsilon = -4t$, but the difference Δ between the energies of the ground state with spin $S = S_{\max} - 1$ and the Nagaoka state is microscopic. We emphasize that this applies both to states with quasimomentum $(0,0)$ and to states with quasimomentum (π,π) . In the macroscopic limit, the levels for both $\alpha_x = \alpha_y = 0$ and $\alpha_x = \alpha_y = \pi$ have distri-

bution density identical to the density of the single-particle excitations of a spinless Fermi gas. For the states with quasimomentum $(0,0)$

$$\frac{\Delta}{4t} = \frac{2\pi^2}{M} + \frac{\ln M}{4\pi^2 M^2},$$

and for the states with quasimomentum (π,π)

$$\frac{\Delta}{4t} = \frac{2\pi^2}{M} - \frac{\ln M}{8\pi^2 M^2}.$$

The Hubbard interaction reduces the energy of the states with spin $S = S_{\max} - 1$ without changing the energy of the states with $S = S_{\max}$. At the same time, the ground state ceases to correspond to the spin $S = S_{\max}$ beginning with the Hubbard energy levels $U = U_c$. To estimate the value of U_c , we write the Hamiltonian of the Hubbard model to terms of order t/U . Then

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \quad (31)$$

where

$$\hat{H}_1 = \frac{t^2}{U} \sum ' \hat{a}_{k\sigma}^+ \hat{a}_{i\sigma'} (1 - \hat{a}_{k\bar{\sigma}}^+ \hat{a}_{k\bar{\sigma}'}) \hat{a}_{i\bar{\sigma}}^+ \hat{a}_{i\bar{\sigma}'} \hat{a}_{j\sigma}^+ (1 - \hat{a}_{j\bar{\sigma}}^+ \hat{a}_{j\bar{\sigma}'}). \quad (32)$$

We obtain a lower bound for the level shift Δ_1 by calculating the diagonal matrix element of H_1 with respect to the function Ψ_0 that corresponds to the ground state for $S = S_{\max} - 1$. For quasimomentum $(0,0)$, we have the obvious inequality

$$\Delta_1 < -4|t|^2/U. \quad (33)$$

Therefore, for $U/t < M/2\pi^2$ the ground state does not have the maximum possible value of the spin. Therefore, the critical value of the Hubbard energy corresponding to crossing of the lowest ferromagnetic level and the ground-state level with $S = S_{\max} - 1$ has macroscopic order of magnitude. For $U < U_c \sim tN^2$, the ground state in the system with one hole is not ferromagnetic.

4. CONCLUSIONS

The aim of this work was to study changes in the energy spectrum that arise in a system with one hole when one spin is flipped. We find that to the levels of the system that correspond to the maximum possible state there are added the levels of states with spin reduced by one. As follows from Nagaoka's proof, all these levels are situated within the interval $[-4t, +4t]$. It follows from our study that at least for states with total quasimomenta $\alpha_x = \alpha_y = 0$ and $\alpha_x = \alpha_y = \pi$ of the system the energy levels are situated between the levels $\varepsilon_{\mathbf{k}}$ of the free quasiparticle. Therefore, the density of states $\Delta n/\Delta\lambda$ of such a system with given value of the quasimomentum at values of $\Delta\lambda$ exceeding the difference of the neighboring levels of the free quasiparticles ceases to depend on the value of the total quasimomentum α . In contrast, in the opposite limiting case of zero Hubbard energy the dependence of $\Delta n/\Delta\lambda$ on α is quite strong.

It follows from the calculation that in the present case, the energy levels are so close to the corresponding energies

of the free quasiparticles that the ratio of the distance between them to the difference between the neighboring levels of the free quasiparticles is microscopically small.

The expressions obtained in this study for the wave functions and energy spectrum of the Hubbard system with one hole and one flipped spin can be used for numerical calculations of the correlation functions, spin susceptibility, and the specific heat.

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APPENDIX A

For definiteness, we sum the expressions for Γ_i over k_x . Let $\theta = \lambda/2 + \cos k_y$, $z = \exp(ik_x)$. Then the denominator of the expressions in the sum vanishes for $z = -\theta \pm \sqrt{\theta^2 - 1}$. Therefore, for $|\theta| > 1$ the summation is readily performed, and for Γ_0 we have [in the expression (A.1), we denote by z_1 the root with largest absolute value, i.e., $z_{1,2} = -\theta \mp (\theta/|\theta|)\sqrt{\theta^2 - 1}$]

$$\Gamma_0 = \frac{1}{N_y} \sum_{k_y} \frac{S_0(k_y)}{z_1 - z_2},$$

$$S_0 = \sum_z \left(\frac{z_1}{z - z_1} - \frac{z_2}{z - z_2} \right) = - \sum_{m=0}^{\infty} \left(\frac{z_1}{z_1} \right)^{N_x m} - \sum_{m=0}^{\infty} \left(\frac{z_2}{z_2} \right)^{N_x m}. \quad (\text{A1})$$

Thus, for N_x even or $z_1 > 0$

$$S_0 = -\coth \left[\frac{N_x}{2} \ln |z_1| \right], \quad (\text{A2})$$

and for N_x odd and $z_1 < 0$

$$S_0 = -\tanh \left[\frac{N_x}{2} \ln |z_1| \right]. \quad (\text{A3})$$

If $|\theta| < 1$, we have $|z_1| = 1$, i.e., $z_1 = \exp(i\vartheta)$. For Γ_0 , we obtain

$$\Gamma_0 = \frac{1}{N_y} \sum_{k_y} \frac{S_0(k_y)}{\sin \vartheta},$$

$$S_0 = -\frac{1}{N_y} \sum_{k_x} \left(\frac{\exp(i\vartheta)}{\exp(ik_x) - \exp(i\vartheta)} - \frac{\exp(-i\vartheta)}{\exp(ik_x) - \exp(-i\vartheta)} \right) \\ = \frac{1}{N_y} \sum_{m=0}^{N_x-1} \frac{\cos(\vartheta/2 - \pi m/N_x)}{\sin(\vartheta/2 - \pi m/N_x)}. \quad (\text{A4})$$

The sum can be calculated, for example, by expanding the trigonometric functions in infinite products. As a result, we obtain

$$S_0 = \cot(N_x \vartheta/2). \quad (\text{A5})$$

APPENDIX B

To prove the relation (20), we represent the expressions for $A(\alpha)$ and $B(\alpha)$ in the form

$$A(\alpha) = C_1 + C_2 \cos \alpha, \quad B(\alpha) = D_1 + D_2 \cos \alpha, \quad (\text{B1})$$

where

$$C_1 = 2\Gamma_1 - 1 + 2\Gamma_1\Gamma_2 - \Gamma_2^2, \quad D_1 = 2\Gamma_1 - 2\Gamma_1\Gamma_2 - \Gamma_2\Gamma_3, \quad (\text{B2})$$

$$C_2 = 2\Gamma_1 + 2\Gamma_1\Gamma_2 - 2\Gamma_2, \quad D_2 = -2\Gamma_1 + 2\Gamma_1\Gamma_2 - \Gamma_3.$$

Therefore, Eq. (18) has the form

$$C_1^2 - D_1^2 + (\cos \alpha_x + \cos \alpha_y)(C_1 C_2 - D_1 D_2) \\ + \cos \alpha_x \cos \alpha_y (C_2^2 - D_2^2) = 0. \quad (\text{B3})$$

Replacing the coefficients C_i and D_i by their expressions (B2), we obtain

$$C_1^2 - D_1^2 = \left(\frac{\lambda}{4} + 1 \right) (-\Gamma_0 + \Gamma_2 - \lambda \Gamma_0 \Gamma_2) \left[-1 - \frac{\lambda \Gamma_2}{4} - 2\Gamma_2^2 + \frac{(\lambda^2 - 16)\Gamma_0 \Gamma_2}{4} \right], \\ C_2^2 - D_2^2 = \left(\frac{\lambda}{4} + 1 \right) \left(1 - \Gamma_0 \Gamma_2 - \frac{\lambda \Gamma_0}{4} \right) \left[-\frac{\lambda}{4} - 3\Gamma_2 + \frac{(\lambda^2 - 16)\Gamma_0}{4} \right], \quad (\text{B4})$$

$$C_1 C_2 - D_1 D_2 = \left(\frac{\lambda}{4} + 1 \right) \left[-\frac{\lambda^3 \Gamma_0^2 \Gamma_2}{4} + \frac{\lambda^2}{4} (2\Gamma_0 \Gamma_2 - 2\Gamma_0^2 \Gamma_2^2 - \Gamma_0^2) + \frac{\lambda}{4} (-\Gamma_2 + 12\Gamma_0 \Gamma_2^2 + 16\Gamma_0^2 \Gamma_2) + \frac{1}{2} + 8\Gamma_0^2 \Gamma_2^2 - \frac{5\Gamma_2^2}{2} + 4\Gamma_0 \Gamma_2^3 + 8\Gamma_0^2 \right].$$

Here, we have introduced the notation

$$\Gamma_0 = \frac{1}{M} \sum_{\mathbf{k}} \frac{1}{\lambda + \varepsilon_{\mathbf{k}}}.$$

and therefore $\Gamma_1 = 1/4 - (\lambda/4 + 1)\Gamma_0$. Since $\lambda = -4$ is not a solution of Eq. (18), we obtain for the determination of λ , canceling the factor $\lambda/4 + 1$, an equation that is invariant under the substitution $\lambda \rightarrow -\lambda$, $\alpha_x \rightarrow \pi - \alpha_x$, $\alpha_y \rightarrow \pi - \alpha_y$ (at the same time $\Gamma_0 \rightarrow -\Gamma_0$, $\Gamma_2 \rightarrow -\Gamma_2$).

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Translated by Julian B. Barbour