СООБЩЕНИЯ
ОБЪЕДИНЕННОГО
ИНСТИТУТА
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Дубна

E4 - 6641

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METAL-INSULATOR TRANSITION AND LIFSHIZ INSTABILITY IN THE HUBBARD MODEL

ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

1972

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1. Introduction

There is considerable interest in the study of electrons in a half-filled narrow energy band. Due to the electron-electron correlation a splitting of the band and magnetic ordering are possible depending on the ratio U/Λ , where U is a measure of the Coulomb repulsion and 2Λ is the band width. A phase diagram is expected which can show in the general case an antiferromagnetic "insulating" phase *(AI)*, an antiferromagnetic "metallic" phase (AM), a paramagnetic "insulating" phase (PI) and a paramagnetic "metallic" phase (PM). Transitions occur by changing U/Λ by means of external pressure or of doping.

We consider in this paper the metal-insulator transition (Mott transition) from a paramagnetic insulating phase to a paramagnetic metallic phase. Both phases are assumed to have the same lattice symmetry. Mott /1/ has proposed that this transition may be discontinuous due to an instability in the free energy corresponding to the instability studied by Lifshiz /2/. Lifshiz considered a metal in which by variation of the external pressure an energy branch passes through the Fermi energy. In our case the narrow band is split into a filled and into an empty subband for large U/Λ. If U/Λ decreases with increasing pressure the gap between the two subbands goes to zero. Thus qualitatively the situations in the case considered by Lifshiz and in our case are the same.

It is the aim of this paper to obtain the Lifshiz instability connected with the metal-insulator transition starting from the Hubbard model. We consider one half-filled nondegenerate band. The Hubbard model is treated by means of the functional integral technique in the static approximation. We neglect higher-order fluctuations in the exponent of the functional integral and develop a self-consistent approximation scheme analogous to the coherent potential approximation (CPA). Similar treatments of the functional integral were given by Cyrot /3/ and Kimball and Schrieffer /4/. The resulting equations are approximately solved by the use of the stationary point approximation for the integrals and of an approximate solution of the CPA condition. In the framework of these approximations the Lifshiz instability can be obtained analytically.

McWhan et al. /5/ have found in $(V_{1-x}Cr_x)_2 O_3$ for $x \simeq 0.01 \div 0.04$ a first order phase transition curve $(PI \rightleftarrows PM)$ terminating at a critical point. Both phases have the same lattice symmetry (α-corundum). Unfortunately the band structure of this system is not well known, and it is not clear therefore whether electron-electron correlation or band shifting (overlapping) is responsible for the transition. Wilson and Pitt /6/ have found a PI $\rightleftarrows$ PM transition in the system $Ni(S_{1-x}Se_x)_2$ for $x \lesssim 0.4$. In this pyrite structure there are

two d-electrons per Ni atom in a well separated twofold degenerate e_g-band[7], so that a model with a half-filled band may be a reasonable approximation.

2. The Functional Integral Method

The Hamiltonian of the Hubbard model[8] is $H = H_0 + H_1$, where

$$H_0 = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} n_{\vec{k}\sigma}, \tag{1}$$

$$H_1 = U \sum_i n_{i\uparrow} n_{i\downarrow} = \frac{U}{4} \sum_i (n_{i\uparrow} + n_{i\downarrow})^2 - \frac{U}{4} \sum_i (n_{i\uparrow} - n_{i\downarrow})^2. \tag{2}$$

$\epsilon_{\vec{k}}$ is the energy of the unperturbed nondegenerate band of band width 2Δ; the chemical potential μ is included into $\epsilon_{\vec{k}}$. The interaction part of the Hamiltonian describes the Coulomb repulsion of two electrons (with antiparallel spins) at the same lattice site. This part is rewritten as suggested by Mühlschlegel[9]. We have preferred the first version proposed by Mühlschlegel because it leads for $U \gg \Delta$ to a gap equal to U. (The second version proposed by Mühlschlegel leads in (11) to the absence of the first term and to $\sqrt{2U}$ instead $\sqrt{U}$; this gives for $U \gg \Delta$ a gap equal to $2U$. The value of the Gibbs potential is for $U \gg \Delta$ the same in both versions).

We apply the integral formula

$$\sqrt{\frac{1}{a}}\, e^{\frac{b^2}{a}} = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{\pi}}\, e^{-ax^2 + 2bx} \tag{3}$$

to the grand partition function of the Hubbard model (Stratonovich-Hubbard transformation[10]):

$$Z = e^{-\beta\Omega} = Tr\{e^{-\beta H}\} = Tr\{T \exp[-i \int_0^{-i\beta} dt\, H(t)]\} =$$

$$= \int \mathfrak{D}x_i(t)\, \mathfrak{D}y_i(t)\, e^{-\beta\Omega(x_i(t),\, y_i(t))}, \tag{4}$$

with

$$e^{-\beta\Omega(x_i(t), y_i(t))} = Tr\{T \exp[-i \int_0^{-i\beta} dt\, H(x_i(t), y_i(t))]\}, \tag{5}$$

$$H(x_i(t), y_i(t)) = \sum_i (x_i^2(t) + y_i^2(t)) + \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} n_{\vec{k}\sigma}(t) -$$
$$- \sqrt{U} \sum_i (n_{i\uparrow}(t) + n_{i\downarrow}(t)) i y_i(t) - \tag{6}$$
$$- \sqrt{U} \sum_i (n_{i\uparrow}(t) - n_{i\downarrow}(t)) x_i(t),$$

$$\mathfrak{D} x_i(t) = \prod_i \prod_{j=1}^{\mathfrak{N}} \left(\sqrt{\frac{\beta}{\pi \mathfrak{N}}}\, dx_i(t_j)\right),$$
$$\mathfrak{D} y_i(t) = \prod_i \prod_{j=1}^{\mathfrak{N}} \left(\sqrt{\frac{\beta}{\pi \mathfrak{N}}}\, dy_i(t_j)\right). \tag{7}$$

For the integration the imaginary time interval $[0, -i\beta]$ is divided into $\mathfrak{N}(\to\infty)$ sub-intervals.

By means of (4) the partition function Z is represented as the average of the partition function of band electrons without electron-electron interaction but under the influence of two stochastic fields x, y. The "magnetic field" x is coupled to the spins of the electrons, the "electric potential" y is coupled to the charge of the electrons.

The spin fluctuation effects are assumed to be more important than the charge fluctuation effects (compare /4,11/). Therefore, the field y is simply treated in the stationary point approximation, that means in $H(x_i(t), y_i(t))$ we use the value of $y_i(t)$ which makes H stationary:

$$0 = \frac{\partial H(x_i(t), y_i(t))}{\partial y_i(t)} = 2y_i(t) - i\sqrt{U}\,(n_{i\uparrow}(t) + n_{i\downarrow}(t)) \approx \tag{8}$$
$$\approx 2y_i(t) - i\sqrt{U}.$$

Furthermore, we treat the field $x_i(t)$ in the static approximation: We neglect the time dependence of the x_i in the interaction part in (6).

In this way the problem is reduced to

$$Z = e^{-\beta\Omega} = \int \mathfrak{D} x_i \; e^{-\beta\tilde{\Omega}(x_i)}, \tag{9}$$

$$H(x_i(t), y_i(t)) = \sum_i (x_i^2(t) + y_i^2(t)) + \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} n_{\vec{k}\sigma}(t) -$$
$$- \sqrt{U} \sum_i (n_{i\uparrow}(t) + n_{i\downarrow}(t)) i y_i(t) - \tag{6}$$
$$- \sqrt{U} \sum_i (n_{i\uparrow}(t) - n_{i\downarrow}(t)) x_i(t),$$

$$\mathfrak{D}x_i(t) = \prod_i \prod_{j=1}^{\mathfrak{N}} \left(\sqrt{\frac{\beta}{\pi \mathfrak{N}}}\, dx_i(t_j)\right),$$
$$\tag{7}$$
$$\mathfrak{D}y_i(t) = \prod_i \prod_{j=1}^{\mathfrak{N}} \left(\sqrt{\frac{\beta}{\pi \mathfrak{N}}}\, dy_i(t_j)\right).$$

For the integration the imaginary time interval $[0, -i\beta]$ is divided into $\mathfrak{N}(\to\infty)$ subintervals.

By means of (4) the partition function Z is represented as the average of the partition function of band electrons without electron-electron interaction but under the influence of two stochastic fields x, y. The "magnetic field" x is coupled to the spins of the electrons, the "electric potential" y is coupled to the charge of the electrons.

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$$O = \frac{\partial H(x_i(t), y_i(t))}{\partial y_i(t)} = 2y_i(t) - i\sqrt{U}\,(n_{i\uparrow}(t) + n_{i\downarrow}(t)) \approx \tag{8}$$
$$\approx 2y_i(t) - i\sqrt{U}.$$

Furthermore, we treat the field $x_i(t)$ in the static approximation: We neglect the time dependence of the x_i in the interaction part in (6).

In this way the problem is reduced to

$$Z = e^{-\beta\Omega} = \int \mathfrak{D}x_i \; e^{-\beta\tilde{\Omega}(x_i)}, \tag{9}$$

with

$$e^{-\beta\tilde{\Omega}(x_i)} = Tr\{\exp[-\beta\tilde{H}(x_i)]\}, \tag{10}$$

$$\tilde{H}(x_i) = -\frac{NU}{4} + \sum_i x_i^2 + \sum_{\vec{k}\sigma} \tilde{\epsilon}_{\vec{k}} n_{\vec{k}\sigma} - \sqrt{U} \sum_{i\sigma} n_{i\sigma}\sigma x_i , \tag{11}$$

$$\tilde{\epsilon}_{\vec{k}} = \epsilon_{\vec{k}} + \frac{U}{2}, \tag{12}$$

$$\mathfrak{D}x_i = \Pi\left(\sqrt{\frac{\beta}{\pi}}\, dx_i\right). \tag{13}$$

For a half-filled band the chemical potential μ can be fixed by requiring electron-hole symmetry (the interaction term in (11) conserves electron-hole symmetry):

$$0 = \frac{1}{N} \sum_{\vec{k}} \tilde{\epsilon}_{\vec{k}}. \tag{14}$$

The magnetic moment of the electrons at a lattice site i is connected with the average of the stochastic field x_i : In view of

$$\int \mathfrak{D}x_i \frac{\partial}{\partial x_i} e^{-\beta\tilde{\Omega}(x_i)} = 0 \tag{15}$$

we obtain from (10,11)

$$\langle n_{i\uparrow} - n_{i\downarrow} \rangle_H = \frac{2}{\sqrt{U}} \int \mathfrak{D}x_i x_i e^{-\beta\tilde{\Omega}(x_i)} \equiv \frac{2}{\sqrt{U}} \langle x_i \rangle_x . \tag{16}$$

Because we have a static field x and no electron-electron interaction, the Gibbs potential $\tilde{\Omega}$ corresponding to the Hamiltonian $\tilde{H}(x_i)$ can be written in the simple form (compare Kimball and Schrieffer /4/)

$$\tilde{\Omega}(x_i) = -\frac{NU}{4} + \sum_i x_i^2 - \frac{1}{\beta}\int_{-\infty}^{\infty} d\omega \rho(\omega, x_i) \ln[1 + e^{-\beta\omega}], \tag{17}$$

where the density of states $\rho(\omega, x_i)$ is given by

$$\rho(\omega, x_i) = -\frac{1}{\pi} \sum_{i\sigma} Im\, G_{ii\sigma}(\omega + i\epsilon, x_i), \tag{18}$$

with the one-electron Green function

$$G_{ii\sigma}(\omega + i\epsilon, x_i) = \frac{1}{i} < T\, a_{i\sigma}(t)\, a^{+}_{i\sigma}(t') >_{\substack{\tilde{H}(x_i), \\ \omega + i\epsilon}} \tag{19}$$

3. The Average with Respect to x

The problem defined by Eq. (9-13) is analogous to the problems considered in the theory of disordered systems (alloys). At each lattice site i we have a static stochastic field x_i (with different sign for different spin direction), and we have to perform the average with respect to these stochastic fields. For this average we use an approximation scheme similar to the coherent potential approximation (/12/; compare also Cyrot /3/, Kimball and Schrieffer /4/).

We write for the Green function

$$G_{ij\sigma}(\omega, x) = \tilde{G}_{ij\sigma}(\omega) + \sum_{\ell\bar{\ell}} \tilde{G}_{i\ell\sigma}(\omega) \mathcal{T}_{\ell\bar{\ell}\sigma}(\omega, x_i) \tilde{G}_{\bar{\ell}j\sigma}(\omega), \tag{20}$$

with

$$(\tilde{G}^{-1}(\omega))_{ij\sigma} = (G^{(0)-1}(\omega))_{ij\sigma} - \Sigma_{i\sigma}(\omega)\, \delta_{ij}, \tag{21}$$

$$\mathcal{T}_{\ell\bar{\ell}\sigma} = \mathcal{T}^{(1)}_{\ell\sigma}\,\delta_{\ell\bar{\ell}} + \mathcal{T}^{(1)}_{\ell\sigma}\,(N\tilde{G}_\sigma)_{\ell\bar{\ell}}\,\mathcal{T}^{(1)}_{\bar{\ell}\sigma} +$$

$$+ \sum_{\ell_1} \mathcal{T}^{(1)}_{\ell\sigma}\,(N\tilde{G}_\sigma)_{\ell\ell_1}\;\mathcal{T}^{(1)}_{\ell_1\sigma}(N\tilde{G}_\sigma)_{\ell_1\bar{\ell}}\,\mathcal{T}^{(1)}_{\bar{\ell}\sigma} + \ldots, \qquad (22)$$

$$\mathcal{T}^{(1)}_{\ell\sigma}(\omega, x_\ell) = \frac{v_{\ell\sigma} - \Sigma_{\ell\sigma}(\omega)}{1 - (v_{\ell\sigma} - \Sigma_{\ell\sigma}(\omega))\,\tilde{G}_{\ell\ell\sigma}}, \qquad (23)$$

$$v_{\ell\sigma} = -\sqrt{U}\,\sigma x_\ell \,. \qquad (24)$$

$G^{(0)}$ is the Green function corresponding to the unperturbed band $\tilde{\epsilon}_{\vec{k}}$; $\Sigma_{\ell\sigma}(\omega)$ is the CPA mass operator and $N\tilde{G}$ is the nondiagonal part of the matrix $\tilde{G}_{ij}$. Eq. (20-24) are exact.

Now we introduce the average with respect to x of the $\mathcal{T}^{(1)}$-matrix for scattering at one lattice site:

$$\langle \mathcal{T}^{(1)}_{\ell\sigma} \rangle_x \,. \qquad (25)$$

We substitute the expression

$$\mathcal{T}^{(1)}_{\ell\sigma}(\omega, x_\ell) = \langle \mathcal{T}^{(1)}_{\ell,\sigma}(\omega) \rangle_x + (\mathcal{T}^{(1)}_{\ell\sigma}(\omega, x_\ell) - \langle \mathcal{T}^{(1)}_{\ell\sigma}(\omega) \rangle_x) \qquad (26)$$

into (22) and neglect higher powers than the first of the fluctuating parts (second term in (26)). The single-site approximation, which is the basis of the CPA, corresponds to the total neglection of the fluctuating parts. It is obtained

$$\mathcal{T}_{\ell\bar{\ell}\sigma} = \langle \mathcal{T}_{\ell\bar{\ell}\sigma} \rangle_x + (\mathcal{T}^{(1)}_{\ell\sigma} - \langle \mathcal{T}^{(1)}_{\ell\sigma} \rangle_x)\,\delta_{\ell\bar{\ell}} +$$

$$+ \sum_{\ell_1} (\mathcal{T}^{(1)}_{\ell\sigma} - \langle \mathcal{T}^{(1)}_{\ell\sigma} \rangle_x)(N\tilde{G}_\sigma)_{\ell\ell_1} \langle \mathcal{T}_{\ell_1\bar{\ell}\sigma} \rangle_x +$$

$$+\sum_{\ell_1} \langle \mathcal{T}_{\ell\ell_1\sigma} \rangle_x (N\tilde{G}_\sigma)_{\ell_1\bar{\ell}} (\mathcal{T}^{(1)}_{\bar{\ell}\sigma} - \langle \mathcal{T}^{(1)}_{\bar{\ell}\sigma} \rangle_x) + \tag{27}$$

$$+\sum_{\ell_2\ell_3} \langle \mathcal{T}_{\ell\ell_1\sigma} \rangle_x (N\tilde{G}_\sigma)_{\ell_1\ell_2} (\mathcal{T}^{(1)}_{\ell_2\sigma} - \langle \mathcal{T}^{(1)}_{\ell_2\sigma} \rangle)(N\tilde{G}_\sigma)_{\ell_2\ell_3} \langle \mathcal{T}_{\ell_3\bar{\ell}\sigma} \rangle_x ,$$

where $\langle \mathcal{T}_{\ell\bar{\ell}\sigma} \rangle_x$ results from (22) by substituting $\mathcal{T}^{(1)}_{\ell\sigma} \to \langle \mathcal{T}^{(1)}_{\ell\sigma} \rangle_x$ everywhere. We further follow the CPA procedure and determine the CPA mass operator $\Sigma_{\ell\sigma}(\omega)$ (or $\tilde{G}_{ij\sigma}(\omega)$) by means of

$$\langle \mathcal{T}^{(1)}_{\ell\sigma}(\omega, \Sigma(\omega), x_\ell) \rangle_x = 0. \tag{28}$$

Eq. (27) is then reduced to

$$\mathcal{T}_{\ell\bar{\ell}\sigma} = \mathcal{T}^{(1)}_{\ell\sigma} \delta_{\ell\bar{\ell}} . \tag{29}$$

In view of (9,17,18,20,29) we obtain for the Gibbs potential of our system

$$e^{-\beta\Omega} = \int \mathcal{D}x_i \, e^{-\beta \sum_i \Omega_i(x_i)} = \left(\int \sqrt{\frac{\beta}{\pi}} \, dx_i \, e^{-\beta \Omega_i(x_i)} \right)^N , \tag{30}$$

with

$$\Omega_i(x_i) = -\frac{U}{4} + x_i^2 + \frac{1}{\pi\beta} \int_{-\infty}^{\infty} d\omega \, \ln [1 + e^{-\beta\omega}] \times$$

$$\times \, Im \sum_\sigma \{ \tilde{G}_{ii\sigma}(\omega) + (\tilde{G}^2_\sigma(\omega))_{ii} \mathcal{T}^{(1)}_{i\sigma}(\omega, x_i) \} . \tag{31}$$

Our expression (31) differs from the corresponding expression of Kimball and Schrieffer /4/ in the factor $(\tilde{G}^2_\sigma)_{ii}$ instead of $(\tilde{G}_{ii\sigma})^2$ in front of $\mathcal{T}^{(1)}_{i\sigma}$. This difference is connected with the assumption made by Kimball and Schrieffer that $\rho_{i\sigma}(\omega, x_j) \equiv$

$\equiv -\frac{1}{\pi} Im \, G_{ii\sigma}(\omega + i\epsilon, x_j)$ depends only on x_i.

In order to get a self-consistent approximation scheme we calculate also the average (25) of $\mathcal{J}^{(1)}$ in the approximation leading to (30,31):

$$<\mathcal{J}^{(1)}_{\ell\sigma}(\omega)>_x = \left(\frac{1}{Z}\right)^{\frac{1}{N}} \int \sqrt{\frac{\beta}{\pi}}\, dx_\ell\, \mathcal{J}^{(1)}_{\ell\sigma}(\omega, x_\ell)\, e^{-\beta\Omega_\ell(x_\ell)} \qquad (32)$$

The problem to be solved self-consistently is given by the Eq. (28,30-32).

It should be noted that our approximation scheme conserves the essential relation in (16). On proving this relation in the framework of the approximation scheme we have to neglect terms of the type

$$\tilde{G}_{\ell i\sigma}\ \tilde{G}_{i\ell\sigma}\ <\left(\mathcal{J}^{(1)}_{\ell\sigma}\right)^2>_x \qquad \text{for} \quad i \neq \ell. \qquad (33)$$

The neglection of these terms is consistent in a CPA-like scheme. The factor $(\tilde{G}^2_\sigma)_{ii}$ in front of $\mathcal{J}^{(1)}_{i\sigma}$ in (31) seems to be necessary in proving (16).

In this paper we consider the metal-insulator transition between two paramagnetic phases. Thus we have to look for solutions with

$$<x_i>_x = 0 \qquad (\text{for paramagnetic phases}). \qquad (34)$$

Furthermore, in the paramagnetic phases $\tilde{G}_{ij\sigma}$ is independent of the spin σ and the CPA mass operator $\Sigma_{\ell\sigma}$ is independent of ℓ and σ. The antiferromagnetic phase will be considered in a further paper.

4. Stationary Point Approximation

We use the stationary point approximation for the calculation of the x-integrals in (28,30) considering β as the large expansion parameter. Because of the sum over σ and the ℓ – σ-independent Σ the potential $\Omega_i(x_i)$ is an even function in x_i. For fixed Σ the minima $\Omega_i(x_i)$ will be at $x_i = \pm|x_{min}|$ (only $|x_{min}| \neq 0$ is of interest).

Then the CPA condition (28) takes the form

$$<\mathcal{J}^{(1)}_{i\sigma}(\omega, \Sigma, x_i)>_x = \frac{1}{2}\mathcal{J}^{(1)}_{i\sigma}(\omega, \Sigma, |x_{min}|) + \frac{1}{2}\mathcal{J}^{(1)}_{i\sigma}(\omega, \Sigma, -|x_{min}|) = 0. \qquad (35)$$

The potential $\Omega_i(x_i)$ (see Eq. (31)) can be written as

$$\Omega_i(x_i) = -\frac{U}{4} + x_i^2 + \frac{1}{\pi\beta}\int_{-\infty}^{\infty} d\omega\, \ell n\,[1+e^{-\beta\omega}] \times$$

$$\times\, Im\{2\tilde{G}_{ii}(\omega) + (\tilde{G}^2(\omega))_{ii}\,(\mathcal{T}_i^{(1)}(\omega, x_i) + \mathcal{T}_i^{(1)}(\omega, -x_i))\}. \qquad (36)$$

Because of the summation over the spin the same combination of the $\mathcal{T}^{(1)}$-matrices as in the CPA condition (35) has appeared in the last term. Thus, at the minima $x_i = \pm|x_{min}|$

$$\Omega_i(\pm|x_{min}|) = -\frac{U}{4} + x_{min}^2 + \frac{2}{\pi\beta}\int_{-\infty}^{\infty} d\omega\, \ell n\,[1+e^{-\beta\omega}]\, Im\,\tilde{G}_{ii}(\omega). \qquad (37)$$

The condition for $|x_{min}|$ is obtained by differentiating $\Omega_i(x_i)$ (Eq. (36)):

$$\frac{\partial}{\partial x_i}\Omega_i(x_i)\Big|_{x_i=\pm|x_{min}|} = 2x_i + \frac{1}{\pi\beta}\int_{-\infty}^{\infty} d\omega\, \ell n\,[1+e^{-\beta\omega}] \times$$

$$\times\, Im\{(\tilde{G}^2)_{ii}\frac{\partial}{\partial x_i}(\mathcal{T}_i^{(1)}(x_i) + \mathcal{T}_i^{(1)}(-x_i))\}\Big|_{x_i=\pm|x_{min}|} = 0. \qquad (38)$$

$\tilde{G}$ is a function of $|x_{min}|$ in view of (35). Instead of determining $|x_{min}|$ from (38) it is also possible to determine $|x_{min}|$ by differentiation of $\Omega_i(|x_{min}|)$ (Eq. (37)) with respect to $|x_{min}|$:

$$\frac{d\Omega_i(|x_{min}|)}{d|x_{min}|} = 2|x_{min}| + \frac{2}{\pi\beta}\int_{-\infty}^{\infty} d\omega\, \ell n\,[1+e^{-\beta\omega}]\, Im\left\{\frac{d\tilde{G}_{ii}(\omega)}{d\Sigma(\omega)}\frac{d\Sigma(\omega)}{d|x_{min}|}\right\} = 0. \qquad (39)$$

On the basis of another reasoning this way of determination of the stationary point value of the stochastic field was also used by Cyrot /3/ . In order to show the equivalence of (38) with (39) we differentiate Eq. (35):

$$\frac{d\langle \mathcal{T}_i^{(1)} \rangle_x}{d\Sigma} \frac{d\Sigma}{d|x_{min}|} + \frac{\partial \langle \mathcal{T}_i^{(1)} \rangle_x}{\partial |x_{min}|} = 0. \tag{40}$$

Straightforward differentiation of the perturbation series for $\mathcal{T}_i^{(1)}$ leads to

$$\frac{d\mathcal{T}_i^{(1)}}{d\Sigma} = -1 - 2\tilde{G}_{ii}\,\mathcal{T}_i^{(1)} + \sum_{\ell \neq i} \tilde{G}_{i\ell}\,\tilde{G}_{\ell i}\,(\mathcal{T}_i^{(1)})^2, \tag{41}$$

where we have used

$$\frac{d\tilde{G}}{d\Sigma} = \tilde{G}^2. \tag{42}$$

The average of (41) over $x_i = \pm |x_{min}|$ is

$$\frac{d\langle \mathcal{T}_i^{(1)} \rangle_x}{d\Sigma} = -1 + \sum_{\ell \neq i} \tilde{G}_{i\ell}\,\tilde{G}_{\ell i}\,\langle (\mathcal{T}_i^{(1)})^2 \rangle_x \approx -1. \tag{43}$$

The last term in the centre of (43) is of the type (33) and has to be neglected in the framework of the CPA x/ . Using (40,42,43) we obtain

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x/ One can see in many ways that this neglection is necessary in order to get a consistent scheme. For example on averaging (22) in the single-site approximation and differentiating we obtain

$$\frac{d\langle \mathcal{T} \rangle_x}{d\Sigma} = \frac{d\langle \mathcal{T}^{(1)} \rangle_x}{d\Sigma}.$$

From the exact relation

$$\frac{d\mathcal{T}}{d\Sigma} = -1 - \tilde{G}\mathcal{T} - \mathcal{T}\tilde{G}$$

we find by averaging

$$\frac{d\langle \mathcal{T} \rangle_x}{d\Sigma} = -1.$$

$$2\frac{d\tilde{G}_{ii}}{d\Sigma}\frac{d\Sigma}{d|x_{min}|}=2(\tilde{G}^2)_{ii}\frac{d\Sigma}{d|x_{min}|}=2(\tilde{G}^2)_{ii}\frac{\partial\langle\mathcal{T}_i^{(1)}\rangle}{\partial|x_{min}|}=$$

$$=(\tilde{G}^2)_{ii}\frac{\partial}{\partial x_i}(\mathcal{T}_i^{(1)}(x_i)+\mathcal{T}_i^{(1)}(-x_i))|_{x_i=|x_{min}|}\quad, \tag{44}$$

showing the equivalence of (38) with (39).

Returning to the integral in (30) we get (a factor 2 comes from the existence of two minima at $x_i=\pm|x_{min}|$)

$$\int_{-\infty}^{\infty}\sqrt{\frac{\beta}{\pi}}\,dx_i\;e^{-\beta\Omega_i(x_i)}=2e^{-\beta\Omega_i(|x_{min}|)}\sqrt{\frac{2}{\Omega_i''(|x_{min}|)}}=$$

$$=\exp\{-\beta[\Omega_i(|x_{min}|)+\frac{1}{\beta}\ln\sqrt{\Omega_i''(|x_{min}|)/8}]\}\approx \tag{45}$$

$$\approx e^{-\beta\Omega_i(|x_{min}|)}\quad,$$

or

$$\Omega=N\,\Omega_i(|x_{min}|), \tag{46}$$

where $\Omega_i(|x_{min}|)$ and $|x_{min}|$ are given by (37) and (39), respectively. (Compare also Cyrot /3/ and Kimball and Schrieffer /4/).

On using this approximation we loose the temperature dependence of the transition (e.g. the spin disorder entropy of the localized moments connected with the factor 2 coming from the two minima). This temperature dependence is essential for the determination of the ordering of the phases (AI, PM, PI) along the temperature axis.

5. Approximative Treatment of the CPA Condition

The unperturbed band given by $\tilde{\epsilon}_{\vec{k}}$ has its centre of gravity at $\omega=0$ (see (14)).Specializing to a parabolic density of states $\rho^{(0)}$ (compare Hubbard /8/)

$$\rho^{(0)}(\omega)=\begin{cases}\frac{4N}{\pi\Delta^2}\sqrt{\Delta^2-\omega^2}\,, & |\omega|\le\Delta\,,\\ 0 & |\omega|>\Delta\,,\end{cases} \tag{47}$$

we obtain for the unperturbed Green function $G_{ij}^{(0)}$ the quadratic equation

$$\omega - \frac{\Delta^2}{I} G_{ii}^{(0)} + \frac{I}{G_{ii}^{(0)}} . \tag{48}$$

For the retarded Green function $(G^{(0)}(\omega + i\epsilon))$ the solution of (48) with negative imaginary part has to be used (note (18)). By means of (21) we get

$$\omega - \Sigma(\omega) = \frac{\Delta^2}{I} \tilde{G}_{ii} + \frac{I}{\tilde{G}_{ii}} \tag{49}$$

It is convenient to use $\tilde{G}$ in the calculations and to eliminate Σ with the help of (49). Thus we obtain for the $\mathcal{T}^{(1)}$-matrix (Eq. (23))

$$\mathcal{T}_{i\sigma}^{(1)}(\omega, x_i) = -\frac{I}{(\tilde{G}_{ii}(\omega))^2} \left\{ \tilde{G}_{ii}(\omega) + \frac{I}{v_{i\sigma} - \omega + \frac{\Delta^2}{I} \tilde{G}_{ii}(\omega)} \right\} , \tag{50}$$

so that the CPA condition (28) is transformed into

$$\tilde{G}_{ii}(\omega) + \left(\frac{I}{N}\right) \sum_{-\infty}^{\infty} \frac{\beta}{\pi} dx_i \, e^{-\beta\Omega_i(x_i)} \frac{I}{v_{i\sigma} - \omega + \frac{\Delta^2}{I} \tilde{G}_{ii}(\omega)} = 0. \tag{51}$$

In the stationary point approximation Eq. (51) reduces to

$$2\tilde{G}_{ii}(\omega) + \frac{I}{\sqrt{U}\,|x_{min}| - \omega + \frac{\Delta^2}{I} \tilde{G}_{ii}} + \frac{I}{-\sqrt{U}\,|x_{min}| - \omega + \frac{\Delta^2}{I} \tilde{G}_{ii}} = 0. \tag{52}$$

Eq. (52) is the version for our problem of the cubic equation given by Velicky et al. [12]. It is convenient to rewrite (52) as

$$\tilde{G}_{ii}(\omega) = \frac{I}{2}(\Gamma_1(\omega) + \Gamma_2(\omega)) . \tag{53}$$

$$\omega - \sqrt{U}\,|x_{min}| - \frac{\Delta^2}{8}(\Gamma_1 + \Gamma_2) = \frac{I}{\Gamma_1} , \tag{54}$$

$$\omega + \sqrt{U}\,|x_{min}| - \frac{\Delta^2}{8}(\Gamma_1 + \Gamma_2) = \frac{1}{\Gamma_2}. \tag{55}$$

We restrict our considerations here to an approximate solution of (54,55), which exhibits the qualitative behaviour of the exact solution of the cubic equation. We neglect in (54,55) the coupling of $\Gamma_{1,2}$ by substituting $\Gamma_1 + \Gamma_2 \to a\Gamma_1$, $\Gamma_1 + \Gamma_2 \to a\Gamma_2$ in (54,55) respectively:

$$\omega - \sqrt{U}\,|x_{min}| = \frac{\tilde{\Delta}^2}{4}\Gamma_1 + \frac{1}{\Gamma_1}, \tag{56}$$

$$\omega + \sqrt{U}\,|x_{min}| = \frac{\tilde{\Delta}^2}{4}\Gamma_2 + \frac{1}{\Gamma_2}. \tag{57}$$

In this approximation $\tilde{G}_{ii}(\omega)$ is the sum of two shifted unperturbed Green functions (compare (48)), each belonging to a subband of width $\tilde{\Delta} = \Delta\sqrt{a/2}$. The number of states in each subband is equal to 1 per lattice site. A gap g in the density of states $\rho(\omega)$ is obtained for $\frac{g}{2} = \sqrt{U}\,|x_{min}| - \Delta > 0$. The parameter a can be fitted to give the best approximation to the exact solution; $a \approx \frac{1}{2} \div 1$. For $a = 1/2$ the gap in the density of states appears at $\sqrt{U}\,|x_{min}| - \frac{\Delta}{2} = 0$, what coincides with the behaviour of the exact solution.

The imaginary parts of the solutions of Eq. (56,57) are

$$-\frac{1}{\pi} Im\,\Gamma_{1,2}(\omega) = \frac{2}{\pi\tilde{\Delta}^2} \sqrt{\tilde{\Delta}^2 - (\omega \mp \sqrt{U}\,|x_{min}|)^2} \tag{58}$$

for ω-values leading to positive radicand (see. Fig. 1).

The appearance of the gap in the density of states may be due to the stationary point approximation. If the integration over x in (51) is performed exactly we expect instead of the gap a minimum in the density of states.

6. The Lifshiz Instability

The Lifshiz instability occurs because of a violation of the thermodynamical stability condition for the total compressibility

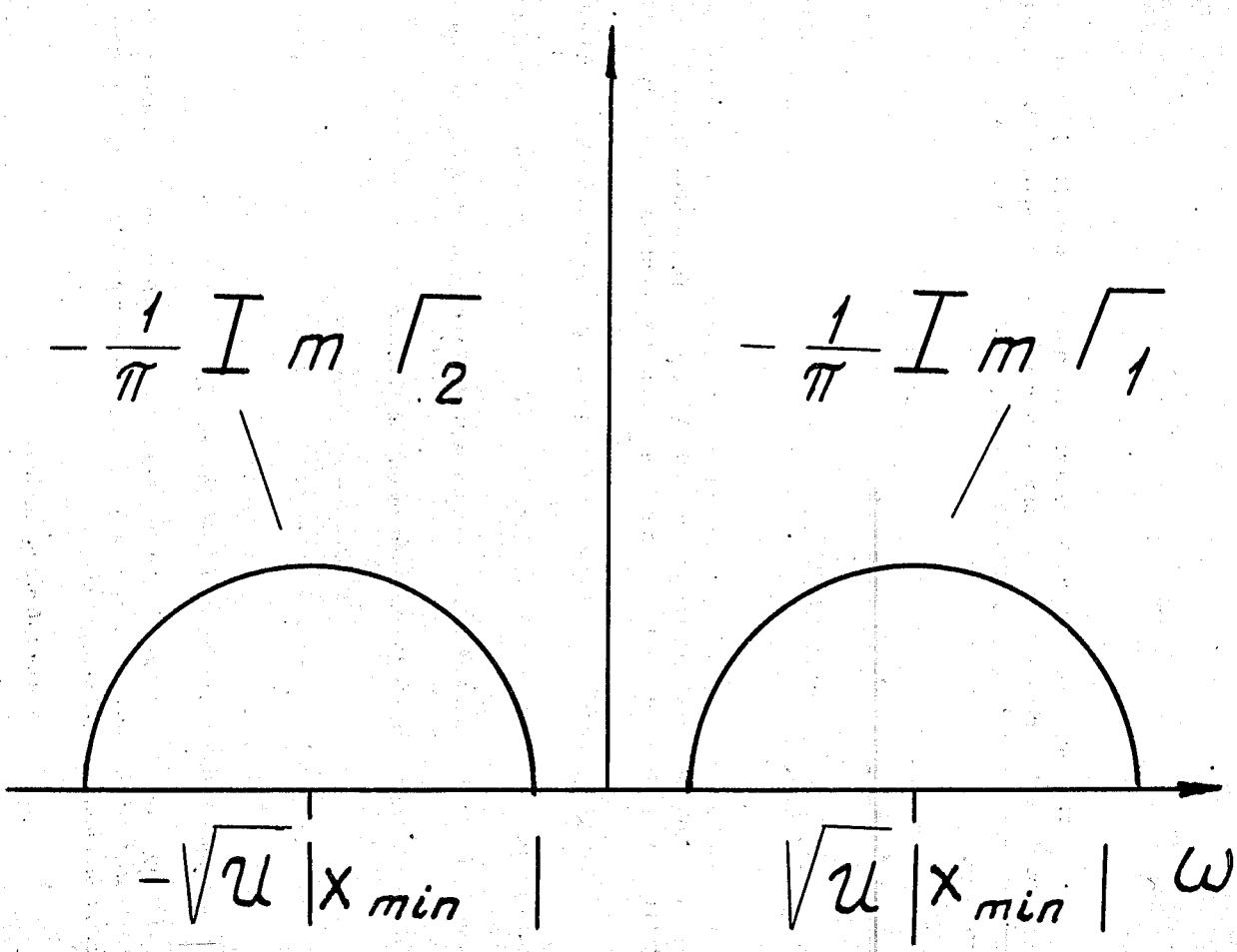

Fig. 1. Density of states with gap.

$$\left(-\frac{\partial^2 F_{tot}}{\partial V^2}\right)_T = \left(\frac{\partial p}{\partial V}\right)_T < 0. \tag{59}$$

F_{tot} is the total free energy of the system. Such a behaviour of the free energy is well known from the case of the van der Waals gas.

We first calculate the Gibbs potential Ω (Eq. (46)) in the limit $\beta \to \infty$. From (37, 53) we get

$$\begin{aligned}
\Omega &= N\Omega_i(|x_{min}|) = \\
&= -\frac{NU}{4} + N x_{min}^2 + \frac{2N}{\pi\beta}\int_{-\infty}^{\infty} d\omega \ln\left[1+e^{-\beta\omega}\right] Im\,\tilde{G}_{ii}(\omega) = \\
&= -\frac{NU}{4} + N x_{min}^2 - \frac{2N}{\pi}\int_{-\infty}^{0} d\omega\ \omega\, Im\,\tilde{G}_{ii}(\omega) = \\
&= -\frac{NU}{4} + N x_{min}^2 + N\int_{-\infty}^{0} d\omega\ \omega\left[-\frac{1}{\pi} Im\left(\Gamma_1(\omega)+\Gamma_2(\omega)\right)\right].
\end{aligned} \tag{60}$$

Substitution of $Im\Gamma_{1,2}$ from (58) leads to

$$\Omega = -\frac{NU}{4} + N x_{min}^2 - N\sqrt{U}|x_{min}|, \quad \text{with gap,} \quad \sqrt{U}\,|x_{min}| > \tilde{\Delta}\ ; \tag{61}$$

$$\begin{aligned}
\Omega = &-\frac{NU}{4} + N x_{min}^2 - N\sqrt{U}|x_{min}| - \\
&-\frac{4N}{\pi\tilde{\Delta}^2}\int_{\sqrt{U}|x_{min}|}^{\tilde{\Delta}} d\xi\left(\xi-\sqrt{U}\,|x_{min}|\right)\sqrt{\tilde{\Delta}^2-\xi^2}, \quad \text{without gap,} \quad \sqrt{U}\,|x_{min}| \le \tilde{\Delta}.
\end{aligned} \tag{62}$$

For small negative gap we obtain for (62)

$$\Omega = -\frac{NU}{4} + N|x_{min}| - N\sqrt{U}|x_{min}| - \frac{16\sqrt{2}N}{15\pi\tilde{\Delta}^{3/2}}\left(\tilde{\Delta}-\sqrt{U}|x_{min}|\right)^{5/2}, \quad \text{without gap.} \tag{63}$$

After determination of $|x_{min}|$ by means of (39) the final result for the Gibbs potential is

$$\Omega = -\frac{NU}{2}, \qquad \text{with gap,} \quad g = U - 2\tilde{\Delta} > 0; \tag{64}$$

and (after iteration)

$$\Omega = -\frac{NU}{2} - \frac{16\sqrt{2}\,N}{15\pi\tilde{\Delta}^{3/2}}\left(\Lambda - \frac{U}{2}\right)^{5/2} \qquad \text{without gap,} \quad g = U - 2\tilde{\Delta} \leq 0. \tag{65}$$

As we already remarked in the introduction the physical situations in the case considered by Lifshiz and in our case are similar. In our approximation even the formulae for Ω are the same in both cases (compare /2/).

Ω in (64,65) is the electronic part of the Gibbs potential. We go over to the total free energy F_{tot} by adding μN and the free energy of the lattice F_L :

$$F_{tot} = \Omega + \mu N + F_L \,. \tag{66}$$

We now consider the dependence of the free energy on the volume V, which can be changed by external pressure. The model parameter U can be considered as independent of V , but the model parameter Λ (half of the unperturbed band width) increases with decreasing V. The gap will approach zero at $\tilde{\Lambda}_0$,

$$\frac{U}{2} - \tilde{\Delta}_0 = 0, \tag{67}$$

and we can expand

$$\frac{U}{2} - \tilde{\Delta} = \frac{a}{N}(V - V_0), \qquad a > 0. \tag{68}$$

We assume that only Ω shows an anomalous behaviour at the point V_0, where the gap disappears, and that the other two terms in (66) can be expanded in the vicinity of V_0. Thus we obtain for the total compressibility

$$\left(\frac{\partial p}{\partial V}\right) =$$

$$= \begin{cases} -\frac{\kappa_0}{N} + \frac{\kappa_1}{N^2}(V - V_0) & \text{for} \quad V > V_0 ; \quad (69) \\ \frac{4\sqrt{2}\,a^{5/2}}{\pi(\tilde{\Delta}_0 N)^{3/2}}(V_0 - V)^{1/2} - \frac{\kappa_0}{N} + \frac{\kappa_1}{N^2}(V - V_0), & \text{for} \quad V < V_0 . \quad (70) \end{cases}$$

$(\kappa_0, \kappa_1 > 0)$. The first term in (70) comes from (65), the other terms come from the expansion of the regular part of the total free energy.

An unstable region $\left(\left(\frac{\partial p}{\partial V}\right)_T > 0\right)$ exists, if

$$\frac{2\sqrt{2}\,a^{5/2}}{\pi\,\tilde{\Delta}_0^{3/2}} > \sqrt{\kappa_0\,\kappa_1} . \quad (71)$$

Such an unstable region leads to a first order transition. At constant pressure the volume jumps from a value V_1 (at the right of the unstable region) to a volume V_2 (at the left of the unstable region). The line $p = \text{const}$ and the volumes $V_{1,2}$ are given by Maxwell's rule of equal areas in the p, V diagram.

A more accurate numerical treatment of the self-consistent system of equations is in preparation. The unstable region resulting from an improved evaluation of the x -integrals, the CPA condition and the corrections for $T \neq 0$ are expected to be smaller than that given by (71). Above the critical point or in cases, where no first order transition line (no unstable region) exists, anomalies similar to the anomalies in the transitions of order 2 1/2(compare Lifshiz[12]) may occur.

Acknowledgements

The author would like to thank Prof. J.R.Schrieffer, Prof. J.B.Goodenough, Dr.J.Czerwonko, Dr. W.Kolley and Dr. T.Siklos for many valuable discussions. In addition he is grateful to Prof. J.R.Schrieffer and Dr. M.Cyrot for making him available preprints of their work.

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Received by Publishing Department
on August 1, 1972.