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The Mott transition in the many-dimensional Hubbard model

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The phase transition problem is solved in the approximation of a large number of nearest neighbors. A phenomenological theory is constructed to find the density of states and the value of the dielectric gap in the neighborhood of the critical point. Concrete calculations are made for the BCC and simple cubic lattices. A detailed comparison with the results of Hubbard's work [Proc. Roy. Soc. A281, 401 (1964)] shows qualitative but not quantitative agreement. The problem of finding the density of states in a metallic phase far from the transition point is discussed.

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INTRODUCTION

We shall study the Hubbard model under the conditions that the number of electrons is equal to the number of sites and the density of states is an even function of the energy. Simple examples that will be considered are the d-dimensional BCC and simple cubic lattices, and also a hypothetical model with the density of states given by Eq. (7), which is the same in zeroth approximation as that used by Hubbard.[1] In all of these cases at $T=0$ the ground state is nearly antiferrodielectric, for any value of the ratio of the energy t for transition of an electron to an adjacent cell to the intraatomic exchange energy I. In papers by Langer, Plischke, and Mattis[2] and by the present writer[3] it has been shown by extrapolation that at the Mott transition point the value of the Neél temperature T_N is at least an order of magnitude smaller than the exchange energy I. Using this as an assumption, we shall consider the metal-dielectric transition (M transition) in a paraphase, regarding the termperature as small compared with I but large compared with T_N.

For this temperature range an attempt has been made to construct a phenomenological theory of the M transition appropriately analogous to the theory of gapless superconductivity.[4] A rigorous calculation can be made only in a space of a large number of dimensions. It will be shown that this scheme checks qualitatively with almost all of the results of the Hubbard theory[1] that are correct above the Neel temperature. It turns out that for the density of states (7) the critical value of the ratio t/I is identical with the value found in Ref. 1, but otherwise the results are quantitatively different.

1. THE APPROXIMATION OF LARGE NUMBER OF NEAREST NEIGHBORS

In a nonmagnetic phase, when $T_N \ll T \ll I$, we can take the Hubbard solution[1] as a zeroth approximation. The corresponding G function will be written in the notation of the previous papers by the writer[3,5]:

$$G^{-1}_{\sigma,\omega}(\mathbf{k}) = \begin{matrix} \\ (0,\sigma) \\ (-\sigma,2) \end{matrix} \begin{matrix} \begin{matrix} (0,\sigma) & \qquad (-\sigma,2) \end{matrix} \\ \begin{pmatrix} -i\omega_n - \varepsilon_0 - {}^1/_2 t(\mathbf{k}), & -{}^1/_2 \sigma t(\mathbf{k}) \\ -{}^1/_2 \sigma t(\mathbf{k}), & -i\omega_n + \varepsilon_0 - {}^1/_2 t(\mathbf{k}) \end{pmatrix} \end{matrix}, \qquad (1)$$

$$t(\mathbf{k}) = t \sum_{(r)}{}' e^{i\mathbf{k}\mathbf{r}}, \quad \varepsilon_0 = {}^1/_2 I, \quad \omega_n = (2n+1)\pi T.$$

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The occupation numbers for opposite spin values ($\sigma = \pm 1$) are each equal to $\frac{1}{2}$. The spectrum of excited states calculated by means of Eq. (1) has a gap (even for $t \sim I$)

$$\varepsilon_p = -{}^1/_2 t(\mathbf{p}) \pm (\varepsilon_0^2 + {}^1/_4 t^2(\mathbf{p}))^{1/2}.$$

If we assume that the number n of nearest neighbors is large ($n \gg 1$), $n^{-1/2}$ is a small parameter of the self-consistent field for the problem. As we shall see later, the M transition in which we are interested occurs at $t \sim I/n^{1/2} \ll I$, where we can use the atomic representation, for which diagram methods for calculating Green's functions have been developed.[3,5] The first approximation in the self-consistent field parameter consists of the set of diagrams containing one loop.

Figure 1 shows the one-loop corrections to the self-energy part. We shall concentrate our attention on diagrams of type a, since diagram d is equal to twice diagram a and the others are equal to zero if we assume that all sums $D_q = \Sigma_p t^q(\mathbf{p})$ with odd q vanish. (The proof is given in Appendix B).

Using the notations adopted in Ref. 3, we write the proper-energy part of diagram a in the following form:

$$\Sigma_{\alpha,\beta,\omega}(\mathbf{k}) = \sum_{\alpha',\beta',\mathbf{p}} t_{-\alpha,\alpha'}(\mathbf{p}) G_{\alpha'\beta'\omega}(\mathbf{p}) t_{-\beta',\beta}(\mathbf{k}) \Gamma_{2\alpha\beta'}. \tag{2}$$

The indices α and β number the transitions. The matrix $t_{-\alpha,\beta}(\mathbf{p})$ is the product of $t(\mathbf{p})$ times the matrix

$$\begin{pmatrix} 1, & \sigma \\ \sigma, & 1 \end{pmatrix}$$

for the spin values $\sigma = \pm 1$.

In the paramagnetic region the lowest energy level contains one electron with either spin up or else with spin down, with equal probabilities. The empty and two-particle levels are separated from the one-particle levels by the energy $\varepsilon_0 = I/2 \gg T$. For this reason the occupation numbers of the upper levels are exponentially small, and the occupation numbers of the lower level are close to $\frac{1}{2}$. Using this fact, we can decidedly simplify the calculation of mean values of products of diagonal operators by taking into account only the low one-particle states. To this accuracy the matrix $\Gamma_{2\alpha,\beta}$ for equal spins is of the form

$$\frac{1}{4}\begin{pmatrix} 1 & -1 \\ -1, & 1 \end{pmatrix}.$$

The result for opposite spins is the same but opposite in sign (see Appendix A).

Direct calculation of the sum over indices in Eq. (2) gives the following result:

$$\Sigma_{\sigma,\omega}(\mathbf{k}) = \frac{t(\mathbf{k})}{4} \sum_{\mathbf{p}} G_\omega^{(\sigma)}(\mathbf{p}) t(\mathbf{p}) \begin{pmatrix} 1, & \sigma \\ -\sigma & 1 \end{pmatrix}, \tag{3}$$

$$G_\omega^{(\sigma)}(\mathbf{p}) = -2\varepsilon_0 / [\varepsilon_0^2 + \omega_n^2 - i\omega_n t(\mathbf{p})]. \tag{4}$$

To construct a phenomenological theory it is necessary only to assume that the function G that appears in Eqs. (2) and (3) is to be replaced with the exact propagator,

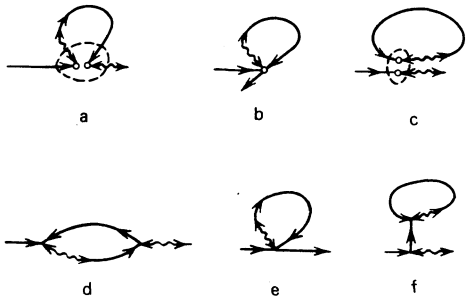

FIG. 1. One-loop self-energy parts

and to write instead of the matrix Γ_2 in Eq. (2) of the coefficient $\frac{1}{4}$ in Eq. (3) an exact vertex part, which we shall take to be constant. Then instead of Eq. (3) we get an equation for determining the self-energy part

$$\lambda_\omega = \frac{\gamma}{4} \sum_{\mathbf{p}} [G_\omega^{(0,\sigma)(0,\sigma)}(\mathbf{p}) - \sigma G_\omega^{(0,\sigma)(-\sigma,2)}(\mathbf{p}) + \sigma G_\omega^{(-\sigma,2)(0,\sigma)}(\mathbf{p}) - G_\omega^{(-\sigma,2)(-\sigma,2)}(\mathbf{p})] t(\mathbf{p}); \tag{5}$$

$$G^{-1} = \begin{pmatrix} -i\omega - \varepsilon_0 - {}^1/_2 t(\mathbf{p}) - \lambda_\omega t(\mathbf{p}), & -{}^1/_2 \sigma t(\mathbf{p}) - \sigma t(\mathbf{p}) \lambda_\omega \\ -{}^1/_2 \sigma t(\mathbf{p}) + \sigma t(\mathbf{p}) \lambda_\omega, & -i\omega + \varepsilon_0 - {}^1/_2 t(\mathbf{p}) + \lambda_\omega t(\mathbf{p}) \end{pmatrix},$$

where γ is the vertex part, which is 3 when we take into account only diagrams a and d in Fig. 1.

In analogy with the transformation used by Abrikosov and Gor'kov[4] we introduce instead of λ_ω an unknown function $\tilde{\omega}$ which depends on the frequency: $i\tilde{\omega} = i\omega - 2\varepsilon_0 \lambda_\omega$. Then instead of Eq. (5) we get an equation for $\tilde{\omega}$:

$$i\tilde{\omega} = i\omega_n + \gamma \sum_{\mathbf{p}} \frac{\varepsilon_0^2 t(\mathbf{p})}{\varepsilon_0^2 + \omega_n^2 - i\tilde{\omega} t(\mathbf{p})}. \tag{6}$$

It is possible to justify a procedure for deriving the closed equation (6) only in a space of a large number of dimensions; this is discussed in Sec. 3. The complete solution of the system of Eqs. (5) and (6) for the special case considered in Hubbard's original paper,[4] for which

$$\nu(x) = \sum_{\mathbf{p}} \delta\left(x - \frac{t(\mathbf{p})}{t}\right) = \frac{2}{\pi}(1-x^2)^{1/2}\theta(1-x^2) \tag{7}$$

is presented in Appendix C.

In the next section we shall obtain the solution of Eq. (6) in the limit of low frequencies; this is precisely where the metal–dielectric transition occurs.

2. PHENOMENOLOGICAL THEORY OF THE M TRANSITION

To find the density of states it is necessary to know the retarded Green's function, which we shall obtain from Eqs. (4)–(6) by analytical continuation into the upper half-plane, $i\omega \to \varepsilon + i\delta$, which corresponds to the replacement $i\tilde{\omega} \to \Omega$.

We assume that all of the quantities D_{2k+1} vanish:

$$D_{2k+1} = \sum_{\mathbf{p}} (t(\mathbf{p}))^{2k+1} = 0.$$

Then the density of states $\nu(x)$ is an even function and Eq. (6) always has a solution that goes to zero as $i\omega_n = \varepsilon \to 0$. The condition that the gap vanish corresponds

to the appearance of a second solution. It is natural to assume that near this point the second solution is small, and therefore after the analtyic continuation we can expand Eq. (6) in a power series in Ω. The second term of the expansion is zero, so that up to terms of third order we find

$$\Omega=\varepsilon+\frac{\varepsilon_0^2\gamma\Omega D_2}{(\varepsilon_0^2-\varepsilon^2)^2}+\frac{\varepsilon_0^2\gamma\Omega^3 D_4}{(\varepsilon_0^2-\varepsilon^2)^4}. \tag{8}$$

In the low-frequency region we get the following equation

$$\Omega^3+p\Omega+q=0;$$
$$p=\frac{\gamma D_2-\varepsilon_0^2}{\gamma D_4}\varepsilon_0^4, \quad q=\frac{\varepsilon\varepsilon_0^6}{\gamma D_4}. \tag{9}$$

A complex solution of Eq. (9) arises for $4p^3=-27q^2$, from which we find the frequency at which a nonvanishing density of states appears in the system, given by

$$\varepsilon_c=^2/_3(\varepsilon_0^2-\gamma D_2)^{1/2}/(3\gamma D_4)^{1/4}. \tag{10}$$

For $p>0$ or $\varepsilon_0^2<\gamma D_2$ there is no gap in the spectrum; this corresponds to the metallic state. In the dielectric phase $p<0$ the spectrum of excitations has a gap $E_g=2\varepsilon_c$. The condition for the transition into the metallic state is of the following form:

$$(t/I)_c=1/2(\gamma n)^{1/4} \quad \text{since} \quad \sum_{\mathbf{p}} t^2(\mathbf{p})=nt^2. \tag{11}$$

Accordingly, for a large number n of nearest neighbors the M transition occurs with $t\ll I$. As has already been remarked, according to perturbation theory $\gamma=3$, and it must be supposed that in the general case this quantity remains finite and positive.

The Green's function differs from the G function by the presence of end factors, which in general depend on the frequency

$$D_{\alpha,\beta}=\sum_{\tau} G_{\alpha\tau}K_{\tau\beta}.$$

In the self-consistent-field approximation it is sufficient to include only the diagrams shown in Fig. 2, a, b, and c. The other diagrams d, e, and f give zero, either because of the condition $D_{2k+1}=0$, or after being summed over the frequencies.

Calculations quite similar to those done in finding the self-energy part lead to the following expression, apart from dependence on σ:

$$\sum_{\alpha\beta} D_{\alpha\beta}={}^1/_2\sum_{\alpha\beta} G_{\alpha\beta}(\mathbf{k})+{}^1/_4\gamma G_\omega(\mathbf{k})\sum_{\mathbf{p}} t(\mathbf{p})G_\omega(\mathbf{p}). \tag{12}$$

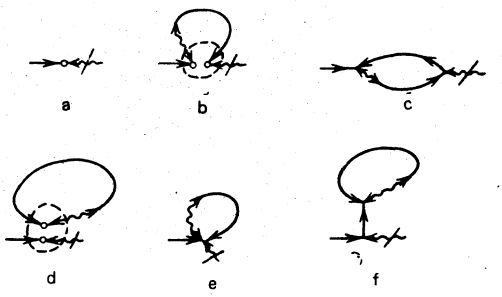

FIG. 2. End diagrams in the one-loop approximation

The expression for $G_\omega(\mathbf{k})$ in terms of $\tilde{\omega}$ is as follows:

$$G_\omega(\mathbf{p})=-2\varepsilon_0/[\varepsilon_0^2+\omega_n^2-i\tilde{\omega}t(\mathbf{p})], \tag{13}$$
$$\sum_{\alpha\beta} G_{\alpha\beta}(\mathbf{p})=2i\omega_n/[\varepsilon_0^2+\omega_n^2-i\tilde{\omega}t(\mathbf{p})]. \tag{14}$$

By means of Eq. (6) we calculate the sum over momenta that appears in Eq. (12). If we now sum the D function over the momentum and use Eq. (6) once more, the retarded Green's function summed over spins can be expressed in terms of Ω:

$$\sum_{\mathbf{k}\alpha\beta\sigma} D_{\alpha\beta}^{(\sigma)}(\mathbf{k})=\frac{2\Omega}{\varepsilon_0^2-\varepsilon^2}\left[1+\frac{\Omega(\Omega-\varepsilon)}{\gamma\varepsilon_0^2}\right]. \tag{15}$$

Apart from a factor $1/\pi$, the density of states is the imaginary part of the expression (15). For example, let us calculate the density of states for $\varepsilon=0$ near the M transition point. Using Eq. (9) at $\varepsilon=0$, we find $\Omega=ip^{1/2}$, so that in the metallic phase

$$I\rho(0)=\frac{4}{\pi}\operatorname{Im}\frac{\Omega}{\varepsilon_0}\left(1+\frac{\Omega^2}{\gamma\varepsilon_0^2}\right)\approx\frac{4\varepsilon_0}{\pi}\left(\frac{\gamma D_2-\varepsilon_0^2}{\gamma D_4}\right)^{1/4}. \tag{16}$$

Let us determine the asymptotic form of the density of states in the limiting case $\varepsilon\to 0$, $t\gg I/n^{1/2}$. For this purpose we introduce the one-particle density of states

$$\nu(x)=\sum_{\mathbf{p}}\delta(x-t(\mathbf{p})/t)$$

and rewrite Eq. (6):

$$i\tilde{\omega}=i\omega_n+\gamma t\varepsilon_0^2\int\frac{x\nu(x)\,dx}{\varepsilon_0^2+\omega_n^2-i\tilde{\omega}xt}. \tag{17}$$

If we suppose that the function $\nu(x)$ is even and that the maximum value of x is approximately n, then the right member of Eq. (17) can be expanded in powers of $\varepsilon_0/|x|t$:

$$i\tilde{\omega}\approx i\omega+\frac{i\gamma\varepsilon_0^2}{\tilde{\omega}}\left[1-\frac{\pi(\varepsilon_0^2+\omega^2)\varepsilon_0\nu(0)}{|t\tilde{\omega}|}\right]. \tag{18}$$

In Eq. (18) let us suppose that $|\omega|\ll\varepsilon_0$; then in zeroth approximation $\tilde{\omega}^2\sim\gamma\varepsilon_0^2$, and in the next approximation

$$\tilde{\omega}^2\approx\gamma\varepsilon_0^2\left\{1-\frac{\pi\varepsilon_0}{\gamma^{1/2}}\sum_{\mathbf{p}}\delta[t(\mathbf{p})]\right\}.$$

As the result of an analytic continuation we get at $\varepsilon=0$

$$\Omega\approx i\gamma^{1/2}\varepsilon_0\left\{1-\frac{\pi\varepsilon_0}{2\gamma^{1/2}}\sum_{\mathbf{p}}\delta[t(\mathbf{p})]\right\}.$$

After substituting this expansion in Eq. (15) we find for $t\gg I/n^{1/2}$

$$\rho(0)\approx 2\sum_{\mathbf{p}}\delta[t(\mathbf{p})]. \tag{19}$$

A comparison of Eqs. (19) and (16) shows that as the M transition point is approached from the high-pressure side (larger values of t/I) the density of states at the Fermi surface increases in proportion to I/t, since

$$\sum_{\mathbf{p}}\delta[t(\mathbf{p})]\sim 1/t.$$

Near the M transition point the density of states goes through a maximum, and then approaches zero according to a law $(t-t_c)^{1/2}$ [see Eq. (16)].

The sum that appears in Eq. (19) depends on the type

of crystal lattice. For example, for a simple cubic lattice

$$\rho(0)\sim\frac{1}{\pi t}\int_0^\infty J_0^d(x)\,dx; \tag{20}$$

J_0 is a Bessel function, and d is the dimensionality. If the sum $\nu(0)$ turns out to be infinite, then the expansion (18) must be carried out again. For example, for the bcc lattice the law of decrease of the density of states for $tn^{1/2}\gg I$ turns out to be slower than I/t:

$$\rho(0)\sim\frac{1}{\pi t}\left[\frac{\ln(tn/I)}{2\pi}\right]^{d-1},\qquad n=2^d. \tag{21}$$

In the dielectric phase $\rho(0)=0$, but for $I\gg\varepsilon\gtrsim\varepsilon_c$ the density of states can be calculated by means of Eqs. (9) and (15):

$$\Omega\approx\left(\frac{q}{2}\right)^{1/3}+\frac{i}{3^{1/2}}\left(p+3\left(\frac{q}{2}\right)^{2/3}\right)^{1/2},\quad \varepsilon-\varepsilon_c\ll\varepsilon_c,$$
$$I\rho(\varepsilon)\approx 2^{3/2}\varepsilon_0(\varepsilon-\varepsilon_c)^{1/2}/3\pi(2\gamma D_4)^{1/2}\varepsilon_c^{1/6}. \tag{22}$$

The quantity ε_c is equal to half the dielectric gap and is given by Eq. (10).

Equations (10), (16), and (22) agree qualitatively with the corresponding results of Hubbard.[1] It must be pointed out, however, that instead of Eq. (9) Ref. 1 gives a different and more complicated result, from which one can derive the asymptotic expansion (19), if the density of states is normalized in precisely the same way. A more detailed comparison with Ref. 1 is given in Appendix C.

3. THE CONDITIONS FOR APPLICABILITY OF THIS METHOD

The simplest diagrams that have been neglected contain three Green's functions; see Fig. 3. In the limit $T\ll\varepsilon_0$ diagram a gives a much larger contribution than diagram b, since it contains a summation over the frequency, which gives an additional factor ε_0/T. For simplicity we confine ourselves to the case of small frequencies $|\omega_n|\ll\varepsilon_0$ and find the correction to the spectrum of excitations

$$t(\mathbf{p})\sum_{\mathbf{p}',\mathbf{p}'',\omega_n} t(\mathbf{p}')t(\mathbf{p}'')t(\mathbf{p}-\mathbf{p}'+\mathbf{p}'')\frac{1}{2\varepsilon_0(\varepsilon_0^2+\omega_n^2)}.$$

In calculating the sum over momenta we use the identity

$$\sum_{\mathbf{p}} t(\mathbf{p})t(\mathbf{p}+\mathbf{q})=tt(\mathbf{q}),$$

and we replace the sum over frequencies with an integral. We thus get a correction $[tt(\mathbf{p})]^2/2T\varepsilon_0^2$, which must be small compared with $t(\mathbf{p})$. The maximum value of the latter is $\max t(\mathbf{p})=nt$, so that we finally have the following restriction on the temperature:

$$t^2n/\varepsilon_0^2\ll T\ll\varepsilon_0. \tag{23}$$

Let us now consider the temperature shift of the M

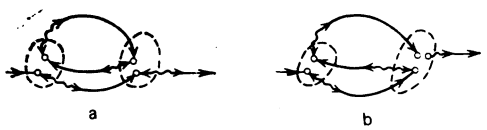

FIG. 3. Intersecting diagrams

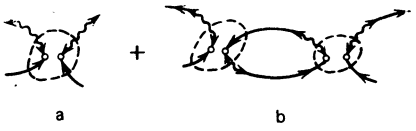

FIG. 4. Correlation corrections

transition line, which arises near the quadrupole point. As has already been pointed out, for $T\ll\varepsilon_0$ the weakly connected diagrams (those which have unconnected parts before the averaging of diagonal operators) contain a factor $(\varepsilon_0/T)^m$, where m is the number of weakly connected parts, which are joined to each other by dashed-line ovals. Starting from this, to find the temperature corrections to the diagram a of Fig. 3 we must perform a summation over the sequence of loops shown in Fig. 4. The result of this summation must be inserted in the diagram a of Fig. 3 instead of the single loop

$$\Pi(\mathbf{k})\to\Pi(\mathbf{k})/(1+\Pi(\mathbf{k})),$$
$$\Pi(\mathbf{k})=1/4\sum_{\mathbf{p}\omega} t(\mathbf{p})t(\mathbf{p}+\mathbf{k})G_\omega(\mathbf{p})G_\omega(\mathbf{p}+\mathbf{k}),$$

where the function $G_\omega(\mathbf{p})$ is given by Eq. (13).

To obtain the equation for the M transition line we have only to solve a linear equation for the function $\tilde\omega$ on which $G_\omega(\mathbf{p})$ depends. Let us therefore expand $\Pi(k)$ in powers of $\tilde\omega$:

$$\Pi(\mathbf{k})\sim\sum_{\mathbf{p},\omega} t(\mathbf{p})t(\mathbf{p}+\mathbf{k})\left(\frac{\varepsilon_0}{\varepsilon_0^2+\omega_n^2}\right)^2+2i\sum_{\mathbf{p}\omega}\frac{\tilde\omega_{\mathbf{p}}t^2(\mathbf{p})t(\mathbf{p}+\mathbf{k})}{(\varepsilon_0^2+\omega_n^2)^3}.$$

As will be seen later, the equation for $\tilde\omega_{\mathbf{p}}$ is very complicated and has no solution independent of the momentum. Therefore to find the eigenvalues we at once resort to a variation method, taking $\tilde\omega_{\mathbf{p}}$ to be a constant. We have $\Pi(\mathbf{k})\sim tt(\mathbf{k})/2\varepsilon_0T$, since

$$\sum_{\mathbf{p}} t^2(\mathbf{p})t(\mathbf{p}+\mathbf{q})=0,$$

and the homogeneous equation for $\tilde\omega_{\mathbf{p}}$ takes the following form:

$$\tilde\omega_{\mathbf{p}}=3\sum_{\mathbf{p}'}\tilde\omega_{\mathbf{p}'}\frac{t^2(\mathbf{p}')}{\varepsilon_0^2}-3\sum_{\mathbf{p}'}\frac{\Pi(\mathbf{p}-\mathbf{p}')\tilde\omega_{\mathbf{p}'}t^2(\mathbf{p}')}{\varepsilon_0^2[1+\Pi(\mathbf{p}-\mathbf{p}')]}. \tag{24}$$

The variational procedure for finding the eigenvalues of Eq. (34) reduces to multiplying the equation by $\tilde\omega_{\mathbf{p}}$ and summing over the momentum $\mathbf{p}$. Since in zeroth approximation $\omega_{\mathbf{p}}$ does not depend on the momentum, to good approximation it can also be treated as a constant in the solution of Eq. (24). By simple manipulations we get

$$\varepsilon_0^2=3\sum_{\mathbf{p}} t^2(\mathbf{p})\left[1-\sum_{\mathbf{p}'}\frac{\Pi(\mathbf{p}')}{1+\Pi(\mathbf{p}')}\right].$$

The condition for the denominator to vanish corresponds to the appearance of antiferromagnetic ordering

$$\min\Pi(\mathbf{k})=-1=-t^2n/2\varepsilon_0T_N. \tag{25}$$

For $T\gg T_N$ Eq. (24) can be expanded in powers of Π. The result is

$$\varepsilon_0^2=3\sum_{\mathbf{p}} t^2(\mathbf{p})\left[1+\left(\frac{t}{2T}\right)^2\sum_{\mathbf{p}'}\frac{t^2(\mathbf{p}')}{\varepsilon_0^2}\right]. \tag{26}$$

Since $\Sigma_p t^2(\mathbf{p}) = nt^2$, the temperature dependent correction is small if the condition (23) holds, but here the correction is of second order in $n^{-1/2}$.

It is interesting to note that the formula (26) agrees qualitatively with experiment, since the critical value $(t/I)_c$ increases with rising temperature. It is clear, however, that the main temperature dependence comes from the interaction with phonons, which requires separate consideration.

4. CONCLUSION

Accordingly, in the approximation of large number of nearest neighbors the M transition is governed by a function $\Omega(\varepsilon)$ which satisfies the equation (9). The transition from the metallic phase to the dielectric phase corresponds to a change of sign of the coefficient of Ω (as in the theory of phase transitions of the second kind). The free coefficient depends on the frequency and is proportional to the deviation from the Fermi level. In the neighborhood of the transition point the imaginary part of $\Omega(\varepsilon)$ determines the density of states.

If we assume that an expansion of Eq. (9) exists also with correlation effects included, we can generalize the theory of the M transition by expanding the coefficients p and q in fractional powers: $p \sim (t-t_c)^2$, $q \sim \varepsilon^{\mu}$. Then instead of the three-halves power law (10) we get $E_g \sim (t_c - t)^{3\nu/2\mu}$, and instead of Eq. (16) we have $\rho(0) \sim (t-t_c)^{\nu/2}$.

The asymptotic form (19) of the density of states does not depend on the interaction energy I and is the density of states at the Fermi surface for free electrons. This fact points to a possibility of using Eq. (6) and the result (15) for all values of ε_0 and for arbitrary lattices with $D_{2k+1}=0$, if the constant γ is properly chosen. The question of the influence of the M transition on magnetic and structural phase transitions deserves special investigation.

The writer is deeply grateful to E. F. Shender for helpful discussions.

APPENDIX A

In Fig. 2, a little circle represents the mean value of the anticommutator of two f-type adjoint operators $X^{(0,\sigma)}$ or $X^{(\sigma,2)}$. Since in our problem the energies of the empty and the two-particle states are equal, and are separated from that of the one-particle state by an a amount ε_0 independent of the spin, we can write

$$\begin{aligned}\langle\{X^{(0,\sigma)}X^{(\sigma,0)}\}\rangle &= \langle\{X^{(\sigma,2)}X^{(2,\sigma)}\}\rangle \\ &= {}^1/_2\langle(X^{(0,0)}+X^{(+,+)}+X^{(-,-)}+X^{(2,2)})\rangle = {}^1/_2.\end{aligned} \tag{A.1}$$

Two circles surrounded by an oval represent the mean square fluctuation of the product of the anticommutators:

$$\langle\{X_\alpha, X_{-\alpha}\}\{X_\beta, X_{-\beta}\}\rangle - \langle\{X_\alpha X_{-\alpha}\}\rangle\langle\{X_\beta X_{-\beta}\}\rangle. \tag{A.2}$$

Direct calculation shows that if α and β correspond to transitions with the same spin change the average of the product of the anticommutators is a unit matrix multiplied by $\frac{1}{2}$. If, on the other hand, α and β correspond to transitions with opposite spin changes, then the matrix elements depend on the temperature, but can differ only in their signs.

The matrix (A.2) is symmetric in the indices (α, β) and does not change when the sign of either of them is changed. For this reason we write out (A.2) only for four independent transitions:

$$\begin{array}{c} \\ (0,+) \\ (-,2) \\ (0,-) \\ (+,2) \end{array} \begin{array}{c} \begin{array}{cccc} (0,+) & (-,2) & (0,-) & (+,2) \end{array} \\ \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} & f & -f \\ -\frac{1}{4} & \frac{1}{4} & -f & f \\ f & -f & \frac{1}{4} & -\frac{1}{4} \\ -f & f & -\frac{1}{4} & \frac{1}{4} \end{pmatrix} \end{array}, \tag{A.3}$$

where $f = -\frac{1}{4}\tanh(\varepsilon_0/2T)$. In the limit with which we are concerned, $T_N \ll T \ll \varepsilon_0$, for which $f = -\frac{1}{4}$, the matrix element changes sign when there is a change of sign of the spin component in one of the two transitions (α or β).

APPENDIX B

The simplest diagram of the type of Fig. 1, a is as shown in Fig. 5. In analytic form the sum of all four of these cases can be expressed as the sum over frequencies of the functions

$$D_{\omega_n}^{(+,-)} = [n(\varepsilon_+) - n(\varepsilon_-)][-i\omega_n + \varepsilon_- - \varepsilon_+]^{-1}; \tag{B.1}$$

here $\omega_n = 2n\pi T$, and

$$\Sigma_{(0,+),\beta,\omega}(\mathbf{k}) = T\sum_{\omega',\mathbf{k}'} \frac{2e_0 t(\mathbf{k}') D^{+-}_{\omega-\omega'}}{\omega'^2 + e_0^2 - i\tilde{\omega}' t(\mathbf{k}')}. \tag{B.2}$$

In the paramagnetic phase $\varepsilon_+ - \varepsilon_-$, so that the D function in (B.1) is nonzero only for $\omega_n = 0$:

$$D_{\omega_n}{}^{+-} \sim \delta(\omega_n)/2T. \tag{B.3}$$

Substitution of (B.3) into Eq. (B.2) gives a correction which is twice the contribution from the diagram shown in Fig. 1, a. The same result can also be obtained for any other incoming and outgoing indices.

We shall show that the contributions from diagrams of the types of Fig. 1, b and e are equal to zero. If we fix the incoming and outgoing indices, we get three different cases [see Fig. 6, where for definiteness the final and initial indices correspond to the transition (0, +) (0, +)]. Since there is to be summation over the indices α', β', γ', we get six diagrams, two of which give zero because the commutators $[X^{(0,+)}\{X^{(0,+)}X^{(+,0)}\}]$ and $[X^{(-,2)}\{X^{(+,0)}X^{(0,+)}\}]$ are equal to zero. The commutators $[X^{(0,-)}, X^{(-,+)}]$ and $[X^{(2,+)}, X^{(0,2)}]$ differ in sign, but the coefficients of the operators $X_\gamma^{(-,0)}X_{\gamma'}^{(0,-)}$ and $X_\gamma^{(+,2)}X_{\gamma'}^{(2,+)}$

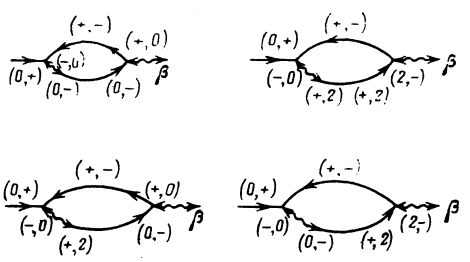

FIG. 5. Diagrams of the type represented by Fig. 1, d

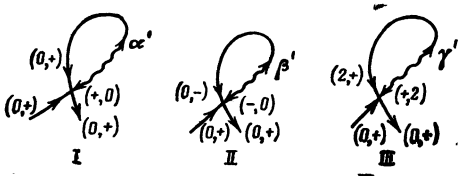

FIG. 6. Diagrams of the type represented by Fig. 1, e

in the Hamiltonian have opposite signs, so that finally we have the following:

$$\delta\Sigma_{\omega}^{(0,+;0,+)}(\mathbf{k})=T\sum_{\omega'\mathbf{k}'}t(\mathbf{k}')\{G_{\omega'}^{(+,2;0,-)}(\mathbf{k}')-G_{\omega'}^{(0,-;0,-)}(\mathbf{k}')-G_{\omega'}^{(2,+;2,+)}(\mathbf{k}')$$
$$+G_{\omega'}^{(-,0;2,+)}(\mathbf{k}')\}=T\sum_{\omega'\mathbf{k}'}t(\mathbf{k}')\{G_{\omega'}^{(+,2;0,-)}(\mathbf{k}')-G_{\omega'}^{(0,-;0,-)}(\mathbf{k}')$$
$$+G_{-\omega'}^{(+,2;+,2)}(\mathbf{k}')-G_{-\omega'}^{(0,-;+,2)}(\mathbf{k}')\}. \qquad (B.4)$$

The second equality can be obtained if we use the relation connecting f-type Green's functions with opposite root vectors:

$$G_{\omega}^{\alpha,\beta}(\mathbf{k})=-G_{-\omega}^{-\alpha,-\beta}(\mathbf{k}).$$

After making the change $\omega'\to-\omega'$ in the last two sums and substituting the G functions from Eqs. (5) and (7) we find

$$\delta\Sigma=T\sum_{\omega',\mathbf{k}'}\frac{2\varepsilon_0 t(\mathbf{k}')}{\varepsilon_0^2+\omega_n'^2-i\tilde{\omega}'t(\mathbf{k}')}. \qquad (B.5)$$

This sum is equal to zero, since $\tilde{\omega}$ is an odd function of the frequency and the sum over momenta of any odd power of $t(\mathbf{p})$ is zero by hypothesis.

It is not hard to show that finding the contribution from the diagrams of Fig. 1, c and d and Fig. 2, d, e, and f reduces to the calculation of the same sum (B.5), independently of the spin direction.

APPENDIX C

For comparison with the results of Hubbard[1] we shall make all of the calculations by means of the density of states (7). Direct calculation of the integral on the right side of Eq. (17) leads to an equation for determining the function $\eta=\tilde{\omega}/\omega$:

$$\eta=1+4a^2\eta/[1+\omega^2+((1+\omega^2)^2+{}^4/_3\omega^2\eta^2a^2)^{1/2}]^2,$$
$$a=t\sqrt{3}/I,\quad \omega=\omega_n/\varepsilon_0. \qquad (C.1)$$

Here and hereafter we set $\gamma=1$, which corresponds to perturbation theory and leads to the same condition for the M transition as in Ref. 1. This equation can be solved for ω^2:

$$\omega^2=-\varepsilon^2=\frac{[a\eta^{1/2}-(\eta-1)^{1/2}]}{(\eta-1)^{1/2}[1+{}^1/_3a\eta^{1/2}(\eta-1)^{1/2}]}. \qquad (C.2)$$

In the limit $\eta\to1$ we have $\omega^2\sim a/(\eta-1)^{1/2}$. In the dielectric phase, with $a<1$, the ratio η varies from unity to $(1-a^2)^{-1}$. In the limit $1-a\ll1$, we have $\eta\leq\eta_c\sim\frac{1}{2}(a-1)^{-1}\gg1$. In the metallic phase, with $a>1$, η varies from 1 to ∞. For large η,

$$\omega^2\sim3(a-1)/\eta^2+3/2\eta^3.$$

We find the equation for the gap as a function of the parameter a from the condition that a branch point of the function appears on the analytic continuation $i\omega\to\varepsilon+i\delta$.

After making this change in Eq. (C.2) we get the branch point from the condition $\partial\varepsilon/\partial\eta=0$. After an elementary differentiation we find

$$a=\frac{t\sqrt{3}}{I}=\frac{4\eta^3-7\eta^2+3\eta-3}{2(\eta-1)^{1/2}\eta^{3/2}(2\eta-1)}. \qquad (C.3)$$

Combining this with Eq. (C.2), we find the value of the gap E_g in parametric form ($E_g=I\varepsilon$):

$$E_g=\frac{I\sqrt{3}}{[\eta(\eta-1)(4\eta-3)]^{1/2}},\quad \frac{t}{I}=\frac{3^{1/2}|1-\varepsilon^{-2}|}{2(\eta-1)^{1/2}\eta^{3/2}(2\eta-1)}$$
$$\eta_{min}\approx1.57<\eta<\infty. \qquad (C.4)$$

The interval $1<\eta<\eta_{\min}$ corresponds to the upper boundary of the allowed zone.

The maximum value $E_g=I$ of the gap is reached for $t/I\to0$, when $\eta=\eta_{\min}$. If, on the other hand, $\eta\gg1$, we have $a\sim1-3/4\eta$, so that the gap goes to zero according to a three-halves power law:

$$E_g\sim{}^4/_3I(1-a)^{3/2}. \qquad (C.5)$$

The dependence of the dielectric gap on the parameter t/I is shown in Fig. 7 and agrees qualitatively with the corresponding curve in Ref. 1.

Let us calculate the density of states in the metallic phase on the Fermi surface ($\varepsilon=0$). For this purpose we set $\Omega=\varepsilon\eta$ in Eq. (C.1) and then go to the limit $\varepsilon\to0$. The result for $a>1$ is

$$\Omega=i\sqrt{3}(1-a^{-1})^{1/2}. \qquad (C.6)$$

By means of the general relation (15) we get

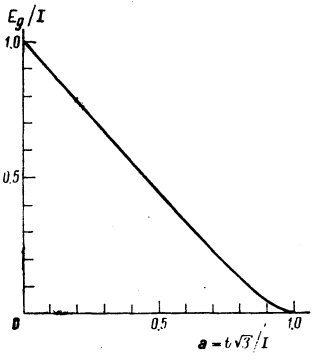

FIG. 7. Dependence of the dielectric constant on the parameter t/I

$$I\rho(0)=4\sqrt{3}(1-a^{-1})^{1/2}/\pi a. \tag{C.7}$$

In our case $\nu(0)=2/\pi$, so that in the limit $a\gg 1$ Eq. (C.7) goes over into (19). On the other hand, if $|a-1|\ll 1$, we get Eq. (C.7) from Eq. (16), where we must set $\gamma=3$, $D_2=t^2/4$, and $D_4=t^4/8$. At $a=\frac{3}{2}$ the quantity (C.6) has its maximum value $8/3\pi\approx 0.85$.

In Ref. 1 a different normalization of the density of states was used, not our present one with the factor $\frac{1}{4}$. If we do use our normalization, we can get from Ref. 1 the following relation instead of Eq. (C.7):

$$I\rho(0)=4\sqrt{3}(1-a^{-2})^{1/2}/\pi a. \tag{C.8}$$

This curve has its maximum at $a=2^{1/2}$, where its value is $2\cdot 3^{1/2}/\pi$. In the limit $A\gg 1$ Eqs. (C.7) and (C.8) give the same value. Near the M transition point the two values differ by a factor $2^{1/2}$.

For small frequencies we can get from (C.1) an expansion of the form of Eq. (9) with the coefficients

$$p=\frac{3}{2}\frac{\varepsilon_0^2(a^2-1)}{a^4},$$
$$q\sim\frac{3}{2}\varepsilon\varepsilon_0^2. \tag{C.9}$$

As was already pointed out, the equation derived in Hubbard's paper[1] is more complicated and cannot be reduced to Eq. (9).

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