Diagram technique and gas approximation in the Hubbard model

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The three-dimensional Hubbard model (Proc. Roy. Soc. **A285**, 542 (1965)) with a narrow band and strong intra-atomic interaction is studied. The critical concentration corresponding to the appearance of ferromagnetic order at $T=0$ is determined for the bcc and fcc lattices. For a concentration close to unity, when the number of particles is slightly less than the number of sites, the spin-wave spectrum is found. In this range of concentration the stability conditions for the ferromagnetic phase for simple, body-centered and face-centered cubic lattices are refined. It is assumed that the system is in thermodynamic equilibrium, and this is the reason why the results differ from the well-known results of Nagaoka (Phys. Rev. **147**, 392 (1966)).

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INTRODUCTION

We shall consider the three-dimensional Hubbard model with the following Hamiltonian:

$$\mathcal{H}=-t\sum_{r,r'\sigma} a_{r\sigma}^{+}a_{r'\sigma}+\sum_{r}[In_r^{(+)}n_r^{(-)}-\mu n_r-H(n_r^{(+)}-n_r^{(-)})]; \qquad (1)$$

here $n_r^{(\sigma)}=a_{r\sigma}^{+}a_{r\sigma}$, $n_r=n_r^{(+)}\pm n_r^{(-)}$, μ is the chemical potential and H is the external field, multiplied by the Bohr magneton. If the intra-atomic exchange energy I is much greater than the tunneling energy t, then, when the concentration c is increased, the system goes over from a paramagnetic phase to a ferromagnetic phase and then, finally, to an antiferromagnetic phase. In these conditions it is natural to go over to the atomic representation of[1] and take the tunneling part of the Hamiltonian (the first term in (1)) as a perturbation.

In this paper it is shown how to construct a diagram technique based on the possibility of expanding in the parameter t/I.

An attempt is made to find the concentration at which the transition from the paramagnetic to the ferromagnetic phase occurs. The results obtained have a qualitative character, since in effect the expansion is performed in powers of the parameter $\nu c^{1/3}$ (ν is the number of nearest neighbors) while the critical concentration corresponds to a value of the parameter of the order of 0.6.

In studying concentrations close to unity we have used the first theorem of Nagaoka,[2] which says that for $I=\infty$ the state of the system is ferromagnetic. Despite the fact that this theorem was proved for the simple cubic and bcc lattices, no contradiction arises if we use it for the fcc lattice too. An investigation of the stability of the magnon spectrum makes it possible to determine the region of existence of the ferromagnetic state (Sec. 2). The results of this section are in quantitative disagreement with the third theorem and directly contradict the second theorem of Nagaoka. Whereas the first theorem has a rather general character, the second and third theorems were proved for a nonuniform state "with one reversed spin." Generally speaking, the stability conditions for such a system are not bound to coincide with the stability conditions for a uniform system which is in complete thermodynamic equilibrium, and the latter is the subject of the present investigation. The methodological part of the paper contains a description of the diagram technique for the Hubbard operators.

1. THE EXCITATION SPECTRUM (LOW TEMPERATURES)

As the zeroth approximation we select the single-cell part of the Hamiltonian (1) (the second sum). The "zeroth" eigenvalues and eigenfunctions have the form

$$\varepsilon_0=0\ \ (\psi_0=|0\rangle),\quad \varepsilon_\pm=-\mu\mp H\ \ (\psi_\sigma=a_\sigma^{+}|0\rangle),$$
$$\varepsilon_2=I-2\mu\ \ (\psi_2=a_-^{+}a_-^{+}|0\rangle).$$

Calculating all possible matrix elements between the states ψ_k, we find the operators a_σ and a_σ^{+} in the atomic representation[1]:

$$a_\sigma=X^{\sigma,0}+\sigma X^{-\sigma,-2},\qquad a_\sigma^{+}=X^{0,\sigma}+\sigma X^{-2,-\sigma}.$$

Here $\sigma=\pm1$ and the operator X^{pq} has its only nonzero matrix element, which is equal to unity, on the intersection of the p-th row and the q-th column.

Thus, the tunneling Hamiltonian is expressed in terms of f-type operators only, which anticommute in different cells:

$$\mathcal{H}_2=-t\sum_{r,r'}{}'\{(X_r^{-,0}-X_r^{2,+})(X_{r'}^{0,-}-X_{r'}^{+,2})+(X_r^{+,0}+X_r^{2,-})(X_{r'}^{0,+}+X_{r'}^{-,2})\}$$
$$=\frac{1}{2}\sum_{\alpha,\beta,r,r'}{}'V_{\alpha,\beta}(\mathbf{r}-\mathbf{r}')X_{\alpha,r}X_{\beta,r'}. \qquad (2)$$

The root vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, which are defined in Appendix B (cf. Fig. 3 there), have the form

$$\alpha(0,\pm)=\left(\mp\frac{1}{\sqrt2},\frac{1}{\sqrt2},1\right)\quad \alpha(\pm,2)=\left(\pm\frac{1}{\sqrt2},\frac{1}{\sqrt2},-1\right),$$
$$\alpha(0,2)=(0,\sqrt2,0).\qquad \alpha(+,-)=(\sqrt2,0,0),\quad \alpha(p,q)=-\alpha(q,p). \qquad (3)$$

In Appendix A it is shown that the diagram technique for the Hubbard operators differs from the technique

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for b-type operators[3] only by a sign rule.[4,5] The excitation spectrum is determined by the poles of the retarded Green function, which we obtain by analytic continuation of the thermodynamic function

$$D_{\alpha,\beta}(\mathbf{k},\omega_n)=\sum_r\int_0^{1/T}\exp(i\omega_n\tau-i\mathbf{kr})\langle T(X_{\alpha r}(\tau)X_{-\beta,0}(0))\rangle d\tau. \qquad (4)$$

If the ground state of the system is known, then, at low temperatures, the fluctuations of the diagonal operators are exponentially small. In this limit our problem reduces to the problem of scattering of weakly-damped excitations. As the bare Green function it is convenient to choose the one determined from the zeroth self-consistent field approximation.[6] In this case we sum all diagrams not containing any loops. The conditions under which the loops make a small contribution will be established below.

In the absence of tunneling the Green function for the transition $p\to q$ is calculated directly:

$$D_{\alpha\beta}^{(0)}(\omega_n)=\delta_{\alpha\beta}\frac{n_q\pm n_p}{-i\omega_n+\varepsilon_{qp}},\quad \varepsilon_{qp}=\varepsilon_p-\varepsilon_q, \qquad (5)$$

$$n_p=e^{-\varepsilon_p/T}\Big/\sum_k e^{-\varepsilon_k/T},\quad \alpha=\alpha(q,p).$$

The quantity ε_{qp} is the scalar product

$$\varepsilon_{qp}=\lambda\alpha(q,p), \qquad (6)$$

where the three-dimensional vector λ is equal to

$$\lambda=\left\{H\sqrt{2},\frac{I}{\sqrt{2}}-\mu\sqrt{2},-\frac{I}{2}\right\}. \qquad (7)$$

The upper sign in (5) refers to f-transitions ($\omega_n=\pi T(2n+1)$) and the lower sign to b-transitions ($\omega_n=2\pi nT$).

In the zeroth self-consistent field approximation we obtain equations of the Dyson type:

$$[D_{\alpha\beta}(\mathbf{k},\omega_n)]^{-1}=[D_{\alpha\beta}^{(0)}(\omega_n)]^{-1}+V_{-\alpha,\beta}(\mathbf{k}),$$
$$V_{\alpha\beta}(\mathbf{k})=\sum_r e^{-i\mathbf{kr}}V_{\alpha\beta}(\mathbf{r}). \qquad (8)$$

In our case $V_{\alpha,\beta}(\mathbf{k})/t(\mathbf{k})$ is the direct product of four matrices. Two matrices have the form

$$\begin{array}{c} \\ \alpha(+,0)\\ \alpha(2,-)\end{array}\begin{array}{c}\begin{array}{cc}\beta(0,+) & \beta(-,2)\end{array}\\ \begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}\end{array}\otimes\begin{array}{c} \\ \alpha(-,0)\\ \alpha(2,+)\end{array}\begin{array}{c}\begin{array}{cc}\beta(0,-) & \beta(+,2)\end{array}\\ \begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}\end{array}; \qquad (9)$$

and the other two are obtained from (9) by transposing and changing the sign. The function

$$t(\mathbf{k})=-t\sum_r{}' e^{i\mathbf{kr}}. \qquad (10)$$

The summation runs over nearest neighbors.

After the replacement $i\omega_n\to\omega+i\delta$ we find the poles of the Green function. In our case we have two types of Bose excitations: magnons, corresponding to transitions $+\rightleftarrows-$, and excitons, corresponding to transitions to the two-particle level ($0\rightleftarrows2$). Namely,

$$\omega_m=\lambda\alpha(+,-)=2H,\qquad \omega_2=\lambda\alpha(0,2)=I-2\mu. \qquad (11)$$

The excitations of the f-type are divided into two groups[1]:

$$\omega_+^{1,2}=\tfrac{1}{2}[\lambda\alpha(0,+)+\lambda\alpha(-,2)+t(\mathbf{k})]\pm\sqrt{D}, \qquad (12)$$

where

$$D=\tfrac{1}{4}[\lambda\alpha(0,+)-\lambda\alpha(-,2)+t(\mathbf{k})[F(0,+)-F(2,-)]]^2$$
$$+F(0,+)F(2,-)t^2(\mathbf{k}),\quad F(p,q)=n_p+n_q.$$

The second pair of branches differs from (12) by the interchange $+\rightleftarrows-$ and corresponds to excitations with the opposite spin. In the limit of a large positive constant I ($I\gg\max(|\mu|,|t(\mathbf{k})|)$ we have the following branches:

$$\omega_m=2H,\ \omega_\pm=-\mu\mp H+F(0,\pm)t(\mathbf{k}). \qquad (13)$$

The energy of the other branches is of the order of I, so that their influence disappears.

In the approximation used the correction to the potential Ω can be calculated as the thermodynamic contribution containing one loop:

$$\Omega\approx\Omega_0+\Omega_1,$$
$$\Omega_0=-NT\ln\left(\sum_k e^{-\varepsilon_k/T}\right), \qquad (14)$$

$$\Omega_1=-T\sum_{k\lambda}\{\ln[1+e^{-\omega_\lambda(\mathbf{k})/T}]-\ln[1+e^{-E_\lambda/T}]\}: \qquad (15)$$

here $E_\lambda=\lim\omega_\lambda(\mathbf{k})$ and $t(\mathbf{k})\to0$; the summation over λ runs over all positive f-type frequencies.

2. HOLE FERROMAGNETISM ($T=0$)

We shall consider the situation when the number of particles is slightly less than the number of cells. According to Nagaoka's theorem,[2] in this case the system is ferromagnetic for $I=\infty$. We shall assume that the single-particle level with spin up has the lowest energy while the level with spin down lies slightly higher ($H>0$). The two other levels ("empty" and two-particle) lie considerably higher. More precisely, $0<\mu<t_m\ll I$, $0<H\ll t_m$ ($t_m=\max t(\mathbf{k})$). The spin-up state is the ground state and, therefore, for $T\ll H$ we must assume that $F(+,0)=F(+,2)=1$, while $F(-,0)=F(-,2)=0$ ($F(p,q)=n_p+n_q=F(q,p)$).

In the limit of large I, in place of (13) we have only one collective f-branch:

$$\omega_+=+t(\mathbf{k})-\mu-H=\xi(\mathbf{k}),\quad \omega_-=-\mu+H,\quad \omega_m=2H. \qquad (13')$$

Concentrations close to unity correspond to almost complete occupation of the band with spin up, i.e., $\mu+H\lesssim t(\mathbf{k})$. This is easily discovered if, using (14) and (15), we calculate the concentration and then take the limits $T\to0$, $H\to0$:

$$c=-\frac{1}{N}\frac{\partial\Omega}{\partial\mu}=1-\frac{1}{N}\sum_k\theta(\xi(\mathbf{k})); \qquad (16)$$

$\theta(x)=1$ for $x>0$ and $\theta(x)=0$ for $x<0$; $\xi(\mathbf{k})$ is defined in (13'). The ground-state energy is calculated from the usual formula

$$E_0=\lim(\Omega+\mu cN)=-\sum_k t(\mathbf{k})\theta(\xi(\mathbf{k})),\quad T\to0,\quad H\to0. \qquad (17)$$

In deriving (16) and (17) we have used the condition $\sum_{\mathbf{k}}t(\mathbf{k})=0$.

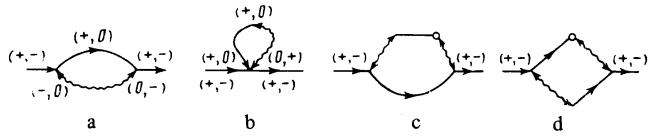

FIG. 1. Single-loop self-energy parts.

Near its maximum the expression $t(\mathbf{k})$ can be expanded as follows: $t(\mathbf{k}) = t_m - p^2/2m$. In place of the chemical potential we introduce the Fermi momentum: $\mu = -H + t_m - p_0^2/2m$ ($p_0 \ll 1$). Expanding (16) and (17) in powers of p_0, we obtain

$$\frac{E_0}{N} = -(1-c)t_m + \frac{3}{10}(6\pi^2)^{2/3}\frac{(1-c)^{5/3}}{m}. \tag{18}$$

We shall write out $t(\mathbf{k})$ for the three cubic lattices: 1) simple cubic, $m = 1/2t$:

$$t(\mathbf{k}) = -2t\sum_{\lambda}\cos k_\lambda, \quad t_m = -t(0) = 6t, \quad \lambda = 1, 2, 3.$$

2) bcc, $m = 1/2t$:

$$t(\mathbf{k}) = -8t\prod_{\lambda}\cos(k_\lambda/2), \quad t_m = -t(0) = 8t.$$

3) fcc:

$$t(\mathbf{k}) = -4t(c_1c_2 + c_2c_3 + c_3c_1),$$
$$t_m = -\tfrac{1}{3}t(0) = 4t, \quad c_\lambda = \cos(k_\lambda/2).$$

In the fcc lattice the hole Fermi surface (near t_m) has a cylindrical shape, with effective mass $m = 1/2t$. For this reason, in place of (18) we have

$$E_0/N = -4t(1-c)[1 - b(1-c)] \quad (b \sim 1). \tag{19}$$

In the one-dimensional case, when $t(k) = -2t\cos k$, formula (17) gives the well-known result of Lieb in the limit $I = \infty$ (cf., e.g., [7]):

$$E_0/N = -(2t/\pi)\sin\pi c. \tag{20}$$

In the three-dimensional case the result (18) coincides with the ground-state energy obtained in [2].

We now calculate the spin-wave spectrum. In the zeroth approximation the spin-wave energy is equal to $2H$. It is not difficult to see that the expansion of the inverse spin-wave Green function proceeds in powers of two parameters: $1-c$ and t/I. In the lowest approximations each loop gives an extra degree of smallness, so that, in the linear approximation, we have the four types of diagram depicted in Fig. 1. The diagrams of order $1-c$ are not difficult to find if we put $I = \infty$ everywhere, i.e., if we disregard diagrams containing a transition to the two-particle level. In the limit $T = 0$ the only nonzero diagrams are those which contain the "collectivized" function $G_{\omega n}^{(+,0)}(\mathbf{k}) = [-i\omega_n - \xi(\mathbf{k})]^{-1}$. The diagrams (c) and (d) should also contain the localized function $G_{\omega n}^{(0,-)} = [-i\omega_n + \varepsilon_-]^{-1}$ in that "shoulder" in which there is no terminal factor $F(0,-)$, since otherwise the diagram will give zero because of the condition $\varepsilon_+ < \varepsilon_- < 0$ ($F(0,-) = 0$). After summing over the frequencies we obtain the following result ($T = 0$):

$$N\Pi_\omega^{(1)}(\mathbf{q}) = \sum_{\mathbf{p}}\theta(\xi(\mathbf{p}))[t(\mathbf{q}-\mathbf{p}) - t(\mathbf{p})] - \sum_{\mathbf{p}}\frac{\theta(\xi(\mathbf{p}))t(\mathbf{p})[t(\mathbf{p}) - t(\mathbf{q}-\mathbf{p})]}{i\omega_n - 2H + t(\mathbf{p})} \tag{21}$$

The diagrams of order t/I can be found if, in the calculation, we assume that $c = 1$, i.e.,

$$\xi(\mathbf{p}) = \bar{\xi}(\mathbf{p}) = t(\mathbf{p}) - t_m < 0.$$

In this case, only those diagrams of the types (c) and (d) which, besides the function $G^{(+,0)}$, also contain $G^{(+,2)}$ will give a nonzero contribution. This happens because the signs of $\bar{\xi}(\mathbf{p})$ and $\varepsilon_+ - \varepsilon_2$ coincide, while the corresponding poles lie on opposite sides of the real axis. After expanding in powers of t/I, we obtain

$$N\Pi_\omega^{(2)}(\mathbf{q}) = \frac{1}{I}\sum_{\mathbf{p}}\theta(-\xi(\mathbf{p}))[t(\mathbf{p}) - t(\mathbf{q}-\mathbf{p})]^2. \tag{22}$$

With the accepted accuracy the sum over $\mathbf{p}$ can be taken over all $\mathbf{p}$, since the region in which $\xi(\mathbf{p}) > 0$ is of order $1-c$.

Diagrams containing two closed loops are of order $(1-c)^2$ in the limit $I = \infty$. In the limit $c = 1$ they are of order $(t/I)^2$. Thus, to within terms of order $1-c$ and t/I we have the following spectrum:

$$\omega_{\mathbf{q}}(\mathbf{q}) = 2H - \Pi_\omega^{(1)}(\mathbf{q}) - \Pi_\omega^{(2)}(\mathbf{q}). \tag{23}$$

Inasmuch as $\max(\omega, 2H) \ll t_m$, in the limit $H \to 0$ we obtain

$$N\omega_{\mathbf{q}}(\mathbf{q}) = 2\sum_{\mathbf{p}}\theta(\xi(\mathbf{p}))[t(\mathbf{p}) - t(\mathbf{q}-\mathbf{p})] - \frac{1}{I}\sum_{\mathbf{p}}[t(\mathbf{p}) - t(\mathbf{q}-\mathbf{p})]^2.$$

Expanding this expression to within terms of order $1-c$, we obtain

$$\omega_{\mathbf{q}}(\mathbf{q}) = -2[t(0) - t(\mathbf{q})][\alpha(1-c) - t/I]. \tag{24}$$

The values of the constant α are given in the table.

In the fcc lattice $\alpha = \frac{1}{3}$ and not 1, since the maximum value t_m is attained not at $-t(0)$ but at $-t(0)/3 = 4t$. For small $\mathbf{q}$ we have the usual ferromagnetic dispersion law $\omega = sq^2$. The spectrum becomes unstable at the same time for all $\mathbf{q}$. The region of existence of the ferromagnetic phase in an fcc lattice is smaller than in the other two lattices ($t/I < (1-c)/3$, in place of $t/I < 1-c$). Similar results were obtained by Penn[8] for the simple cubic lattice (for the corresponding graph see[9]).

At first sight it may appear that all the results obtained are valid only in an extremely narrow range of

	sc	bcc	fcc
ν	6	8	12
α	1	1	1/3
β	1.516...	1.393...	1.345...
c_0	?	0.25	0.068
p_{0c}	$>\pi/2$	1.96	1.26

Note: Here ν is the number of nearest neighbors, β are the Watson integrals and p_{0c} is the Fermi momentum for the critical concentration c_0.

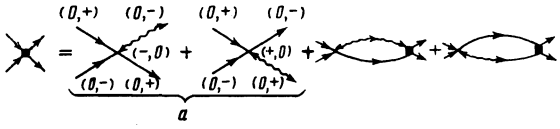

FIG. 2. The Bethe-Salpeter equation.

temperatures $T \ll H$. But this is not so. The introduction of the magnetic field is necessary in order that the state of each cell be already nondegenerate in the zeroth approximation. If we can then calculate the corrections to the Fermi-excitation spectrum for finite H (diagrams of the type depicted in Fig. 1), it turns out that these corrections depend weakly on the field and the level ε_- lies above the middle of the "conduction band" $\xi(p)$ by an amount of the order of $t_m(1-c)$. Thus, even in the absence of the field, the spin-down states are localized and remain unfilled, while the spin-up states form an almost completely filled band. As we should expect, the difference between the mean energy of the spin-up states and that of the spin-down states is equal to the ground-state energy per cell (18). It is clear that, in order of magnitude, this energy is the phase-transition temperature T_c. Thus, the results of this section have a range of applicability that is independent of the field:

$$T \ll t_m(1-c) \sim T_c, \quad H \ll t_m.$$

3. GAS APPROXIMATION

We shall consider the case of low concentrations, when $\mu + H < 0$. In this case all levels lie above the zeroth level and the ground state is nondegenerate. Putting $H = 0$ throughout, in place of (13) we obtain two branches with the same energy:

$$\omega_\pm = \xi(\mathbf{p}). \tag{25}$$

The potential Ω from (15) goes over into the potential of an ideal Fermi gas. The situation is such that for large t/I the results obtained in the atomic representation should coincide with the usual "gas" perturbation theory.[10,11] In the Born approximation, of course, we have different results. In the usual theory $\Gamma^0 = I$, while, in the limit $I = \infty$,

$$\Gamma^0 = -[t(\mathbf{p}_3) + t(\mathbf{p}_4)], \tag{26}$$

(cf. Fig. 2a).

As usual, it is necessary to solve an equation of the ladder type:

$$\Gamma(p_1, p_2; p_3, p_4) = \Gamma^0(\mathbf{p}_3, \mathbf{p}_4) - \frac{T}{N}\sum_{\omega' \mathbf{p}'} \Gamma^0(\mathbf{p}', \mathbf{s}-\mathbf{p}') G_{s_0-\omega'}(\mathbf{s}-\mathbf{p}') G_{\omega'}(\mathbf{p}') \Gamma(p', s-p'; p_3, p_4); \tag{27}$$

$$s_0 = \omega_1 + \omega_2 = \omega_3 + \omega_4, \quad \mathbf{s} = \mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}_3 + \mathbf{p}_4, \quad G_\omega^{-1}(\mathbf{p}) = -i\omega + \xi(\mathbf{p}).$$

In writing Eq. (27) we have taken into account that Γ^0 either does not depend on the momenta at all or depends only on the third and fourth arguments. We write the auxiliary equation conjugate to (27), in which we put $s_0 = 0$, $\mu = t(0)$ and $T = 0$:

$$\Gamma(p_1, p_2; p_3, p_4) = \Gamma^0(\mathbf{p}_3, \mathbf{p}_4) - \frac{1}{N}\sum_{\mathbf{p}'} \Gamma(p_1, p_2; p', s-p') \frac{\Gamma^0(\mathbf{p}_3, \mathbf{p}_4)}{\xi^{(0)}(\mathbf{p}') + \xi^{(0)}(\mathbf{s}-\mathbf{p}')},$$

$$\xi^{(0)}(\mathbf{p}) = t(\mathbf{p}) - t(0). \tag{28}$$

Noting that $\tilde{\Gamma}$ and Γ depend only on the third and fourth arguments, we obtain an equation that does not contain Γ^0:

$$\Gamma(p_3, p_4) = \tilde{\Gamma}(\mathbf{p}_3, \mathbf{p}_4) - \frac{1}{N}\sum_{\mathbf{p}'} \Gamma(\mathbf{p}', \mathbf{s}-\mathbf{p}') \left\{ \frac{1 - n(\xi(\mathbf{p}')) - n(\xi(\mathbf{s}-\mathbf{p}'))}{\xi(\mathbf{p}') + \xi(\mathbf{s}-\mathbf{p}')} - \frac{1}{\xi^{(0)}(\mathbf{p}') + \xi^{(0)}(\mathbf{s}-\mathbf{p}')} \right\} \Gamma(p_3, p_4); \tag{29}$$

$n(x)$ is the Fermi distribution.

The kernel of the new equation goes to zero far from the Fermi surface; near the Fermi surface it has a rather sharp maximum. For this reason, we shall expand all the quantities appearing in (29) about the Fermi surface. In the gas situation, when $p \lesssim p_0 \ll 1$, we can write

$$\xi(\mathbf{p}) \approx \frac{p^2}{2m} - \frac{p_0^2}{2m}, \quad \xi^{(0)}(\mathbf{p}) \approx \frac{p^2}{2m}. \tag{30}$$

We denote $\tilde{\Gamma}(0, 0; 0, 0) = \bar{\Gamma}$; then

$$\Gamma = \bar{\Gamma} / [1 + g W_T(s/2p_0)], \tag{31}$$

where $g = mp_0\bar{\Gamma}/2\pi^2$, $s = |\mathbf{p}_3 + \mathbf{p}_4|$ and the function $W_T(x)$ is well-known in the theory of superfluid Fermi systems. In the following we shall need the asymptotic expansion of $W_T(x)$ for $T = 0$ and $x \ll 1$, calculated in the pole approximation,[12] when $g^{-1} \sim -W_T(x) < 0$:

$$W_0(x) \sim -\ln x - {}^4/_3 + {}^1/_3 \ln 2. \tag{32}$$

For finite I we have

$$\Gamma = I \Big/ \left[1 + \frac{1}{N}\sum_{\mathbf{p}} \frac{I}{2\xi^{(0)}(\mathbf{p})} \right]. \tag{33}$$

Using (28) we immediately obtain the limiting value of the expression (33) when $I = \infty$:

$$\Gamma_\infty = 2 \Big/ \frac{1}{N}\sum_{\mathbf{p}} \frac{1}{t(\mathbf{p}) - t(0)}. \tag{34}$$

The sum in the denominator reduces in the three simplest cases to the well-known Watson integrals, and, therefore,

$$\Gamma = \frac{I}{1 + I/\Gamma_\infty}, \quad \Gamma_\infty = \frac{2\nu t}{\beta}. \tag{35}$$

Here ν is the number of nearest neighbors and the coefficients β are listed in the table.

We can try to substitute the results (31) and (35) in the well-known condition for the appearance of ferromagnetism:

$$(mp_0/2\pi^2)\bar{\Gamma} = 1 \tag{36}$$

(the bar denotes averaging over the directions of the momenta $\mathbf{p}_3$ and $\mathbf{p}_4$ on the Fermi surface). Using (31), it is not difficult to obtain

$$\int_0^1 \frac{dy}{g_c^{-1} + W_T(y)} = 1, \quad y = s^2/4p_0^2. \tag{37}$$

Substituting the asymptotic expansion (32) into this, we find $g_c = 0.57$. It now becomes simple to obtain the Fermi momentum and critical concentration, since for all three cubic lattices $m = 1/2t$ and the vertex part $\tilde{\Gamma}$ is known.

Since $c = p_0^3/3\pi^2$, in the limit of small t/I and for $T = 0$ we obtain the following expansion:

$$c = c_0 + 21.8 c_0^{2/3} t/I. \tag{38}$$

The constants c_0 are written out in the table. For a simple cubic lattice the critical concentration is so large that it is necessary in all cases to allow for the anisotropy of the Fermi surface. This result does not contradict the extrapolation of Kanamori, which gives a critical concentration c_0 in the range from 20 to 35%.[13] In the other two cases the critical concentration corresponds to momenta in the region of weak anisotropy ($p_0 < \pi$). The difference in the critical concentrations is connected in an obvious way with the difference in the number of nearest neighbors.

Unlike the results of the preceding section, the coefficients in the expansion (38) are tentative in character, since in the averaging over the Fermi surface in (37) the integral is taken not only in the region of small values of $x = s/2p_0$ but also in the region of values $x \sim 1$, where the formula (31), for $g = g_c = 0.57$, is no longer valid.

CONCLUSION

We note that as the temperature is raised from zero to the Fermi level the vertex part Γ increases (cf. (31)), since the function $W_T(x)$ decreases with increasing temperature. For this reason, on heating, the critical concentration first falls and then begins to increase. This form of the dependence evidently indicates the presence of a first-order phase transition.

The question of the phase transition at concentrations of order unity must be regarded as not completely solved. The point is that we do not yet know which phase the ferromagnetic phase is contiguous with. It may turn out that a phase transition occurs before the spin-wave instability arises at $t/I = \alpha(1-c)$.

It is necessary to note that the diagram technique used makes it possible to obtain the high-temperature expansion in the paramagnetic phase. For an fcc lattice and for $I = \infty$ the results of Plischke[14] are obtained. However, his extrapolation of the results into the region $T \ll t$ is in no way justified.

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APPENDIX A

The Hubbard operators X_r^{pq} can be divided into two classes: operators of the Fermi type (f-operators) and operators of the Bose type (b-operators). All the f-operators are nondiagonal while the b-operators are divided into diagonal and nondiagonal operators.

The basis of the derivation of the diagram technique is the rule for bringing nondiagonal operators outside the T-product (cf.[3-6]):

$$\langle T(X_1(\tau_1)\dots X_m(\tau_m) X_\alpha(\tau) X_{m+1}(\tau_{m+1})\dots X_n(\tau_n))\rangle_0 = \sum_{k=1}^{n} (-1)^{p_k} G_\alpha(\tau-\tau_k) \times \langle T(X_1(\tau_1)\dots X_{k-1}(\tau_{k-1})[X_\alpha X_k]_{\pm}|_{\tau_k} X_{k+1}(\tau_{k+1})\dots X_n(\tau_n))\rangle_0. \tag{A.1}$$

If X_α is an operator of the b-type, then

$$G_\alpha(\tau) = \exp[-(\lambda\alpha)\tau] \begin{cases} 1+N(\lambda\alpha), & \tau>0 \\ N(\lambda\alpha), & \tau<0 \end{cases}.$$

The notation is taken from[3]. Inside the average is a commutator; $p_k = 0$. But if X_α is an operator of the f-type, then

$$G_\alpha(\tau) = \exp[-(\lambda\alpha)\tau] \begin{cases} 1-n(\lambda\alpha), & \tau>0 \\ -n(\lambda\alpha), & \tau<0 \end{cases};$$

$n(x)$ is the Fermi distribution and $\lambda\cdot\alpha(p,q) = \varepsilon_q - \varepsilon_p$. Inside the average we have the anticommutator if X_k is an f-type operator, or the commutator if X_k is a b-type operator. The signature p_k is the number of interchanges of f-operators required to get from the original sequence to the sequence in which the operator X_α stands immediately to the left of the operator X_k:

$$X_1 X_2 \dots X_{k-1} X_\alpha X_k X_{k+1} \dots X_n.$$

In[3] it was shown that for Bose operators a conservation law for the resultant root vector is fulfilled at each vertex; this law follows from the well-known commutation relation[15]

$$[X_\alpha, X_\beta] = N_{\alpha,\beta}^{(-)} X_{\alpha+\beta} \quad (N_{\alpha,\beta}^{(-)} = 0, \pm 1). \tag{A.2}$$

We can obtain an analogous relation for the anticommutator if we use the second Jacobi identity

$$[h_i\{X_\alpha, X_\beta\}] = \{X_\alpha[h_i X_\beta]\} - \{X_\beta[h_i X_\alpha]\}. \tag{A.3}$$

We have

$$\{X_\alpha, X_\beta\} = N_{\alpha,\beta}^{(+)} X_{\alpha+\beta} \quad (N_{\alpha,\beta}^{(+)} = 0 \text{ или } 1). \tag{A.2'}$$

Hence it follows that the diagram technique containing f-operators does not differ in its external form from the technique for b-operators.[3] A difference arises because of the coefficients $N_{\alpha,\beta}^{(\pm)}(-1)^{p_k}$, and also from the coefficient $f_k(\alpha)$, which originates from the anticommutator of two conjugate f-operators:

$$\{X_\alpha, X_{-\alpha}\} = f(\alpha) + \sum_k f_k(\alpha) h_k. \tag{A.4}$$

In practice, in calculating any given diagram, in place of the general relations of the type (A.2) and (A.4) it is convenient to use Hubbard's form of the commutation relations:

$$[X_r^{pq}, X_{r'}^{nm}]_{\pm} = \delta_{rr'}[\delta_{qn} X_r^{pm} \pm \delta_{mp} X_r^{nq}], \tag{A.5}$$

since in this case the root vectors, the coefficients $N_{\alpha,\beta}^{(\pm)}$, $f(\alpha)$ and $f_k(\alpha)$ are determined automatically.

APPENDIX B

All the diagonal operators in the four-level model (1) can be expanded in the following set of three operators:

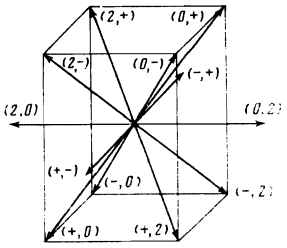

FIG. 3. Root system of the group $SU(4)$.

$$h_1=\frac{1}{\sqrt{2}}\begin{pmatrix}0&&&\\&1&&\\&&-1&\\&&&0\end{pmatrix},\quad h_2=\frac{1}{\sqrt{2}}\begin{pmatrix}1&&&\\&0&&\\&&0&\\&&&-1\end{pmatrix},$$
$$h_3=\frac{1}{2}\begin{pmatrix}1&&&\\&-1&&\\&&-1&\\&&&1\end{pmatrix}. \tag{B.1}$$

The components of the root vectors are determined from the well-known relation (cf., e.g., [15])

$$[h_k, X_\alpha]=\alpha_k X_\alpha, \tag{B.2}$$

from which we obtain all twelve root vectors of the group $SU(4)$ (cf. (3) and Fig. 3). To within a constant, the single-particle Hamiltonian (1) can be written in the form of a linear combination of the operators (B.1):

$$H_1=-\sum_{r,k}\lambda_k h_{kr}. \tag{B.3}$$

The components of the vector λ are given in (6). In the interaction Hamiltonian (2) only nondiagonal operators appear. For this reason, in the determination of the Green functions of such operators diagonal operators appear only as a result of interchanging two mutually conjugate operators. In the diagrams, a stopping-point of a solid line corresponds to this situation (see Figs. 4a and 4b).

A crossed wavy line corresponds to a terminal diagram and in place of the stopping point there arises

$$\begin{aligned}&\sum_k \alpha_k h_k - \text{ for } b\text{-operators}\\ &f(\alpha)+\sum_k f_k(\alpha)h_k - \text{ for } f\text{-operators}\end{aligned} \tag{B.4}$$

The result of independent averaging of these sums is depicted by a small circle (see Figs. 4c and 4d), to which correspond the factor

$$b(\alpha)=\sum_k \alpha_k\langle h_k\rangle_0=n_p-n_q$$

for b-operators, and the factor

$$F(\alpha)=f(\alpha)+\sum_k f_k(\alpha)\langle h_k\rangle_0=n_p+n_q$$

for f-operators. The averaging of several diagonal

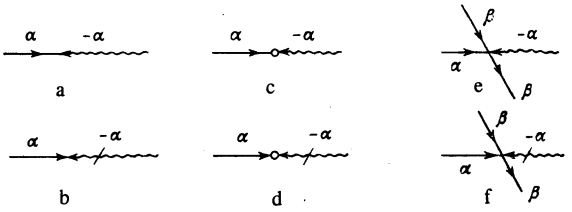

FIG. 4. Averaging of vertices containing diagonal operators ($T=0$).

operators reduces, after subtraction of all possible disconnected diagrams, to the calculation of semi-invariants, which are proportional to derivatives of the partition function.[6,3] In the limit of low temperatures, these quantities are exponentially small, because the averaging is performed over the ground state of the system and the semi-invariants are proportional to the fluctuations of the diagonal operators. There is also a third possibility, when, in the process of taking any nondiagonal operator outside the average, one commutes it with the sum (B.4). It is clear that in this case we have vertices of the type in Figs. 4e and 4f, after which a nondiagonal operator remains in place of the diagonal one.

Thus, at $T=0$, as a result of averaging the diagonal operators vertices of the type in Figs. 4c–f remain. At finite temperatures, we must add to these the result of averaging the different diagrams containing several stopping points pertaining to the same cell.

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