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Isostructural instability and physical properties of the Hubbard long-range model

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The use of the large-number-of-nearest-neighbor approximation enables us to evaluate the polarization operator which defines the permittivity and the phonon spectrum renormalization. We evaluate the long-range correction to the free energy in the vicinity of the metal-dielectric transition (*M*- or Mott-transition). We show that in the region of strong correlations the system loses its mechanical stability so that the *M*-transition is accompanied by a first-order isostructural transition. Far from the transition and for sufficiently low temperatures the singularities of the thermodynamic quantities are weakened and remind us of those near a second-order transition.

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INTRODUCTION

In the theory of structural transformations which accompany the transition from the metallic to the dielectric state one uses in an essential way the assumption that the electron-electron interaction is small. For instance, in the theory of an exciton dielectric^{1,2} all calculations of the irreducible vertex part are restricted to the second order of perturbation theory. In Adler's theory³ one assumes that the cause of the structural transition is the strong electron-phonon interaction. The direct electron-electron interaction does not occur at all in this theory. In the Hubbard model⁴ the strong interaction of the electrons (u) is taken into account right from the beginning. One can therefore expect that a correct allowance for the electron-phonon and electron-electron interactions (in different cells) in that model will lead us appreciably closer to an understanding of the physical effects which take place in the oxides, sulfides, and nitrides of transition metals.

We assume that the energy for the transition to a neighboring cell (t) is smaller than the energy of the electron interaction in one and the same cell (u). One

can then easily show⁵ that in the Hubbard model there occurs a structural transition if the electron-phonon interaction energy reaches a value of the order of u . Such a situation may be an exception—as a rule the opposite situation occurs. The electron-phonon interaction is equivalent to an attraction which is of the same order of magnitude as (or less than) the Coulomb interaction between different cells which, in turn, is less than the energy u . Because of this we shall neglect in the present paper the ion motion, assuming that its role reduces to providing electro-neutrality on the whole. Taking the long-range part of the Coulomb interaction into account makes our model close to the well known Shubin-Vonsovskii model⁶ where the problem was posed of finding the ground state of a system with an arbitrary interaction between different cells.

We shall consider in the present paper the first-order isostructural transition which accompanies the Mott transition. We shall show that the rearrangement of the electron spectrum near the *M*-transition line strongly changes the long-range part of the Coulomb interaction. The permittivity increases in the dielectric phase when the pressure increases and becomes infinite at the Mott

transition point. The screening radius decreases in the metallic phase when the pressure is lowered far from the transition point, and afterwards starts to increase as one approaches the M -transition point due to the decrease in the density of electron states. We shall show that as one approaches the metal-dielectric transition point the hydrostatic stress modulus changes sign so that the system loses its mechanical stability. Hence one may conclude that close to the M -transition line there occurs a first-order phase transition. The proposed model enables us to find the corrections to the free energy in the disordered magnetic phase when the temperature is large compared to the Néel temperature, but less than the energy u .

1. CHOICE OF MODEL AND HAMILTONIAN

The problem of the metal-dielectric transition was solved by the present author⁷ by the self-consistent field method. The Hubbard Hamiltonian was written in the atomic representation so that we would use as the zeroth approximation the one-cell part of the Hamiltonian

$$H = H_1 + H_2 = \sum_{r,\sigma} u \hat{n}_{r\sigma} \hat{n}_{r-\sigma} - \sum_{r\sigma} \mu \hat{n}_{r\sigma} + \sum_{r,r',\sigma} t(r-r') a_{r\sigma}^+ a_{r'\sigma}, \quad (1)$$

where σ is the spin, index, $\hat{n}_{r\sigma} = a_{r\sigma}^+ a_{r\sigma}$, μ is the chemical potential which below is chosen in such a way that the number of electrons turns out to equal the number of sites ($\mu = u$). In Ref. 7 we reproduced Hubbard's main result⁴ consisting in that near the M -transition point the electron Green function has a branch point kind of singularity and there occurs a phase transition as the result of electron scattering by the spin fluctuations in the paramagnetic phase. The electron Green function, summed over all indices, has a rather simple form

$$D_\omega(p) = i\bar{\omega} / [u^2 + \omega_n^2 - i\bar{\omega}t(p)]. \quad (2)$$

The quantity $\bar{\omega}$ depends on the frequency ω_n and satisfies a self-consistency condition (vide infra). In the limit $u \rightarrow 0$ $\bar{\omega} = \omega_n$ so that we get from (2) the usual Green function. In the opposite limiting case $|t(p)| \ll u$ we get after an analytical continuation, $i\omega_n \rightarrow \varepsilon$, the D -function with a gap $E_g = 2u$.

It is shown in Ref. 7 that close to the M -transition point $\bar{\omega}(\omega)$ satisfies a Landau type equation. In the dielectric phase, as $\omega_n \rightarrow 0$, $\bar{\omega}$ also tends to zero. In the metallic phase the function $\bar{\omega}$ is finite for $\omega_n = 0$ and it tends to zero as the square root as function of the pressure, $\bar{\omega}(0) \propto (p - p_c)^{1/2}$. We shall show below that such a behavior of the Green function in the limit $T \rightarrow 0$ leads to a phase transition of order $3\frac{1}{2}$, which contradicts the general Peierls-Landau and Zel'dovich considerations.⁸ This is explained by the fact that in the Hubbard model the Coulomb interaction between neighboring cells is neglected and especially in the dielectric phase the long-range part of the Coulomb interaction is not screened and it is necessary to take it into account together with the tunnel part of the Hamiltonian (1). The operator of the direct Coulomb interaction has the form

$$V = \frac{1}{2} \sum_{r,r'} \hat{n}_r \hat{n}_{r'} \frac{e^2}{|r-r'|}, \quad \hat{n}_r = \sum_{\sigma} \hat{n}_{r\sigma}. \quad (3)$$

In the present paper we take the interaction (3) into ac-

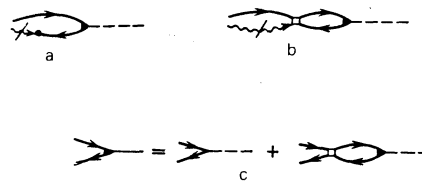


FIG. 1. a) Polarization operator without corrections to the end diagrams; b) corrections to the end diagrams; c) equation for the vertex part.

count in the Debye-Hückel approximation, using afterwards the ε -expansion. The polarization operator will be evaluated in the same approximation as the electron Green function (2) when we can neglect all intersecting diagrams, while the Coulomb interaction is taken into account through perturbation theory.

2. POLARIZATION OPERATOR

To find the permittivity and the phonon spectrum it is necessary to know the polarization loop summed over the spins (see Fig. 1). The Green function, evaluated in the large number of closest neighbors approximation, has the following form (for spin "up"):

$$G^{-1} = \begin{pmatrix} -i\omega - u - \frac{1}{2}t(p) - \lambda_u t(p) & -\frac{1}{2}t(p) - \lambda_u t(p) \\ -\frac{1}{2}t(p) + \lambda_u t(p) & -i\omega + u - \frac{1}{2}t(p) + \lambda_u t(p) \end{pmatrix};$$

u is half the Hubbard energy I , the quantity λ depends on the frequency and is determined by the following self-consistency condition:

$$i\bar{\omega} = i\omega - 2u\lambda_u = i\omega + \gamma \sum_p [t(p)/V_\omega(p)], \quad (4)$$

$$V_\omega(p) = u^2 + \omega_n^2 - i\bar{\omega}t(p), \quad t(p) = \sum_{r(r \neq 0)} \exp(ipr) t(r);$$

γ is a positive quantity of order unity, $\omega_n = (2n+1)\pi T$. The vertex part, irreducible with respect to two electron lines of opposite directions, can be calculated in the same approximation as the Green function when one can neglect the contribution of the intersecting diagrams. An estimate of the omitted diagrams is made in Ref. 7. Performing simple calculations and summing over spins one easily understands that the simplest taking into account of scattering by static spin fluctuations in the para-phase makes it possible to express the vertex part in terms of the same parameter γ which occurs in the definition of the Green function (2) (see Fig. 2a, b). Thus, for instance, for spin "up" the vertex part Γ_0 shown in Fig. 3 is independent of the index of the outgoing lines and changes sign when the index of the incoming lines are changed:

$$\Gamma_0 = \gamma(-1)^{\alpha+\beta} t(p_2) t(p_1). \quad (5)$$

In this case $\omega_1 = \omega_3$ and $\omega_2 = \omega_4$, as in the approximation

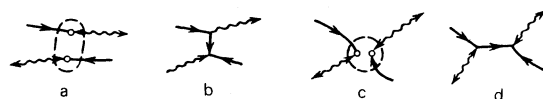


FIG. 2. Simplest irreducible vertex parts. The total contribution from diagrams a and b leads to the value $\gamma = 3$. The contribution from the diagrams c and d vanishes after summation over spins in the Coulomb vertex part.

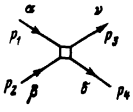


FIG. 3.

used we take into account scattering by static spin fluctuations.

The electrostatic vertex shown in Fig. 1 by a dashed line is determined by the commutator $[X_\alpha, \sum_{\sigma} \sigma a_{\sigma\alpha}^* a_{\sigma\beta}]$, the magnitude of which is independent of the spin:

$$[X^{\alpha\pm}, \hat{n}] = X^{\alpha\pm}, \quad [X^{\pm\alpha}, \hat{n}] = X^{\pm\alpha}.$$

Direct evaluation of the Π -operator leads to a sum of two terms corresponding to Figs. 1a and b:

$$\Pi_i(q) = \Pi_i^{(a)}(q) + \Pi_i^{(b)}(q),$$

where

$$\begin{aligned} \Pi_i^{(a)}(q) &= T \sum_{\omega, p} \frac{2u^2 + \omega_+^2 + \omega_-^2 - (\omega_+ + \omega_-)(\tilde{\omega}_+ + \tilde{\omega}_-)}{V_{\omega_+}(p_+) V_{\omega_-}(p_-)} \\ \Pi_i^{(b)}(q) &= \frac{\gamma u^2 T}{2} \sum_{\omega, p} \left\{ \frac{t(\omega_+ + \omega_-)(t(p_+) + t(p_-)) + 2t(p_+)t(p_-)}{V_{\omega_+}(p_+) V_{\omega_-}(p_-) [1 - \varphi_\omega(q, \varepsilon)]} \right. \\ &\quad \left. \times \sum_{p'} \frac{2u^2 + \omega_+^2 + \omega_-^2}{V_{\omega_+}(p_+') V_{\omega_-}(p_-')} \right\}; \end{aligned} \quad (6)$$

here

$$\begin{aligned} V_{\omega_\pm}(p_\pm) &= u^2 + \omega_\pm^2 - i\tilde{\omega}_\pm t(p_\pm), \\ \varphi_\omega(q, \varepsilon) &= \gamma \sum_p \frac{u^2 t(p_+) t(p_-)}{V_{\omega_+}(p_+) V_{\omega_-}(p_-)} \end{aligned}$$

$$\omega_\pm = \omega \pm \varepsilon/2, \quad p_\pm = p \pm q/2, \quad \tilde{\omega}_\pm = \tilde{\omega}(\omega_\pm), \quad \varepsilon = 2n\pi T.$$

The quantities $\tilde{\omega}_\pm$ satisfy condition (4) which we used to transform the second sum in (6). If $\varepsilon = 0$ and $q = 0$, the polarization operator can be expressed in terms of the complete Green function

$$\Pi_0(0) = -iT \sum_{\omega, p} \frac{\partial D_\omega}{\partial \omega}(p), \quad (7)$$

$$D_\omega(p) = \sum_{\alpha\beta} G^{\alpha\beta}(p) K_{\alpha\beta} = \frac{2i\tilde{\omega}}{u^2 + \omega_n^2 - i\tilde{\omega}t(p)}. \quad (8)$$

One can easily check Eq. (7) by differentiating the D -function (8) and using Eq. (4) and afterwards comparing it with what one obtains from (6):

$$\Pi_0(0) = 2T \sum_{\omega, p} V_{\omega_n}^{-2}(p) \left\{ -2\tilde{\omega}\tilde{\omega} + \frac{u^2 + \omega_n^2}{1 - \varphi_\omega} \left[1 + 2i\tilde{\omega}\gamma \sum_{p'} u^2 t(p') V_{\omega_n}^{-2}(p') \right] \right\}; \quad (9)$$

here $\varphi_\omega = \varphi_\omega(q=0, \varepsilon=0)$. Equation (7) enables us to express $\Pi_0(0)$ in terms of the density of states

$$\rho(\omega) = \text{Im} \frac{1}{\pi} \sum_p D_\omega^R(p). \quad (10)$$

$D_\omega^R(p)$ is the retarded Green function which we can obtain from (8) through an analytical continuation in the upper half-plane, $i\omega_n \rightarrow \omega + i\delta$.

We change in (7) from a sum to an integration:

$$\Pi_0(0) = \frac{1}{4\pi i} \int_\Gamma \sum_p \text{th} \frac{z}{2T} \frac{\partial D_z}{\partial z}(p) dz.$$

The contour Γ encloses all singularities of the function $\text{th}(z/2T)$. If we now expand it along the real axis, the

upper half gives the integral of the retarded and the lower half the integral of the advanced Green function $D_\omega^A(p)$. We have

$$\Pi_0(0) = \frac{1}{4\pi i} \sum_p \int_{-\infty}^{+\infty} \text{th} \frac{\omega}{2T} \left[\frac{\partial D_\omega^R(p)}{\partial \omega} - \frac{\partial D_\omega^A(p)}{\partial \omega} \right] d\omega.$$

On the real axis $D_\omega^A(p) = [D_\omega^R(p)]^*$ so that we get after integrating by parts

$$\Pi_0(0) = -\frac{\text{Im}}{4\pi T} \sum_p \int_{-\infty}^{+\infty} D_\omega^R(p) \text{ch}^{-2} \left(\frac{\omega}{2T} \right) d\omega = -\frac{1}{4T} \int_{-\infty}^{+\infty} \rho(\omega) \text{ch}^{-2} \left(\frac{\omega}{2T} \right) d\omega. \quad (11)$$

In the limit $T \rightarrow 0$, $\Pi_0(0) = -\rho(0)$ so that there is no screening in the dielectric phase, while in the metallic phase the screening radius has a minimum as a function of the ratio t/u (see Refs. 4, 7). Close to the M -transition point the screening radius becomes infinite like $(t - t_c)^{-1/4}$.

If we assume that for all p there exists a Q such that the condition $t(p+Q) = -t(p)$ is satisfied, the polarization operator at $\varepsilon = 0$ and $q = Q$ determines the condition of stability against an increase in the period of the structure:

$$\begin{aligned} \Pi_0(Q) &= 2T \sum_{\omega, p} \left\{ \frac{u^2 + \omega_n^2}{|V_{\omega_n}(p)|^2 [1 - f_\omega]} - \frac{2\tilde{\omega}\omega}{|V_\omega(p)|^2} \right\}, \\ f_\omega &= -\gamma \sum_p u^2 t^2(p) |V_\omega(p)|^{-2}. \end{aligned} \quad (12)$$

In the limit $t \ll u$, $T \rightarrow 0$ we have

$$\Pi_0(Q) = -4\gamma T D_2 \sum_{\omega_n} u^6 (u^2 + \omega_n^2)^{-4}, \quad D_2 = \sum_p t^2(p)/u^2. \quad (13)$$

If, however, $t \gg u$, we have

$$\Pi_0(Q) = -2T \sum_{\omega_n, p} [\omega_n^2 + t^2(p)]^{-1} = -\sum_p \text{th} \left(\frac{t(p)}{2T} \right) t^{-1}(p). \quad (14)$$

A comparison of (13) and (14) shows that the quantity $u\Pi_0(Q)$ has a negative minimum when $t \sim u$. In the limit $T \rightarrow 0$ the function (14) has a logarithmic singularity which determines the structural transition in an exciton dielectric. However, for any finite u in the limit $T \rightarrow 0$ the integral is cut off in frequency so that we get instead of (14) as $T \rightarrow 0$

$$\Pi_0(Q) \sim -\int_u \nu(\varepsilon) \frac{d\varepsilon}{\varepsilon}, \quad \nu(\varepsilon) = \sum_p \delta(\varepsilon - t(p)), \quad (15)$$

where $\nu(\varepsilon)$ is the single-particle density of states.

3. PERMITTIVITY AND SOUND

We showed above that in the dielectric phase as $T \rightarrow 0$

$$\lim_{q \rightarrow 0} \Pi_0(q) = 0.$$

The next term of the expansion in powers of q^2 determines the permittivity

$$\varepsilon = 1 - \frac{4\pi e^2}{a} \lim_{q \rightarrow 0} \frac{\partial \Pi_0(q)}{\partial q^2} \quad (16)$$

(a is the size of the crystal cell which we assume to be cubic).

In the "dielectric" limit $t \ll u$ one can show that the polarizability vanishes as $T \rightarrow 0$ with an accuracy up to

terms of second order in the parameter $(t/u)^2$. For this it is sufficient to expand the first sum in (6) in powers of q^2 as the second sum of (6) gives corrections of order $(t/u)^4$ and higher:

$$\Pi_{\perp}(q) \sim 2T \sum_{\mathbf{p}} \frac{u^2 - \omega_n^2}{(u^2 + \omega_n^2)^2} + \frac{T}{2} \sum_{\mathbf{p}} \frac{\omega_n^2 (u^2 - \omega_n^2)}{(u^2 + \omega_n^2)^4} \sum_{\mathbf{p}} \left(q \frac{\partial t}{\partial \mathbf{p}} \right)^2.$$

As $T \rightarrow 0$ both sums over ω_n vanish as the summed functions are total derivatives.

When the pressure increases the dielectric permittivity increases and becomes infinite near the M -transition point. The occurrence of this singularity is connected with the factor $1 - \varphi_{\omega}(\mathbf{q}, \varepsilon)$ which vanishes in that point where both its arguments vanish. We shall assume that all odd moments

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

vanish and we expand the "dangerous" denominator in powers of $\tilde{\omega}$ and ω :

$$1 - \varphi_{\omega} \approx 1 - \gamma D_2 + 2\gamma D_2 \omega_n^2 u^{-2} + 3\gamma \tilde{\omega}^2 D_2 u^{-2}. \quad (17)$$

This expansion determines the behavior of all polarization loops near the M -transition point when $|1 - \gamma D_2| \ll 1$. It is convenient to introduce instead of ω a new variable $\psi = \omega/\tilde{\omega}$. To express $\tilde{\omega}$ in terms of it we use an expansion of the self-consistency condition (4) in powers of ω , $\tilde{\omega}$ and $|1 - \gamma D_2|$:

$$1 - \varphi_{\omega} = \gamma D_2 [1 - 2\omega^2 u^{-2}] - \gamma D_2 \omega^2 \varphi_{\omega}^{-2} u^{-2}.$$

Hence we have near the M -transition point

$$\omega_n = \psi u \left(\frac{\psi - 1 - \gamma D_2}{\gamma D_2} \right)^{1/2}, \quad (18)$$

$$\frac{d\omega}{d\psi} = u \frac{3\psi + 2(\gamma D_2 - 1)}{2(\gamma D_2)^{3/2} (\psi - 1 + \gamma D_2)^{3/2}}.$$

In the metallic phase the parameter ψ changes from 0 to 1. In the dielectric phase ψ changes from $1 - \gamma D_2$ to 1. Substitution of (18) into the expansion (17) leads to the following result:

$$1 - \varphi_{\omega} \approx 2(\gamma D_2 - 1) + 3\psi_{\omega}. \quad (19)$$

In the limit $\psi \rightarrow \psi_{\min}$ we get from (19) a "pair law":

$$\min(1 - \varphi_{\omega}) = 2(\gamma D_2 - 1) + 3(\gamma D_2 - 1) + (1 - \gamma D_2) \theta(1 - \gamma D_2).$$

It follows from Eq. (18) that when we integrate over ψ the important region is of the order $|1 - \gamma D_2|$, so that the main part of the expansion of the Π -operator originates from the factor $1 - \varphi_{\omega}$:

$$1 - \varphi_{\omega}(q, \varepsilon=0) \sim 1 - \varphi_{\omega} - \frac{\gamma u^2}{4} \sum_{\mathbf{p}} \left[t(\mathbf{p}) q_{\alpha} q_{\beta} \frac{\partial^2 t}{\partial p_{\alpha} \partial p_{\beta}} - \left(q_{\alpha} \frac{\partial t}{\partial p_{\alpha}} \right)^2 \right] V_{\omega}^{-2}(\mathbf{p}).$$

We do not write down here an expansion of the denominator $V_{\omega}(\mathbf{p}_{\pm})$ in powers of q as each differentiation of this function gives an extra factor $\tilde{\omega} \propto \psi^{1/2}$. Taking this fact into account we put everywhere where it is at all possible ω and $\tilde{\omega} = 0$ so that the main term in the expansion of the Π -operator in powers of q^2 has the following form

$$\frac{\partial \Pi_{\perp}(q)}{\partial q^2} = -\frac{\gamma T}{6} \sum_{\mathbf{p}} u^{-2} D_2 \left(\frac{\partial t}{\partial \mathbf{p}} \right)^2 [1 - \varphi_{\omega}]^{-3}.$$

We integrated here by parts and used the cubic symmetry of the crystal. In the limit $T \rightarrow 0$ we can integrate over ψ rather than sum over ω [see (18) and (19)]:

$$\frac{\partial \Pi_{\perp}(q)}{\partial q^2} = -\frac{D_2 (\gamma^3)}{u^2 (D_2)}^{1/2} \sum_{\mathbf{p}} \left(\frac{\partial t}{\partial \mathbf{p}} \right)^2 \frac{1}{12\pi} \int_{\psi_c}^1 \frac{d\psi}{(\psi - 1 + \gamma D_2)^{3/2} [3\psi + 2(\gamma D_2 - 1)]^2} \quad (20)$$

where $\psi_c = 1 - \gamma D_2$ in the dielectric phase and $\psi_c = 0$ in the metallic phase. The evaluation of the integral (20) gives the following expression:

$$\frac{\partial \Pi}{\partial q^2} = -\left(\frac{\gamma^3}{3D_2 |1 - \gamma D_2|} \right)^{1/2} \frac{D_2}{6u^2} \sum_{\mathbf{p}} \left(\frac{\partial t}{\partial \mathbf{p}} \right)^2 \times \left\{ \frac{\theta(1 - \gamma D_2)}{2} + \frac{\theta(\gamma D_2 - 1)}{2\pi} \ln \left(\frac{3^{3/2} + 1}{3^{3/2} - 1} \right) \right\}. \quad (21)$$

Hence we find by means of (16)

$$\varepsilon_{\omega} = 1 + \frac{\pi e^2 D_2}{3au^3} \left(\frac{\gamma^3}{3D_2 |1 - \gamma D_2|} \right)^{1/2} \sum_{\mathbf{p}} \left(\frac{\partial t}{\partial \mathbf{p}} \right)^2, \quad (22)$$

so that the permittivity becomes infinite according to the rule

$$(1 - \gamma D_2)^{-1/2} \propto 1/(t_c - t)^{1/2}.$$

To find the spectrum of the collective (sound and plasma) excitation we expand the Π -operator in ε^2 . To do this we perform an expansion of the product which occurs in the "dangerous" denominator $1 - \varphi_{\omega}(q, \varepsilon)$:

$$V_{\omega}^{-1}(\mathbf{p}) V_{\omega}^{-1}(\mathbf{p}) = V_{\omega}^{-2}(\mathbf{p}) \left\{ 1 - \left(\frac{\varepsilon}{2} \right)^2 \left[\frac{1}{V} \frac{\partial^2 V}{\partial \omega^2} - \frac{1}{V^2} \left(\frac{\partial V}{\partial \omega} \right)^2 \right] \right\} \quad (23)$$

we use the definition (4) of the quantities $V_{\omega}(\mathbf{p})$ and $\tilde{\omega}$:

$$\frac{d\tilde{\omega}}{d\omega} = 1 + \gamma u^2 i \sum_{\mathbf{p}} t(\mathbf{p}) V_{\omega}^{-2}(\mathbf{p}) \frac{\partial V_{\omega}(\mathbf{p})}{\partial \omega},$$

$$V_{\omega}(\mathbf{p}) = u^2 + \omega_n^2 - i\tilde{\omega} t(\mathbf{p}).$$

Hence we find

$$\frac{d\tilde{\omega}}{d\omega} = \left[1 + 2i\omega \gamma u^2 \sum_{\mathbf{p}} t(\mathbf{p}) V_{\omega}^{-2}(\mathbf{p}) \right] R_{\omega},$$

where

$$R_{\omega} = (1 - \varphi_{\omega})^{-1}.$$

Similarly we can determine also the second derivatives, but near the M -transition point one can considerably simplify the calculations if everywhere in the numerators we put $\tilde{\omega}$ and ω equal to zero. As a result we get the following expression:

$$\frac{\partial V_{\omega}(\mathbf{p})}{\partial \omega} \approx -it(\mathbf{p}) R_{\omega}, \quad \frac{d\tilde{\omega}}{d\omega} = R_{\omega},$$

$$\frac{\partial^2 V_{\omega}(\mathbf{p})}{\partial \omega^2} \approx -it(\mathbf{p}) \frac{d^2 \tilde{\omega}}{d\omega^2} = 2\gamma u^2 R_{\omega}^3 \sum_{\mathbf{p}} t^3(\mathbf{p}) V_{\omega}^{-3}(\mathbf{p}).$$

Substituting this into (23) we find $[\sum_{\mathbf{p}} t^3(\mathbf{p}) = 0]$

$$1 - \varphi_{\omega}(0, \varepsilon) \approx 1 - \varphi_{\omega} + \gamma \frac{u^2 \varepsilon^2}{4} \sum_{\mathbf{p}} t^4(\mathbf{p}) V_{\omega}^{-4}(\mathbf{p}) [1 - \varphi_{\omega}]^{-4}. \quad (24)$$

Finally we perform the expansion of (6) in ε^2 :

$$\frac{\partial \Pi_{\perp}(0)}{\partial \varepsilon^2} = -\frac{D_2 D_2 \gamma^2}{2u^4} T \sum_{\mathbf{p}} [1 - \varphi_{\omega}(0)]^{-4}.$$

After changing from a summation over ω to an integration over ψ by means of (18) we have

$$\frac{\partial \Pi_{\perp}(0)}{\partial \varepsilon^2} = -\frac{\gamma^2 D_2 D_2}{u^3 \pi} \int_{\psi_c}^1 \frac{d\psi}{(\gamma D_2)^{3/2} (\psi + \gamma D_2 - 1)^{3/2} [3\psi + 2(\gamma D_2 - 1)]^2}.$$

We determine the main term of the expansion of (24) in powers of $|1 - \gamma D_2|^{-1/2}$:

$$\frac{\partial \Pi_{\perp}(0)}{\partial \varepsilon^2} = -\frac{\gamma^2 D_2 (3D_2)^{3/2}}{|1 - \gamma D_2|^{3/2} 32\pi u^3} \times \begin{cases} \pi - \text{in the dielectric phase} \\ \ln [(3^{1/2} + 1)/(3^{1/2} - 1)] - 2/3^{1/2} - \text{in the metallic phase} \end{cases} \quad (25)$$

Combining these results with (21) we find the following expression for the sound velocity in the dielectric phase, the value of which vanishes linearly:

$$c_s^2 = \frac{\partial \Pi}{\partial q^2} / \frac{\partial \Pi}{\partial \varepsilon^2} = 8 \sum_p \left(\frac{\partial t}{\partial p} \right)^2 \frac{(1 - \gamma D_2)^2}{9 D_4}. \quad (26)$$

In the metallic phase the expansion of the Π -operator contains a constant part. After an analytical continuation, $\varepsilon^2 \rightarrow -\omega^2$, one obtains easily the spectrum of the optical kind of oscillations:

$$\omega^2 = \left[\Pi_0(0) + q^2 \frac{\partial \Pi_0(q)}{\partial q^2} \right] / \frac{\partial \Pi_0(0)}{\partial \varepsilon^2}. \quad (27)$$

Near the transition point $\Pi_0(0) \propto (\gamma D_2 - 1)^{1/2}$ so that the frequency of the plasma oscillations vanishes as $(t - t_c)^{3/2}$.

4. METAL-DIELECTRIC PHASE TRANSITION

If we neglect the direct Coulomb interaction, the free energy in the Hubbard model is calculated by means of the following general formula:

$$t \frac{\partial F}{\partial t} = \sum_{r, r'} t(r-r') \langle a_{r\sigma}^\dagger a_{r'\sigma} \rangle. \quad (28)$$

To obtain this relation it is sufficient to assume that $t(r)$ is proportional to the integral for the transition to a neighboring cell which, in turn, is a decreasing function of the mutual distance between the atoms. The average of the two operators in (28) is evaluated in terms of the complete Green function (2):

$$t \frac{\partial F}{\partial t} = T \sum_{\mathbf{p}} t(\mathbf{p}) D_\omega(\mathbf{p}) = 2iT \sum_{\mathbf{p}} \bar{\omega} t(\mathbf{p}) V_\omega^{-1}(\mathbf{p}). \quad (29)$$

We use (4) to evaluate the sum over the momenta:

$$t \frac{\partial F}{\partial t} = -\frac{2T}{\gamma u^2} \sum_{\omega} \bar{\omega}(\bar{\omega} - \omega). \quad (30)$$

Near the M -transition point it is convenient to use the variable ψ [see (18)]. In the absolute zero limit we get $F = E$ and

$$t \frac{\partial E}{\partial t} = -\frac{4u}{3\gamma} (\gamma D_2)^{-1/2} \int_{\psi_c}^1 (\psi + \gamma D_2 - 1)^{1/2} d\psi. \quad (31)$$

After integrating we arrive at the conclusion that without a long-range Coulomb interaction the M -transition is a transition of order $3\frac{1}{2}$ and

$$t \frac{dE_{\text{abs.z.}}}{dt} \sim \theta(\gamma D_2 - 1) \frac{8u(\gamma D_2 - 1)^{1/2}}{15\gamma(\gamma D_2)^{3/2}}, \quad (32)$$

$$E_{\text{abs.z.}} \sim \theta(\gamma D_2 - 1) (\gamma D_2 - 1)^{1/2}.$$

The contribution from the long-range Coulomb part is well determined by the well known formula from the "ring" approximation⁸:

$$F_{\text{Coul}} = T \sum_{\mathbf{q}} \ln \left[1 - \frac{4\pi e^2}{aq^2} \Pi_0(\mathbf{q}) \right]. \quad (33)$$

We first of all determine the correction coming from the polarization operator:

$$F_1 = -\frac{4\pi e^2 T}{a} \sum_{\mathbf{q}} \Pi_0(\mathbf{q}) q^{-2}. \quad (34)$$

Sufficiently close to the transition point the largest contribution to the sum in (33) and (34) comes from the term with $\varepsilon = 0$. Due to the Coulomb factor close to the

transition point the sum over \mathbf{q} in (34) then comes from the small \mathbf{q} region. This fact is connected with the singularity of the Π -operator which contains a denominator $1 - \varphi_\omega(\mathbf{q})$. We use its expansion in powers of q^2 :

$$1 - \varphi_\omega(q) \sim 1 - \varphi_0 + \frac{\gamma q_\alpha q_\beta}{2u^2} \sum_p \frac{\partial t}{\partial p_\alpha} \frac{\partial t}{\partial p_\beta}.$$

For cubic crystals this expansion has the following form, if we use (19):

$$1 - \varphi_\omega(q) = 2(\gamma D_2 - 1) + 3\psi + bq^2, \quad b = \frac{\gamma}{6u^2} \sum_p \left(\frac{\partial t}{\partial p} \right)^2. \quad (35)$$

Making the same simplifications as when we evaluated the permittivity we find

$$\Pi_0(q) \sim \frac{2T\gamma}{u^2} \sum_{\mathbf{p}} \frac{D_2}{2(\gamma D_2 - 1) + 3\psi_\omega + bq^2}.$$

After changing to integration in the small q^2 region we get instead of (34) the following expression:

$$F_1 = -\frac{2\gamma e^2 T^2 D_2}{au^2 b^{1/2}} \sum_{\mathbf{p}} [2(\gamma D_2 - 1) + 3\psi_\omega]^{-1/2}. \quad (36)$$

To estimate the sum in (36) we evaluate it for $T = 0$ using the substitution (18):

$$F_1 = -\frac{e^2 T D_2 \gamma^{1/2}}{\pi au (b D_2)^{1/2}} \int_{\psi_c}^1 \left(\frac{3\psi + 2(\gamma D_2 - 1)}{\psi + \gamma D_2 - 1} \right)^{1/2} d\psi$$

$$= -\frac{e^2 T D_2 \gamma^{1/2}}{2\pi au (3b D_2)^{1/2}} \{ (\gamma D_2 - 1) \ln |1 - \gamma D_2| + 6 \}. \quad (37)$$

The particular properties of the obtained expression are connected with the increase of the polarizability near the M -transition point. At finite temperatures the logarithmic singularity in (37) is smeared out so that as the simplest interpolation we must take instead of $|1 - \gamma D_2|$ under the logarithm sign the larger of the two quantities: $|1 - \gamma D_2|$ or T/u . For the final evaluation of the correction (33) we subtract from it the sum (34):

$$F_2 = T \sum_{\mathbf{q}} \left\{ \frac{4\pi e^2}{aq^2} \Pi_0(\mathbf{q}) + \ln \left[1 - \frac{4\pi e^2}{aq^2} \Pi_0(\mathbf{q}) \right] \right\}. \quad (38)$$

If the number of dimensions is less than four, all the integrals in (38) come from small q so that one must everywhere in (38) put $\Pi_0(q) \approx \Pi_0(0)$. For not too low temperatures it is sufficient to take from the sum over ε the term with $\varepsilon = 0$. As a result we get after elementary integrations

$$F_2 = -\frac{T}{6\pi} \left[\frac{4\pi e^2}{a} |\Pi_0(0)| \right]^{1/2}. \quad (39)$$

The quantity $\Pi_0(0)$ is given in (11); in the case $T \ll u$ it is non-vanishing only in the metallic phase:

$$\Pi \sim -\rho(0) = -2(\gamma D_2 - 1)^{1/2} / (\pi u (\gamma D_2)^{1/2})$$

[see Ref. 7 and (18)]. In the metallic phase the main contribution comes therefore from F_2 —the Debye-Hückel correction to the free energy which is appreciably larger than (32) and F_1 , as for $T \ll \varepsilon_0$

$$F_2 \propto -(t - t_c)^{1/2}.$$

In the dielectric phase the main contribution comes from (37) as according to (11) the density of states at low temperatures turns out to be exponentially small. At low temperatures

$$|F_1| \sim \frac{Te^2}{au^2} (t_c - t) \ln \left(\frac{t_c}{t_c - t} \right) > |F_2|$$

in the dielectric phase. The correction to the equation of state is obtained by differentiating the free energy with respect to the volume, taking into account the fact that the parameter t is a decreasing function of the mean distance between the atoms $V \partial t / \partial V < 0$:

$$\Delta p = - \frac{\partial F^{\text{abs.z.}}}{\partial V} = V \frac{\partial t}{\partial V} \left\{ \frac{\gamma^2 T e^2 D_2^2}{\pi a t u (3b \gamma D_1)^{1/2}} \ln |1 - \gamma D_2| + \frac{T (4\pi e^2)^{1/2}}{a^{1/2} 4\pi} |\Pi_0(0)|^{1/2} \frac{\partial |\Pi_0(0)|}{\partial t} \right\}. \quad (40)$$

In the dielectric phase the pressure increases logarithmically due to the first term in Eq. (40). The second term gives a large negative contribution in the metallic phase, $\propto (t - t_c)^{-1/4}$ which for $t > t_c$ is always larger in absolute magnitude than the first term.

Equations (37) and (39) show that for some range of temperatures a phase transition is possible in the system which is close to a first order transition. When the temperature is lowered appreciably below u the nature of the singularity changes. However, even at $T=0$ the singularity originating from the Coulomb interaction turns out to be stronger than the one occurring in the Hubbard model (32). At $T=0$ all sums over frequencies must be replaced by integrals and one must expand the dangerous denominator in powers of q^2 and ε^2 . Using (24) and (35) we get

$$1 - \varphi_0(q, \varepsilon) \approx 1 - \varphi_0 + b q^2 + c \varepsilon^2 / (1 - \varphi_0)^2. \quad (41)$$

As a result of integrating over the momentum q^2 we have instead of (36)

$$F_1 = - \frac{\gamma^2 D_2^2}{\pi^2 a b^{1/2}} \int_0^\infty \frac{d\omega d\varepsilon}{u^2} \left\{ 1 - \varphi_0 + \frac{c \varepsilon^2}{(1 - \varphi_0)^2} \right\}^{-1/2}.$$

The logarithmic divergence in ε at the upper limit is cut off at some maximum frequency which is independent of t . Using the expansion (19) and the change of variable (18) we easily make the integral obtained dimensionless using the substitutions

$$\varepsilon \rightarrow |\gamma D_2 - 1|^{1/2} \varepsilon, \quad \psi \rightarrow |\gamma D_2 - 1| \psi,$$

as a result of which we shall have (with logarithmic accuracy)

$$F_1 = - \frac{3e^2 D_2}{2a u \pi^2} \left(\frac{\gamma}{bc D_1} \right)^{1/2} \int_{\psi_c}^1 \frac{(2\tau + 3\psi)^2}{(\psi + \tau)^{1/2}} \ln \left[\frac{(c^{1/2} \varepsilon_{\text{max}})^{1/2}}{2\tau + 3\psi} \right] d\psi, \quad (42)$$

$$F_1^{\text{abs.z.}} = - \frac{12e^2 D_2}{5\pi^2 a u} \left(\frac{\gamma}{bc D_1} \right)^{1/2} \theta(\tau) \tau^{1/2} \ln \tau;$$

$$\tau = \gamma D_2 - 1.$$

A comparison of this result with (37) shows that the extra integration over ε gives an additional small factor $|1 - \gamma D_2|^{3/2}$. For this reason we get as $T \rightarrow 0$ instead of (39) the following result:

$$F_2 = - \frac{B u}{6\pi^2} |\gamma D_2 - 1|^{3/2}. \quad (43)$$

In the metallic phase the coefficient B is of order unity; in the dielectric phase it is different from zero but somewhat smaller. This fact is connected with the simple fact that after the analytical continuation the integration in (38) will take place over that region of energies where the density of states is non-vanishing. In the dielectric phase this region decreases fast as we get away from the M -transition point.

electric phase this region decreases fast as we get away from the M -transition point.

5. LONG-RANGE CORRELATION EFFECTS AND CONDITIONS OF APPLICABILITY

Equations (43) and (42) are valid for sufficiently low temperatures and not too close to the M -transition point:

$$T_N \ll T \ll u [|t - t_c| / |t_c|]^u \ll u. \quad (44)$$

The left-hand inequality arises from the fact that at sufficiently low temperatures ($< T_N$) the system becomes unstable against the occurrence of antiferromagnetic ordering⁹ which was neglected in the present paper.

The results (37), (39), and (40) apply at sufficiently high temperatures. It is, however, clear that when we approach the transition point the formulae obtained above cease to be applicable because of critical fluctuations.

We shall depict by a wavy line the Coulomb interaction:

$$V(q) = 4\pi e^2 / (q^2 + \kappa^2), \quad \kappa^2 = -4\pi e^2 \Pi_0(0) / a. \quad (45)$$

The basic correlation corrections are determined by the ternary and quaternary vertex parts E_3 and E_4 , as shown in Fig. 4. One shows easily that in our case of a half-filled band the vertex part E_3 vanishes as an odd power of q_1 . The vertex part E_4 , calculated in the static and long-wavelength limit $\omega_i = 0$ and $q_i \rightarrow 0$, corresponds to repulsion and depends strongly on the ratio t/u . In the vicinity of the Mott transition which is of interest to us it has a very weak singularity which we must neglect and evaluate E_4 for $t = t_c$:

$$E_4 = T \sum_{\mathbf{p}} \psi_0^4 D_0^4(\mathbf{p}) \sim u^{-2} g(T/u, t/u). \quad (46)$$

Here $g(x, y)$ is a dimensionless positive-definite function which we shall use in the limit $T \ll u$, $t \sim t_c$, $g(0, t_c/u) = g$. The simplest account of the correlation corrections shown in Fig. 4a to c leads to the following estimate ($q_i = 0$):

$$\Delta V^{(a)} \sim \Delta V^{(b)} \sim \Delta V^{(c)} \sim \sum_q \frac{(4\pi e^2 g)^2 T}{a^2 u^9 (q^2 + \kappa^2)^2}. \quad (47)$$

Here a is the size of the cell; and the factor T arises because in the summation over the energy transfer we restrict ourselves to the static term corresponding to $\omega = 0$.

In the three-dimensional case comparison of (47) and (46) leads to the following inequality:

$$\frac{T g}{8\pi u} \left(\frac{4\pi e^2}{a u} \right)^4 \ll \left| \frac{t - t_c}{t_c} \right|^u.$$

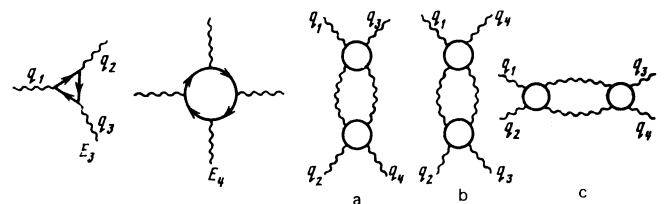


FIG. 4. Ternary (E_3) and quaternary (E_4) unpaired Coulomb potential, a to c: corrections to the quaternary potential.

Combining this inequality with the condition for the use of the quasi-static approximation we get the region of applicability of the results (37) to (40):

$$u \left| \frac{t-t_c}{t_c} \right|^{\frac{1}{2}} \ll T \ll \frac{8\pi u}{g} \left(\frac{au}{4\pi e^2} \right)^{\frac{1}{2}} \left| \frac{t-t_c}{t_c} \right|^{\frac{1}{2}}. \quad (48)$$

We note that in fact the parameter $g \sim 1$, but it is always multiplied by the factor $[4\pi e^2/ua]^2$ which is the square of the ratio of the size of an atom to the size of the elementary cell.

It is interesting to note that in four-dimensional space all corrections become logarithmic so that our problem can be solved in the parquet approximation.¹⁰ In the three-dimensional case our problem is equivalent to the single-component Ising model where the dimensionless parameter $\tau = |(T - T_c)/T_c|$ must be replaced by κ^2 . The critical indexes in that model are well known:¹¹ $\alpha = 0.08$, $\beta = 0.33$, $\gamma = 1.26$, $\eta = 0.04$. In the dielectric phase $\kappa^2 = 0$ and the correlation function is determined by Fisher's parameter η :

$$V(q) \propto q^{-2+\eta}, \quad V(r) \propto r^{-1.04}. \quad (49)$$

In the metallic phase when $\kappa^2 > 0$,

$$V(q) \propto [q^{2-\eta+\kappa^{2\eta}}]^{-1}. \quad (50)$$

The second derivative of the free energy with respect to the parameter κ^2 (in the metallic phase) is determined by the index α^{10} :

$$\delta^2 F / \delta (\kappa^2)^2 = -\kappa^{-2\alpha}. \quad (51)$$

Because of this we have in the region of strong Coulomb correlations instead of (39)

$$\Delta F \sim - \left[\frac{4\pi e^2}{a} |\Pi_0(0)| \right]^{2-\alpha}. \quad (52)$$

In the region of strong Coulomb correlations when

$$1 \gg \frac{gT}{8\pi u} \left(\frac{4\pi e^2}{au} \right)^{\frac{1}{2}} \gg \left| \frac{t-t_c}{t_c} \right|^{\frac{1}{2}}, \quad (53)$$

the absolute value of the Debye-Hückel correction (39) is thus overestimated (since $2 - \alpha \sim 1.92 > 3/2$).

In the dielectric phase in the region of (53) the dielectric permittivity is infinite as according to (49) at large distances the Coulomb interaction decreases somewhat faster than $1/r$ —as $r^{-1.04}$. When the temperature is low-

ered the region of applicability of the "high-temperature" results is diminished, but the extrema on the isotherms (40) become steeper and the amount of heat released at the transition diminishes. The nature of the transition is not changed at any finite temperature, but as $T \rightarrow 0$ this transition is in a wide range of pressures close to a second-order transition [according to (42) and (44) it has the character of order $2\frac{1}{4}$ to $2\frac{1}{2}$].

The Coulomb interaction in the Hubbard model thus changes the nature of the Mott transition considerably. It is transformed from a transition of order $3\frac{1}{2}$ to a first-order isostructural transition [see (32) and (40)]. When we approach the transition point the dielectric permittivity grows and the frequency of the plasma oscillations and the sound speed decrease. The Coulomb interaction necessarily leads to a structural instability near the Mott transition point. This result agrees qualitatively with all experiments where a metal-dielectric transition occurs.

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