Hubbard model with strong correlation. The equivalent Hamiltonian

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A Hubbard model with infinite repulsion at the center is considered. The purpose is a reformulation and simplification of the problem from the very beginning. An equivalent Hamiltonian is obtained (in two forms) and it is shown that in a number of cases it is more illustrative and convenient for calculations than the original Hubbard Hamiltonian.

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1. INTRODUCTION

The Hamiltonian corresponding to the Hubbard model[1] is

$$H=\sum_{nn'\nu} t_{nn'} a_{n\nu}^{+} a_{n'\nu} + U \sum_{n} (a_{n\uparrow}^{+} a_{n\uparrow})(a_{n\downarrow}^{+} a_{n\downarrow}). \tag{1}$$

The quantity $U>0$ characterizes the interaction at one center; $a_{n\nu}$ and $a_{n\nu}^{*}$ are the annihilation and creation operators for an electron with spin $\nu=\uparrow,\downarrow$ at the center n and satisfy the usual Fermi commutation relations. A periodic arrangement of the center is implied. The matrix element $t_{nn'}$ couples the nearest neighbors:

$$t_{nn'}=\begin{cases} t \text{ for nearest neighbors} \\ 0 \text{ in all other cases} \end{cases}. \tag{2}$$

At

$$U\to\infty \tag{3}$$

not more than one electron can be situated on each center—this is the case of the extreme strong correlation. The present paper is devoted to just such a model (1)–(3).

A number of the basic properties of the model (1)–(3) have by now been established. When the number of electrons N equals the number of centers N_0 (half-occupied band) everything is simple: there is one electron on each center and all levels have the same energy, while the states differ only in the values of the spin on each site. If, however, the number of electrons is less than the number of centers, $N<N_0$, the properties of the system depend substantially on the type of lattice.

Lattices can be divided into two classes. Some lattices consist of two sublattices such that the nearest neighbors of each atom are only atoms of the other sublattice. These are the so-called divisible (alternating) lattices (e.g., simple cubic and body-centered cubic). The other class is that of indivisible (non-alternating) lattices (e.g., face-centered cubic). A distinction must be made between two cases:

(a) lattices indivisible at $t>0$ and lattices divisible regardless of the sign of t;

(b) indivisible lattices at $t<0$.

Nagaoka[2] considered the problem with one unoccupied center, i.e., with one vacancy ($N_0-N=1$), and proved that in case (a) the ground state has a maximum possible spin $\frac{1}{2}N$, but in the case (b) this is not so. Nagaoka obtained next the spectrum of a spin wave in case (a) (for a simple cubic lattice) at a low vacancy density:

$$n_v=(N_0-N)/N_0\ll 1. \tag{4}$$

Iordanskiĭ[3] and Iordanskiĭ and Smirnov[4] investigated case (b) and obtained the spin structure and the ground-state energy for one vacancy in a triangular and hexagonal close-packed lattice.

The main purpose of the present paper is to construct a Hamiltonian equivalent to the Hubbard Hamiltonian (1), (2) under the condition (3) (Sec. 2). A reformulation of the Hubbard problem is needed because the existing methods are too complicated to use for further study of the properties of the Hubbard model. This pertains both to the Nagaoka method[2] and to that of Zaĭtsev[5]; the complexity is due in part to the fact that the interaction U considered in Refs. 2 and 5, while large, is finite, and the authors attempt to take into account terms of order t/U; in the limit (3) of interest to us one can hope for a substantial simplification. In fact, as shown in Sec. 3, the use of the equivalent Hamiltonian greatly simplifies in some cases the solution of the problem. For example, an equation for the dispersion of a spin wave is easily obtained [case (a), limit (4)]. In the same section we obtain the vertex part that describes the interaction of a spin wave and a vacancy, i.e., a property needed to ascertain the influence of the spin waves on the conductivity. An interesting although obvious property of spin waves is established and points to a possible rearrangement of the magnetic structure in the presence of a vacancy flux.

2. THE EQUIVALENT HAMILTONIAN

As already noted, an obvious property of the Hubbard model under condition (3) is the absence of doubly occupied centers. This circumstance can be taken into account explicitly, without introducing an infinite interaction into the Hamiltonian, in the following manner. We consider the Hamiltonian

$$H_e=\sum_{nn'\nu} t_{nn'} a_{n\nu}^{+} (1-a_{n,-\nu}^{+} a_{n,-\nu}) a_{n'\nu} (1-a_{n',-\nu} a_{n',-\nu}). \tag{5}$$

This Hamiltonian forbids the tunneling of a particle to an occupied center, whereas a transition to an empty site from a single-occupany center is described in the

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same manner as by the operator (1). The Hamiltonian (5) does not forbid double occupancy of a center, but such a center cannot decay. In other words, the Hamiltonian H_e conserves the number N_2 of the doubly occupied centers, i.e., the corresponding operator

$$\hat{N}_2=\sum_n (a_{n\uparrow}^+ a_{n\uparrow})(a_{n\downarrow}^+ a_{n\downarrow}) \tag{6}$$

commutes with H_e. It is clear after these remarks that any eigenstate of the Hamiltonian (1), (3) is an eigenstate (with the same energy) of the Hamiltonian (5) with the quantum number

$$N_2=0, \tag{7}$$

and vice versa. Thus, the Hamiltonian (1) subject to conditions (3) is fully equivalent to (5) under condition (5). The transition from (1), (3) to (5), (7) is the basis of the new approach to the problem.

It might seem at first glance that we have gained nothing from this approach. Although H_e does not contain infinite terms explicitly the direct use, e.g., of standard diagram methods[6] is impossible as before, this time because of the need to take the additional condition (7) into account. Actually this is not so. We shall show how the Hamiltonian (5), (7) can be used in limiting cases.

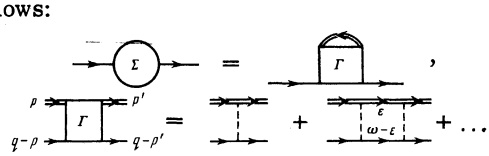
A. The first limiting case is when the number of electrons is small compared with the number of lattice sites:

$$N/N_0 \ll 1. \tag{8}$$

It is easy to see that the ground state corresponds to (7). We reason in the following manner. Assume, for example, that we have a doubly occupied center. The electron energy at this center is zero, whereas the energy of two electrons located at different centers and capable of tunneling from site to site is negative and is close to double the energy of the bottom of the band. The absence of doubly occupied centers is therefore energywise favored.

What is valid for the ground state holds also for not too highly excited states, i.e., for sufficiently low temperatures (the energy of the excitations and the temperature should be less than the band width). We see thus that in the limit (8), at not too high temperatures, the additional condition (7) can be disregarded, and the problem can be solved, for example, by a diagram technique[7] (this is obviously valid up to some ratio $N/N_0 \sim 1$).

The considered limiting case is of no particular interest, and we shall discuss it only briefly. One can use here the well worked out so-called gas approximation. A solution of the problem by a diagram technique was presented for Fermi system by Galitskiĭ.[7] As applied to our problem, the results are the following: the electronic self-energy part Σ is connected with the vertex part Γ calculated in the ladder approximation as follows:



(9)

The single and double lines pertain here to electrons with different spins, and the dashed line to the interaction. Knowing Σ we can obtain the electron spectrum in the usual manner as the pole of a single-particle Green's function.

It should be noted that so long as the ladder approximation is used for Γ, we can start out with the Hamiltonian (1) (Ref. 8); the results are the same when $U \to -\infty$. It is difficult, however, to go outside the framework of this approximation for the Hamiltonian (1), (3), i.e., to take higher powers of the density into account. It is not simple to justify formally even the ladder approximation in the case of an infinite interaction, since in principle diagrams of all order in the interaction must be taken into account, and only then it is possible to take the limit as $U \to -\infty$ and see what is left. The fact that no such questions arise when H_e is used is an undisputed advantage.

B. The second limiting case is that of few vacancies (4). In this limit, the condition (7) is certainly not satisfied for the ground state of the Hamiltonian H_e, so that the direct use of H_e is impossible. We can, however, to go over with the aid of H_e to another equivalent Hamiltonian which is free of the above difficulty. This is done in the following manner.

We assume a ground state ("vacuum") with the maximum possible number of electrons ($N = N_0$) and spin ($N_0/2$); for the sake of argument let all electrons have spin $\uparrow$. The vacancy is then simply a hole against the background of electrons with spin $\uparrow$, and it corresponds to annihilation and creation operators α_n and α_n^+ connected in the usual manner with the electron operators

$$\alpha_n = a_{n\uparrow}^+, \quad \alpha_n^+ = a_{n\uparrow}. \tag{10}$$

That Hamiltonian component $\tilde{H}_1$ that describes the vacancy tunneling (in the absence of electrons with spin $\downarrow$) takes the simple form

$$\tilde{H}_1 = -\sum_{nn'} t_{nn'} \alpha_n^+ \alpha_{n'}. \tag{11}$$

We consider now the Hamiltonian component H_2, which describes the displacement of the particles with spin $\downarrow$; this component is contained in H_e (5) and corresponds to $\nu = \downarrow$; changing from electron operators with spin $\uparrow$ to vacancy operators in accord with (10), we obtain

$$H_2 = \sum_{nn'} t_{nn'} \beta_n^+ \alpha_n \alpha_{n'}^+ \beta_{n'}, \tag{12}$$

where

$$\beta_n = \alpha_n a_{n\downarrow}, \quad \beta_n^+ = a_{n\downarrow}^+ \alpha_n^+. \tag{13}$$

Let us clarify the meaning of the introduced operators. In view of the assumed definition of the vacuum and the exclusion of double occupancy of the center, a particle $\downarrow$ is produced only by spin flip, i.e., via production of a vacancy plus production (on the same site) of a particle $\downarrow$. This is precisely the condition satisfied by the operator β_n^+. The meaning of H_2 is clear—this operator gives tunneling of the particle β only if there is a vacancy alongside (in which case they exchange places).

The operators β and β^+ at different sites commute with each other, while on the same site they are subject to

the condition

$$\beta_n^2=(\beta_n^+)^2=0.$$

These are precisely the properties of the operators S_{nx}, S_{ny} and of S_{nz} of spin $\frac{1}{2}$ if the following correspondence is assumed

$$\beta_n^+ \leftrightarrow S_n^-, \quad \beta_n \leftrightarrow S_n^+, \quad S^\pm=S_x\pm iS_y. \tag{14}$$

Each site is thus assigned its own pseudospin. In this notation, the pseudospin projection corresponding to a center with particle β is $-\frac{1}{2}$, and that to a free center is $+\frac{1}{2}$. We note that a transition of similar type to spin $-\frac{1}{2}$ operators was used in various papers (see, e.g., the paper by Anderson[9]).

Next, the operators β and β^* commute with α and α^* at different sites, while on the same site

$$\alpha_n\beta_n=\beta_n^+\alpha_n^+=0.$$

This condition that there be no two particles on the same site can be taken into account by using the procedure already used at the beginning of this section, i.e., by forbidding the transition of a vacancy (particle α) to a center occupied by particle β. This condition is obviously satisfied by the operator

$$H_1=-\sum_{nn'} t_{nn'}\alpha_n^+(1/2+S_{nz})\alpha_{n'}(1/2+S_{n'z}), \tag{15}$$

which must be used in lieu of the operator $\tilde{H}_1$ (11).

The sought Hamiltonian is thus

$$\mathcal{H}=H_1+H_2=-\sum_{nn'} t_{nn'}\alpha_n^+\alpha_{n'}\{(1/2+S_{nz})(1/2+S_{n'z})+S_n^+S_{n'}^-\}. \tag{16}$$

This Hamiltonian commutes with the operator of the number of doubly occupied centers

$$\hat{\mathcal{N}}_2=\sum_n \alpha_n^+\alpha_n(1/2-S_{nz}), \tag{17}$$

and, as before, we are interested only in states with quantum number

$$\mathcal{N}_2=0. \tag{18}$$

The very method of constructing the Hamiltonian (16) shows that it is equivalent [subject to condition (18)] to the initial Hamiltonian (1), (3). This can be verified also directly, by calculating the matrix elements of these Hamiltonians from the corresponding functions and verifying that they coincide.

Some of the quantities in $\varkappa$ are: α are Fermi operators, S are spin $-\frac{1}{2}$ operators that commute at different sites, while α and S commute with one another. In the vacuum (all sites occupied by spin $\uparrow$ electrons) there are no vacancies, and the pseudospins are directed up. All the states of the system can be enumerated by generating vacancies and reversing the pseudospins [but not at the same site, owing to condition (18)]. If a vacancy appears at some site, the pseudospin in this place is directed up as before; therefore the pseudospins have no direct physical meaning, although the pseudospin on a center free of vacancies shows the direction of the spin of the electron located on this center. This means that the spin operator σ_n is connected with the pseudospin in the following manner:

$$\sigma_n=S_n(1-\alpha_n^+\alpha_n). \tag{19}$$

The operator of the total spin of the system

$$\sigma=\sum_n \sigma_n$$

commutes with the Hamiltonian (16) and with the operator (17).

The advantage of the Hamiltonian (16) over (5) is that the ground state of the Hamiltonian (16) has a quantum number $\mathcal{N}_2=0$, so that there is no need to take into account this additional condition. This statement can be proved in the following manner. Consider a state with one flipped pseudospin, and let a vacancy be located on the same site; this cannot be a ground state, since it is possible to indicate another state that is certainly lower in energy. The energy of the considered state (with double occupancy of a certain site) coincides with the average energy of the state in which all the pseudospins are directed up and one of the vacancies is localized at the site. The last is not an eigenstate for the Hamiltonian (16), and can therefore not be the ground state (in any ground state, all the vacancies are delocalized if the pseudospins are directed up). Similar arguments can be advanced also for several flipped spins. We verify by the same token the validity of the statement made.

Our main purpose has therefore been achieved: we have obtained an equivalent Hamiltonian (16) that does not contain explicitly infinite terms, and can be used at sufficiently low temperatures [the temperature must be lower than the width of the band in the limit (4)], without the need to satisfy the additional condition (18). It appears that this Hamiltonian is particularly useful for the study of the ferromagnetic state (with maximum possible spin). This Hamiltonian contains explicitly vacancies, spin waves (the "embryo" of the spin wave is the flipped pseudospin), and their interaction. The difficulty in using the Hamiltonian (16), just as magnetism theory in general (see, e.g., Ref. 10), is the presence of spin operators, which are considerably more difficult to use than particle operators. In some cases, however, this difficulty can be circumvented (see the next section).

We emphasize that although we have arrived at the Hamiltonian (16) by considering the limit (4) and tacitly implying the case (a) of Sec. 1, this Hamiltonian is nevertheless suitable in principle for any case; the problem is to know when it is more convenient to use the Hamiltonian (16) in place of the initial Hamiltonian (1), (3) or the Hamiltonian (5), (7).

3. VERTEX PART

In this section we study the interaction of vacancies with spin waves in the limit (4) of low vacancy density. Knowing this interaction, we can find, for example, the spectrum of the spin wave.

We change first from pseudospin operators to Bose operators. The transition might be effected, say, using the known Holstein-Primakoff transformation. In the case of single spin wave (one flipped pseudospin), how-

ever, there is a simpler method, namely, we can use a Hamiltonian expressed in terms of the operators β and β^+ (13). These are Bose-type operators, and the condition that there be no transition of a vacancy to a site occupied by the particle β is taken into account, as in the preceding section; the suitably modified operator $\bar{H}_1$ (11) when added to (12) gives the sought Hamiltonian

$$H_0=-\sum_{nn'} t_{nn'}\alpha_n^+\alpha_{n'}\{(1-\beta_n^+\beta_n)(1-\beta_{n'}^+\beta_{n'})+\beta_{n'}^+\beta_n\}. \tag{20}$$

It is easily understood that this Hamiltonian is fully equivalent to (16) in the considered case of one magnon; β and β^+ are magnon operators.

The Hamiltonian (20) can be rewritten with the three-particle interaction discarded, since one particle β is considered:

$$H_0\to-\sum_{nn'} t_{nn'}\alpha_n^+\alpha_{n'}(1-\beta_n^+\beta_n-\beta_{n'}^+\beta_{n'}+\beta_{n'}^+\beta_n). \tag{21}$$

This is the initial Hamiltonian for the study of the interaction of a vacancy with a spin wave.

We change in (21) to the momentum representation by means of the usual formulas

$$\alpha_n=\frac{1}{N_0^{1/2}}\sum_{\mathbf{k}}\alpha_{\mathbf{k}}\exp(i\mathbf{k}\mathbf{R}_n),\quad \alpha_{\mathbf{k}}=\frac{1}{N_0^{1/2}}\sum_n\alpha_n\exp(-i\mathbf{k}\mathbf{R}_n), \tag{22}$$

where $\mathbf{k}$ is the quasimomentum and $\mathbf{R}_n$ is the radius vector of the site n (and similarly for β). In place of (21) we obtain

$$H_0=\sum_{\mathbf{k}}\varepsilon(\mathbf{k})\alpha_{\mathbf{k}}^+\alpha_{\mathbf{k}}+\frac{1}{N_0}\sum_{\mathbf{k}_t}\{\varepsilon(\mathbf{k}_3-\mathbf{k}_1)-\varepsilon(\mathbf{k}_1)-\varepsilon(\mathbf{k}_4)\}\alpha_{\mathbf{k}_1}^+\beta_{\mathbf{k}_2}^+\beta_{\mathbf{k}_3}\alpha_{\mathbf{k}_4}. \tag{23}$$

Here $\varepsilon(\mathbf{k})$ is the energy of the free (noninteracting) vacancy, i.e., the single-particle energy for a system with Hamiltonian (11); for a primitive cubic lattice

$$\varepsilon(\mathbf{k})=-2t(\cos k_x+\cos k_y+\cos k_z) \tag{24}$$

(the lattice constant is taken to be unity). In (23) we imply the usual quasimomentum conservation law, and the summation over $\mathbf{k}_t$ is within the confines of the Brillouin zone.

We use next the diagram technique of Ref. 6. The Green's functions G of the vacancy and D of the magnon take in the frequency representation the form

$$G(\varepsilon,\ \mathbf{p})=[\varepsilon-\xi(\mathbf{p})+i\delta\ \mathrm{sign}\,\xi(\mathbf{p})]^{-1},\quad \xi(\mathbf{p})=\varepsilon(\mathbf{p})-\mu, \tag{25}$$

$$D(E,\mathbf{k})=1/(E-E_{\mathbf{k}}+i\delta), \tag{26}$$

where μ is the chemical potential of the vacancies, and E_k is the magnon energy still to be determined. The interaction of the vacancy with the magnon is described by the vertex part Γ, which in the limit (4), when the gas approximation can be used, is given by the ladder diagrams (9) (a single line corresponds to a magnon, and a double one to a vacancy). In this approximation we can neglect the dispersion of the spin wave E_k, which is proportional to the small parameter n_v (if the magnon damping is of no interest). The vertex part Γ depends on the total frequency ω and the total quasimomentum $\mathbf{q}$ and, for example, on the incoming and outgoing quasimomenta $\mathbf{p}$ and $\mathbf{p}'$ of the vacancy. The integral equation for Γ is of the form

$$\Gamma(\mathbf{p},\mathbf{p}')=\varepsilon(\mathbf{q}-\mathbf{p}-\mathbf{p}')-\varepsilon(\mathbf{p})-\varepsilon(\mathbf{p}')+\frac{1}{N_0}\sum_{k>p_F}\frac{\varepsilon(\mathbf{q}-\mathbf{p}-\mathbf{k})-\varepsilon(\mathbf{p})-\varepsilon(\mathbf{k})}{\omega-\xi(\mathbf{k})+i\delta}\Gamma(\mathbf{k},\mathbf{p}'). \tag{27}$$

Here ω, $\mathbf{q}$, and $\mathbf{p}'$ are parameters (we have left out of Γ, for simplicity, the dependences on ω and q); p_F is the Fermi momentum. Elementary integration has been carried out in (27) with respect to the internal frequency ε [see the second diagram of (9)], on which Γ does not depend. The vertex part, strictly speaking, is Γ/N_0 [see (23)].

The restriction $k>p_F$ in the sum of (27) means integration outside the Fermi sphere; this restriction is sometimes an exaggeration of the accuracy. It was retained in (27), since it is necessary to determine first when it can be lifted [as $|\omega|-0$ the sum in (27) diverges logarithmically].

Equation (27) becomes somewhat simpler when a change is made to another function

$$\mathcal{T}(\mathbf{p},\mathbf{p}')=\Gamma(\mathbf{p},\mathbf{p}')-\frac{[\xi(\mathbf{p})-\omega][\xi(\mathbf{p}')-\omega]}{\mu+\omega+i\delta}, \tag{28}$$

after which we obtain the following equation for the function $\mathcal{T}$ and for its mean value λ:

$$\mathcal{T}(\mathbf{p},\mathbf{p}')=\varepsilon(\mathbf{q}-\mathbf{p}-\mathbf{p}')+\frac{1}{N_0}\sum_{k>p_F}\frac{\varepsilon(\mathbf{q}-\mathbf{p}-\mathbf{k})\mathcal{T}(\mathbf{k},\mathbf{p}')}{\omega-\xi(\mathbf{k})+i\delta}+\lambda, \tag{29}$$

$$\frac{1}{N_0}\sum_{k>p_F}\frac{\mathcal{T}(\mathbf{k},\mathbf{p}')}{\omega-\xi(\mathbf{k})+i\delta}+1=0, \tag{30}$$

where, by definition,

$$\lambda=\frac{1}{N_0}\sum_{\mathbf{k}}\mathcal{T}(\mathbf{k},\mathbf{p}'),$$

which follows directly from (29) after averaging over p and taking into account the relation

$$\frac{1}{N_0}\sum_{\mathbf{k}}\varepsilon(\mathbf{k})=0.$$

We note that if the restriction $k>p_F$ is taken into account in the last sum, we obtain a quantity of the order of tn_v, which can be neglected. Equation (29) does not contain these terms.

In the gas approximation, the spin-wave self-energy part Σ is connected with the vertex part in accord with (9). In the lowest approximation in the gas parameter, we must find the function $\mathcal{T}_0(\mathbf{p})$ connected with $\mathcal{T}$ by the relation

$$\mathcal{T}_0(\mathbf{p})=\mathcal{T}(\mathbf{p},0)\big|_{\substack{\omega=0\\ \mu=\varepsilon(0)}}=\Gamma(\mathbf{p},0)\big|_{\substack{\omega=0\\ \mu=\varepsilon(0)}}. \tag{31}$$

We put here for the sake of argument $t>0$, since we are interested in case (a) of Sec. 1; the minimum of the vacancy band is located therefore at the point $p=0$ and corresponds to an energy $\varepsilon(0)$. For the function $\mathcal{T}_0$ we obtain from (29) and (30)

$$\mathcal{T}_0(\mathbf{p})=\varepsilon(\mathbf{q}-\mathbf{p})-\frac{1}{N_0}\sum_{\mathbf{k}}\frac{\varepsilon(\mathbf{q}-\mathbf{p}-\mathbf{k})\mathcal{T}_0(\mathbf{k})}{\varepsilon(\mathbf{k})-\varepsilon(0)}+\lambda,$$
$$\frac{1}{N_0}\sum_{\mathbf{k}}\frac{\mathcal{T}_0(\mathbf{k})}{\varepsilon(\mathbf{k})-\varepsilon(0)}=1 \tag{32}$$

(the restriction $k>p_F$ was lifted. The magnon energy,

which coincides with the self-energy part, is determined by the value of $\mathcal{T}_0$ at zero:

$$E_q = n_v \mathcal{T}_q(0). \tag{33}$$

Relations (32) and (33) follow also from Eqs. (5.8) and (5.5) of Ref. 2. Thus, Eq. (5.8), corrected for misprints, can be written in the form

$$[E_q - t(\mathbf{p}) + t(\mathbf{k})]\Phi_q(\mathbf{p}|\mathbf{k}) = \frac{1}{N}\sum_{k'<}[t(\mathbf{k}') - t(\mathbf{k}'+\mathbf{k}-\mathbf{p}-\mathbf{q})] \times \Phi_q(\mathbf{p}|\mathbf{k}') + [t(\mathbf{k}-\mathbf{q}) - t(\mathbf{p})]\frac{1}{N}\sum_{k'<}\Phi_q(\mathbf{p}|\mathbf{k}') \tag{5.8}$$

[in our notation we should replace $t(\mathbf{p})$ by $-\varepsilon(\mathbf{p})$, let $N - N_0$, and the restriction $k <$ means $k > p_F$]. The variable $\mathbf{k}$ changes in a wide range of $k <$, and the parameter $\mathbf{p}$ in a narrow region of $p >$, so that we can simplify the equation by neglecting the dependence on $\mathbf{p}$ (by putting $\mathbf{p} = 0$) and lifting the restriction $k <$, as well as by discarding the small quantity E_q (these simplification are in fact made in Ref. 2 in the actual calculations). We then obtain from (5.8) our Eq. (32) by introducing the function

$$\mathcal{T}_q(\mathbf{k}) = [t(0) - t(\mathbf{k})]\Phi_q(0|\mathbf{k}) \Big/ \frac{1}{N}\sum_{\mathbf{k}'}\Phi_q(0|\mathbf{k}').$$

Eq. (5.5) goes over then into (33) [it is necessary to correct (5.5) by replacing $t(\mathbf{p}-\mathbf{q})$ by $t(\mathbf{k}-\mathbf{q})$]. Notice must be taken here of the following. As seen from the last equation, $\Phi_q(0|\mathbf{k})|_{k\to 0} \to \infty$, since the quantity $\mathcal{T}_0(0)$ that determines the magnon spectrum is finite. The fact that the function $\Phi_q(\mathbf{p}|\mathbf{q})$ is large at small $\mathbf{k}$ follows also from the original equation (5.8), since the right-hand side of the equation is generally speaking not small at small $\mathbf{k}$ and arbitrary $\mathbf{q}$, while the coefficient of $\Phi_q(\mathbf{p}|\mathbf{k})$ in the left-hand side of the equation is small. After the simplification this function is not merely large, but becomes infinite as $\mathbf{k} \to 0$. Refinement of the behavior at small $\mathbf{k}$ would mean inclusion of higher powers of the gas parameter in the magnon spectrum, something not included in our purpose.

When it comes to comparison with Nagaoka's results, we note the following. Refinement of the results in our approach within the framework of the same ladder approximation leads to the appearance of damping of the spin wave because particle-hole pairs are knocked out of the Fermi background of the vacancies. This is not so easy to discern in the Nagaoka method. Further, Eqs. (29) and (30) can be used to investigate the bound state of a single [in the absence of a Fermi background, $\mu = \varepsilon(0)$] vacancy with a magnon. This calls for solving the homogeneous equations and seeking a solution at $\omega < 0$. It turns out that for indivisible lattices at $t < 0$ there actually exists such a bound state (this was verified for triangular and face-centered cubic lattices), thus clarifying the meaning of Nagaoka's statement that the ground state of such structure is not the state with maximum possible spin (for a triangular lattice, the bonding of a single vacancy with a large number of flipped spins is according to Refs. 3 and 4 stronger than with one flipped spin). A bound state of vacancies with a magnon arises also in case (a) in the presence of a Fermi background; in the limit (4) the binding energy is exponentially small (because of the aforementioned logarithmic divergence), and since the bond arises only at a finite summary quasimomentum, the total energy of such a complex is positive, the ground state does not change, and one more type of elementary excitation appears.

We proceed now to study the scattering of a vacancy by a magnon. This is necessary to determine, for example, the influence of spin waves on the conductivity. At low densities of the vacancies (4) and of the magnons (low temperatures) it suffices to know the vertex part $\mathcal{T}$ at small values of the momenta [the difference between $\mathcal{T}$ and Γ, see (28), turns out to be negligible]. Leaving out the straightforward calculations, we present only the result for a simple cubic lattice:

$$\frac{\mathcal{T}(\mathbf{p},\mathbf{p}')}{2t} = \frac{p^2+p'^2}{2} + \frac{1}{1+\gamma}\left\{\mathbf{p}\mathbf{p}' - (\mathbf{p}+\mathbf{p}')\mathbf{q} + \frac{1-\gamma}{2}q^2\right\} - \left(\frac{\omega}{2t} + \frac{p_F^2}{2}\right), \tag{34}$$

where the dimensionless quantity γ is given by the expression

$$\gamma = \frac{2t}{N_0}\sum_{k>p_F}\frac{\sin^2 k_x}{\xi(\mathbf{k}) - \omega - i\delta}. \tag{35}$$

We are interested in the scattering of a vacancy with energy near the Fermi surface. In place of ω it is necessary to substitute in (34) the combined energy of the vacancy of the magnon, which is small: $|\omega| \ll tp_F^2$, because the role of the vacancy energy is assumed by the quantity $\xi(\mathbf{p})$, and the frequency ω can be neglected in the last term. Recognizing that $p \approx p' \approx p_F$ and introducing the initial magnon momentum $\mathbf{k} = \mathbf{q} - \mathbf{p}$, we obtain in place of (34) in this case

$$\frac{\mathcal{T}}{2t} = \frac{1}{1+\gamma}\left\{\frac{1-\gamma}{2}k^2 - \gamma(\mathbf{k}\mathbf{p}) - (\mathbf{k}\mathbf{p}')\right\}. \tag{36}$$

As for the dependence of γ on ω, it may turn out to be appreciable. Indeed, if we disregard terms of order n_v in γ, we can write at small $|\omega|$

$$\gamma = \gamma_0 + \gamma_1,$$

where γ_0 does not depend on the frequency:

$$\gamma_0 = \frac{2t}{N_0}\sum_{\mathbf{k}}\frac{\sin^2 k_x}{\varepsilon(\mathbf{k}) - \varepsilon(0)} \approx 0.208 \tag{37}$$

(we have presented here Nagaoka's numerical result for a simple cubic lattice), and the dependence on ω is contained in γ_1:

$$\gamma_1 \sim n_v \ln\frac{tp_F^2}{|\omega|}.$$

At sufficiently low temperatures, allowance for γ_1 may be necessary.

Equation (34) can be used also for other purposes: let us obtain once more the magnon spectrum (at small k)—this is found to make sense. The result of the principal approximation can be written as

$$E_k = \frac{1}{N_0}\sum_{\mathbf{p}}\mathcal{T}(\mathbf{p},\mathbf{p})|_{\omega=\varepsilon(\mathbf{p})} f(\mathbf{p}), \tag{38}$$

where $f(\mathbf{p})$ is the vacancy distribution function, and the vacancy momentum $\mathbf{k} = \mathbf{q} - \mathbf{p}$ in $\mathcal{T}$ is fixed. If we replace γ by γ_0 in $\mathcal{T}$, and this can be done under the summation sign, than (38) practically coincides with Eq. (25) of

Ref. 7, apart from an exchange term, which is obviously missing from (38) because of the presence of the factor 2. From (34) we have for the vertex part contained in (38)

$$\frac{1}{2t}\mathcal{T}(\mathbf{p},\mathbf{p})|_{\omega=\varepsilon(\mathbf{p})}=\frac{1}{2}\frac{1-\gamma}{1+\gamma}k^2-\mathbf{kp}. \tag{39}$$

In the equilibrium state we obtain from (38), taking (39) into account, Nagaoka's result for the spectrum

$$\frac{E_k}{2t}=n_v\frac{1}{2}\frac{1-\gamma_0}{1+\gamma_0}k^2. \tag{40}$$

If, however, a vacancy flux is present, we obtain in place of (40)

$$\frac{E_k}{2t}=n_v\left\{\frac{1}{2}\frac{1-\gamma_0}{1+\gamma_0}k^2-\mathbf{k}\langle\mathbf{p}\rangle\right\}, \tag{41}$$

where $\langle\mathbf{p}\rangle$ is the average momentum of the vacancies. It is seen therefore that the magnon spectrum is substantially altered—its energy becomes negative at certain $\mathbf{k}$.

The cause of the change in the dispersion (41) is easily understood. We consider the precession equation

$$\frac{d\sigma(\mathbf{r},t)}{dt}=-\left[\sigma\times\frac{\delta W}{\delta\sigma}\right], \tag{42}$$

where $\sigma(\mathbf{r},t)$ is the spin density and W is the energy of the ferromagnet; in the simplest isotropic case we have

$$W=A\int d^3r\frac{\partial\sigma_i}{\partial x_k}\frac{\partial\sigma_i}{\partial x_k}. \tag{43}$$

In the presence of a vacancy flux there is a countercurrent of spin momenta, so that the left-hand side of (42) takes the form

$$\frac{d\sigma}{dt}=\left(\frac{\partial}{\partial t}+(\mathbf{v}\nabla)\right)\sigma, \tag{44}$$

where $\mathbf{v}$ is the velocity of the spin liquid and is determined by the vacancy flux:

$$\frac{\mathbf{v}}{2t}=\frac{-n_v\langle\mathbf{p}\rangle}{1-n_v}\approx-n_v\langle\mathbf{p}\rangle\quad(n_v\ll1) \tag{45}$$

(we recall that the momentum is a dimensionless quantity and the velocity has the dimension of energy). From (42), with allowance for (43)–(45), we obtain for the oscillation frequency an expression of the type (41), and the increment linear in $\mathbf{k}$, which is of interest to us, remains exactly the same.

The change of the spectrum (41) is thus a direct consequence of the motion of the spin liquid and is therefore general in character, i.e., it does not depend on the model. One cannot exclude the possibility that the magnons produced in the presence of a vacancy flux will accumulate predominantly in a single state and form a condensate (this would mean formation of a spin superstructure). This question, as well as that of the conductivity, calls for a special analysis.

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