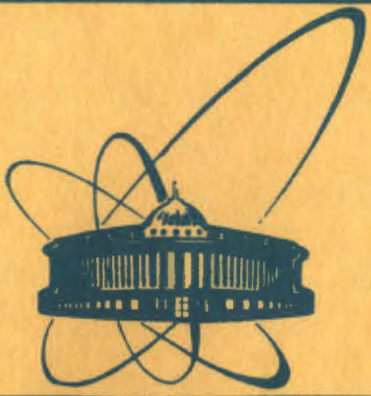

сообщения
объединенного
института
ядерных
исследований
дубна

E17-83-425

U.Lindner*, W.Schumacher

TO MAGNETIC SOLUTIONS OF THE HUBBARD MODEL

*Sektion Physik, Karl-Marx-Universitat, DDR

1983

1. INTRODUCTION

Several years ago in 1977 we investigated magnetic solutions of the Hubbard model using Hartree-Fock approximation[1]. Among others we found the surprizing result that for the antiferromagnetic case for nearest-neighbour overlap and simple cubic lattice the so-called heat magnetization can occur. The Hubbard model in Wannier representation is given by

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 - \mu N \qquad (1)$$

$$= \sum_{i \neq j \sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} + \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} - \mu \sum_{i\sigma} n_{i\sigma} ,$$

$\mathcal{H}_0 = \sum_{i \neq j, \sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} n_{\vec{k}\sigma}$ describes an s band

where $t_{ij} = \begin{cases} t & \text{if i and j are nearest neighbour lattice sites,} \\ 0 & \text{otherwise;} \end{cases}$

and

$$\epsilon_{\vec{k}} = 2t(\cos k_x a + \cos k_y a + \cos k_z a)$$

for s.c.l. (band width $W = 12\ t$).

$$\mathcal{H}_1 = \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}$$

is the Coulomb or correlation term, where U represents the repulsion energy between electrons with spin σ and $-\sigma$ at the i-th lattice place. $N = \sum_{i\sigma} n_{i\sigma}$ is the total number operator of electrons and μ denotes the chemical potential. If we want to include an external magnetic field, then instead of t_{ij} we use $t_{ij} - \theta_{ij}\ \sigma h(\vec{R}_i)$, where $h(\vec{R}_i)$ represents the z-component of this field (in energy units) at lattice point i characterized by position vector $\vec{R}_i$.

The fact that this Hamiltonian (1) in Hartree-Fock approximation (HFA) for the antiferromagnetic case for certain parameter combinations admits heat magnetization is demonstated by the following figures[1]. Fig.1 shows the temperature depen-

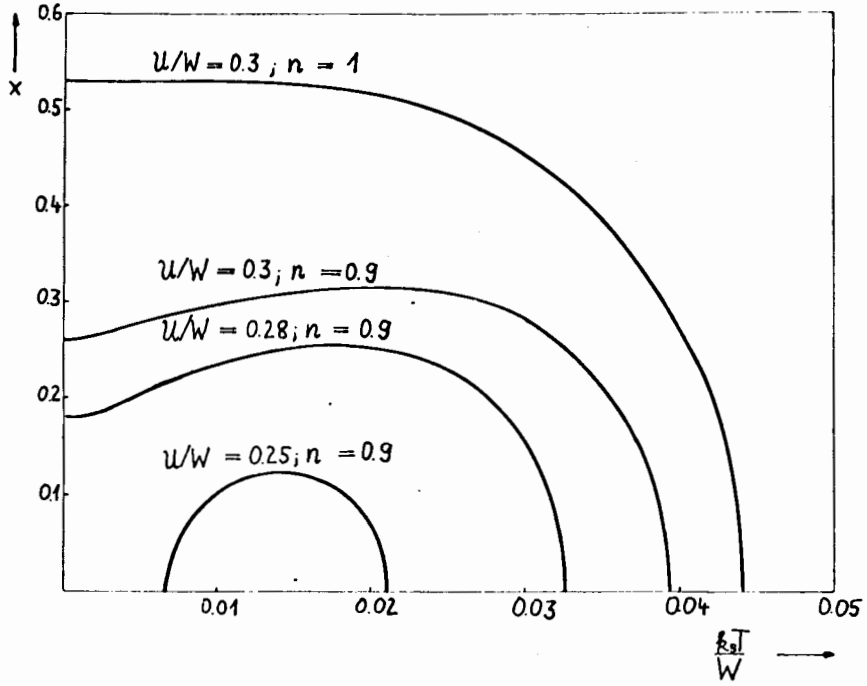

Fig.1. Order parameter x of the afm phase versus temperature T (in units of k_B/W) in HFA for different values of the ratio of correlation energy U to band width W and of the mean occupation number n.(1) U/W = 0,3, n = 1; (2) 0.3, 0.9; (3) 0.28, 0.9; (4) 0.25, 0.9.

dence of the order parameter x. It is to see that for non-half-filled band ($n \neq 1$) and certain values of the ratio of correlation energy U to band width W magnetic ordering ($x \neq 0$) can appear in a finite temperature region even if for the temperature T = 0 no magnetic order exists. This phenomenon is known under the notation heat magnetization. The region where this effect occurs is characterized by double solutions of the Neel temperature T_N (comp. Fig.2). The temperature dependence of the reciprocal static zero-field susceptibility $\chi^{-1}(\vec{q} = \vec{g}/2)$ for the same parameter values like in fig.1 is plotted in fig.3. (μ_B denotes the Bohr magneton and $\vec{g}$ is a vector of the reciprocal lattice). In the region in which $x \neq 0$ it follows $\chi(\vec{q} = \vec{g}/2) < 0$, i.e., the paramagnetic (pm) phase is unstable as against the antiferromagnetic (afm) phase. (We remark that for this parameter range no ferromagnetic phase exists). Figure 4 represents the difference of the free energy per lattice point of pm and afm phases versus the

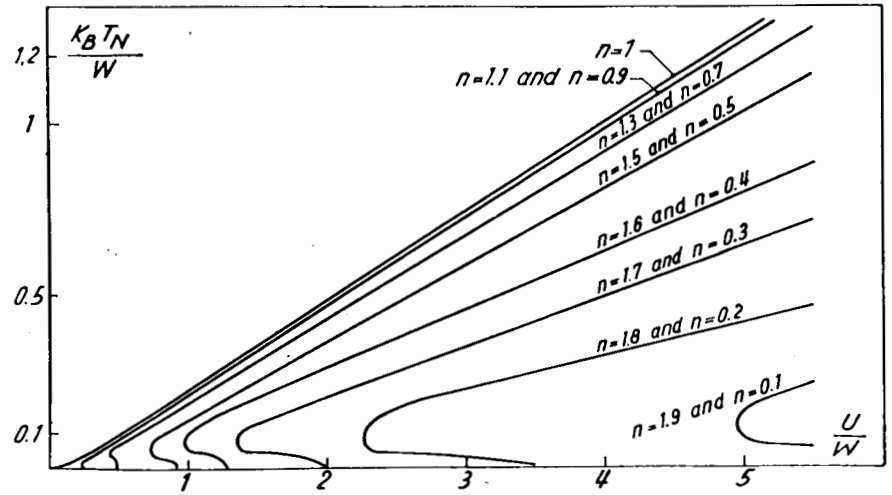

Fig.2. Neel temperature T_N (in units of k_B/W) in HFA as a function of U/W for different values of n. (1) n = 1; (2) 1.1 and 0.9; (3) 1.3 and 0.7; (4) 1.5) and 0.5; (5) 1.6 and 0.4; (6) 1.7 and 0.3; (7) 1.8 and 0.2; (8) 1.9 and 0.1.

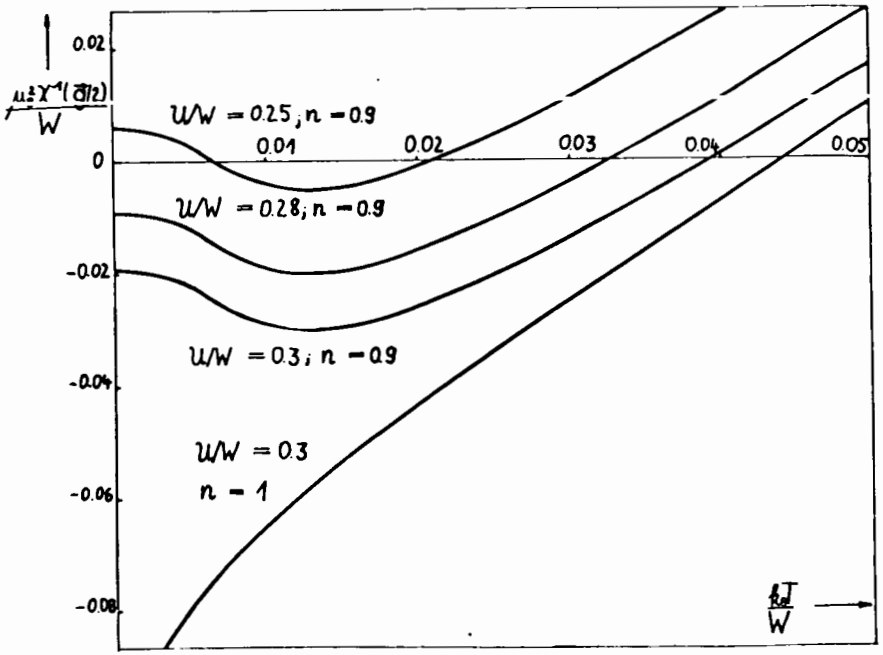

Fig.3. Zero-field susceptibility $\mu_B^2 \chi^{-1}(|\vec{g}/2|)/W$ in HFA as a function of $\frac{k_B T}{W}$ for the same parameters as in fig.1.

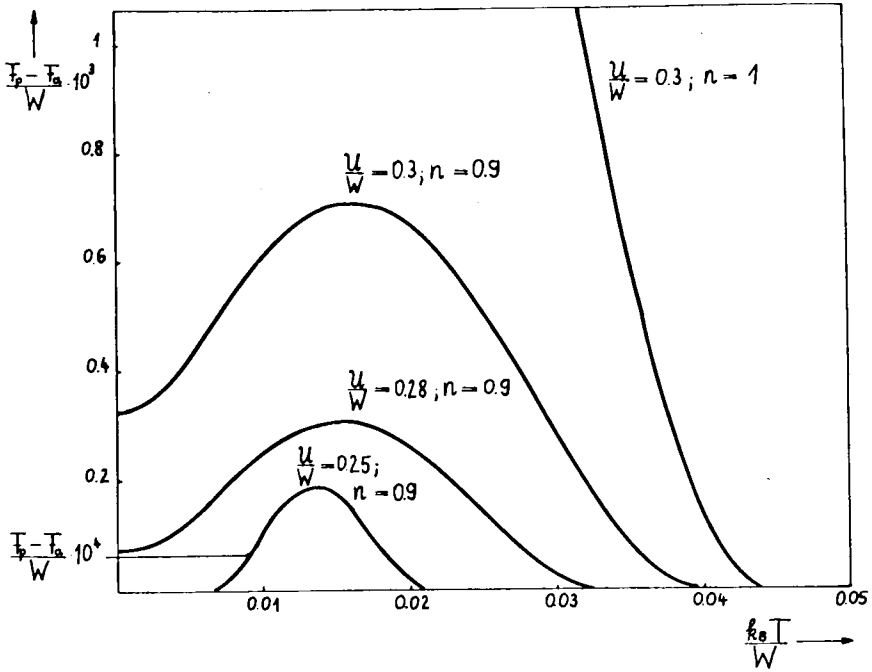

Fig.4. Difference of the free energy per lattice point of pm and afm phase in HFA versus temperature T (in unit of k_B/W) for the same parameters as in fig.1.

the temperature T for the same parameters as fig.1. One sees that the free energy of the afm solution is always less than that of the pm solution, i.e., the afm phase is stable, and furthermore, that no first order phase transition exists. The question which we want to answer here is the following: Is it possible to observe this effect of afm heat magnetization or

(i) is the heat magnetization destroyed by other exited states with much lower energy or,

(ii) is the heat magnetization an effect of the used HFA?

In order to answer these questions we investigate in section 2 the possibility of the existence of further magnetic solutions in the framework of HFA and in section 3, we consider another approximation (the so-called unified theory) using the functional integral formalism to take into account spin functions.

2. HARTREE-FOCK APPROXIMATION

That which one does if one uses HFA is a linearization of the interaction term

$$\mathcal{H}_1 = \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \Rightarrow U \sum_{i\sigma} \langle n_{i-\sigma} \rangle n_{i\sigma} - \frac{1}{2} U \sum_{i\sigma} \langle n_{i\sigma} \rangle \langle n_{i-\sigma} \rangle \quad (2)$$

$$= \sum_{i\sigma} \epsilon_{i\sigma} n_{i\sigma} - \frac{1}{2} U \sum_{i\sigma} \langle n_{i\sigma} \rangle \langle n_{i-\sigma} \rangle$$

with $\epsilon_{i\sigma} = \frac{1}{2} U (n_i - \sigma m_i)$, this means exchange field $\frac{1}{2} U m_i$ is postulated. $n_i = \langle n_{i\uparrow} + n_{i\downarrow} \rangle$ is the mean occupation number of electrons at the lattice point i and $m_i = \langle n_{i\uparrow} - n_{i\downarrow} \rangle$ is proportional to the z-component of the magnetization at i. If we restrict ourselves to long range order, then in the so-called itinerant picture we can put

$$n_i = n \quad \text{and} \quad m_i = m e^{i\vec{q}\vec{R}_i} . \quad (3a)$$

Magnetic effects are introduced ad hoc. For $\vec{q} = 0$, $m \neq 0$ we obtain ferromagnetism; for $\vec{q} = \vec{g}/2 \equiv \vec{Q}$, $m \equiv x \neq 0$, antiferromagnetism; and for $m = 0$, paramagnetism. From (3a) it is clear, if we look for further magnetic solutions, we have to investigate m_i for arbitrary $\vec{q}$ (commensurable and incommensurable modulated phases).

In the so-called localized picture one assumes (see, e.g. /2/) instead of (3a)

$$n_i = n \quad \text{and} \quad m_i = \pm m. \quad (3b)$$

Then $\epsilon_{i\sigma}$ is considered as random variable and the lattice is divided in A and B sites with $\epsilon^A_\uparrow = \frac{1}{2}(n - m) = \epsilon^B_\downarrow$, and $\epsilon^B_\uparrow = \frac{1}{2} U (n + m) = \epsilon^A_\downarrow$. If one uses for the probability P that an A-site has a B-site as nearest neighbour $P = 0$, then it yields for $m \neq 0$ ferromagnetism, for $P = 1$ and $m \neq 0$ antiferromagnetism, and for $m = 0$ paramagnetism. For describing the modulated phases the localized picture is not favourable but it is possible to describe with this picture the magnetic short range order. We restrict ourselves to long range order.

Summarizing one can give the following interpretation (3) for the HFA: It is postulated the existence of an exchange field which leads to different band structures for the up and down spin electrons and which is itself generated by the

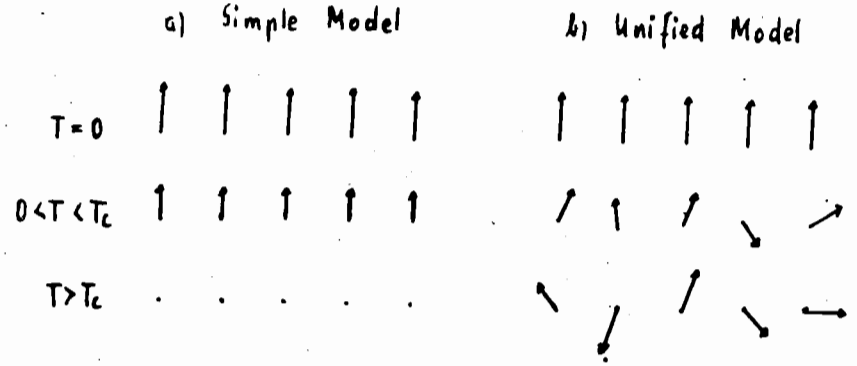

Fig.5. Exchange field configurations for the fm case in (a) simple model, e.g., HFA and (b) unified model.

resulting differences in up and down spin electron occupation numbers. In the fm case, e.g., (comp. fig.5a) the field is the same at all atoms. It has the maximal amount for $T = 0$, decreases for increasing temperatures, and becomes zero at the critical temperature T_c and above T_c. The exchange field corresponds to the spin ordering, i.e., to the order parameter. Because of (2) one believes that HFA is reasonable, if at all, for $\frac{U}{W} \ll 1$, only. Charge and spin fluctuations are not included because of assumption (3a).

In the case of arbitrary $\vec{q}$ we calculate the isothermal static zero-field susceptibility

$$\chi(\vec{q}) = \frac{\partial M(\vec{q})}{\partial h}\Big|_{h=0}, \tag{4}$$

where

$$M(\vec{q}) = \frac{1}{N}\sum_i M(\vec{R}_i)\, e^{i\vec{q}\vec{R}_i} = \frac{1}{N}\sum_{\vec{k}\sigma} \sigma \langle c^+_{\vec{k}+\vec{q},\sigma} c_{\vec{k}\sigma}\rangle , \tag{5}$$

and

$$\vec{h} = (0, 0, h(\vec{R}_i)) \qquad \text{with} \quad h(\vec{R}_i) = h e^{i\vec{q}\vec{R}_i}$$

denotes the external field in the pm phase. (The exchange field has the same structure; $m_i = M(\vec{R}_i)\, e^{i\vec{q}\vec{R}_i}$). We obtain

$$\chi(\vec{q}) = \frac{2\chi_0(\vec{q})}{1 - 2U\chi_0(\vec{q})}$$

and

$$\chi_0(\vec{q}) = -\frac{1}{2N}\sum_{\vec{k}} \frac{1}{(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}})} \{f(E_{\vec{k}+\vec{q}}, T) - f(E_{\vec{k}}, T)\} > 0, \tag{6}$$

where $f(E, T) = [\exp\{\frac{E}{k_B T}\} + 1]^{-1}$ is the Fermi function and $E_{\vec{k}+\vec{q}} = \frac{1}{2}Un - \mu + \epsilon_{\vec{k}+\vec{q}}$.

If $\chi(\vec{q})^{-1} \leq 0$, the pm phase is unstable and goes over to a phase modulated by $\vec{q}$ ($\vec{q}$ phase). For given parameter n, $\frac{U}{W}$, and $\vec{q}$ the transition temperature T_c and the chemical potential μ follow from (6) and (3):

$$\frac{1}{2U} = \chi_0(\vec{q}; T_c), \tag{7}$$

$$n = \frac{2}{N}\sum_{\vec{k}} f(E_{\vec{k}}, T_c).$$

At $T = 0$, i.e., in the ground state, from (7) one gets the results of Penn (4). For fixed values of n and U/W it yields the critical $\vec{q}$ vector and if n and $\vec{q}$ are fixed, then (7) gives the critical ratio U/W above of which the pm phase does not exist. For a half-filled band ($n = 1$) one obtains antiferromagnetism for each ratio U/W. For non-half-filled bands ($n \neq 1$) the pm phase goes over to a modulated phase which with increasing $n (n < 1)$ or increasing U/W goes over to afm of fm phase. Figure 6 shows these results. The model (1) possesses electron-hole symmetry therefore the picture is symmetrical relative to $n = 1$. The upper part of the picture represents the critical values U/W, at which the pm phase goes over to the modulated phase, as function of n and the lower part represents the $\vec{q}$ vector which belongs to that modulated phase. For $0.42 \leq n \leq 1$ the $\vec{q}$ vector is of the type $\vec{q} = \frac{\pi}{a}(1,1,\xi)$; for $0,14 \leq n \leq 0,42$, of the type $\vec{q} = \frac{\pi}{a}(1, \xi, 0)$ and for $0 \leq n \leq 0.14$ we have $\vec{q} = \frac{\pi}{a}(\xi, 0, 0)$ with $0 \leq \xi \leq 1$.

In the range in which we found double solutions for T_N the transition does not occur from pm to afm phase with $\vec{Q} = \frac{\pi}{a}(1,1,1)$ immediately but at first to modulated phases with $\vec{q} = \frac{\pi}{a}(1,1,\xi)$ or $\vec{q} = \frac{\pi}{a}(1, \eta, 0)$ where $0 \leq \xi, \eta \leq 1$ (incommensurable phases mostly) such that the existence of double solutions of T_N is related with the existence of incommensurable phases.

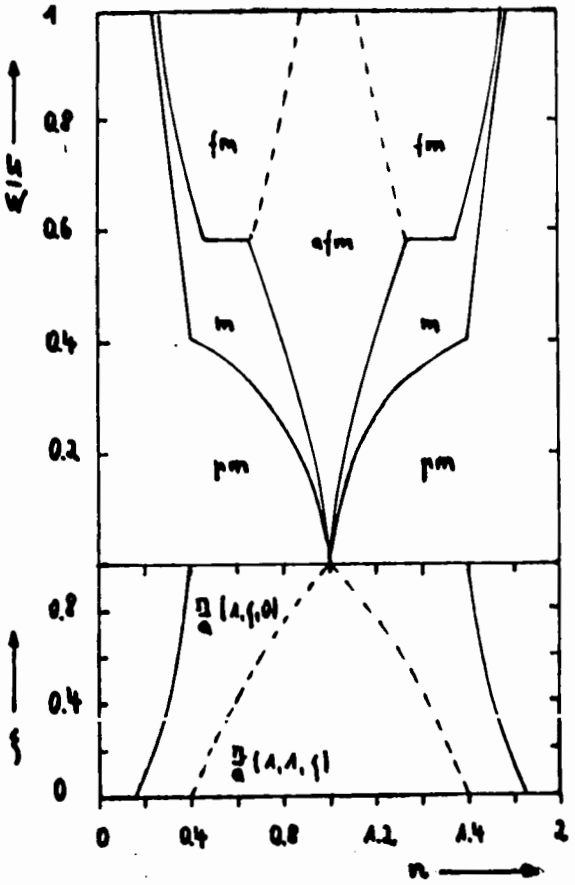

Fig.6. Phase diagram for the pm, fm, and afm phase in HFA at T = 0. At the boundary to the with m denoted region the pm phase (for certain $\frac{U}{W}$ and n) is unstable and goes over to a $\vec{q}$ phase. The lower part of fig.6 represents the critical $\vec{q}$ vector as function of n. Solid lines indicate second-order phase transitions, dashed lines indicate first-order phase transitions.

Thus, we have found the answer to our question (i): It is necessary to consider modulated phases and to discuss the temperature dependence of every $M(\vec{q})$ ($M(\vec{Q}) \hat{=} x$). Unfortunately the free energy F in HFA can be calculated without further approximation for the fm case ($\vec{q} = 0$) and the afm case ($\vec{q} = \vec{Q} = \frac{\vec{g}}{2}$) only thus that the temperature behaviour and the region of stability (phase diagram) of modulated phases is an open problem yet.

Since, on the other, hand, it is known that the values for the transition temperatures calculated in the framework of itinerant electron theory, e.g., HFA (without modulated phases), are too large compared with the observed Curie temperature T_c for iron or the Neel temperature T_N for nickel [5], one must conclude from this fact, too, that it is necessary to regard other excited states which are capable of reducing the magnetic order. These excited states might be, beside the spinwave-like collective modes ($\vec{q}$ phases) which we have considered till now, states in which the atomic moments are no longer oriented parallel to each other. In order to take into consideration such states we have to extent the approximation. We use the so-called unified theory and we have now to answer our question (ii).

3. UNIFIED THEORY

The extension of our physical picture is represented for the ferromagnetic case in fig.5b. In the ground state, at T = 0 we have the same situation like before (comp. fig.5a), in the language of the itinerant picture - the exchange field is the same at all atoms or in the language of localized picture - all spins are parallel directed. Because the exchange field at an atom depends on the spin of this atom, the exchange field is a vector quantity (in spin space) and it must not be parallel at all lattice points but it can vary in direction and strength from atom to atom if the temperature T increases. Then above T_c the exchange field may not vanish, but it has to be merely randomized in direction and strength producing a total zero magnetization, this means in the language of localized picture, we admit localized moments above T_c.

This unified model contains the simple model which we have considered before (comp. fig.5a) as a special case. In the language of itinerant picture now we can say, we have to investigate electrons which move from atom to atom under influence of different exchange fields or under influence of a stochastic potential, and in the language of localized model, we have to regard different exchange field configurations which correspond to spin configurations, e.g., like in Heisenberg model, but more general because they can vary in direction and magnitude. To describe such a physical picture one can use the functional integral formalism. The basic mathematical formulation was provided by Schrieffer et al. [6] and Cyrot [7]. One writes the grand partition function

$$Z = \mathrm{sp}\{e^{-\beta \mathcal{H}}\} = e^{-\beta \Omega} \tag{8}$$

in a functional integral over classical fields using time order in τ on $(0, \beta)$,

$$\exp\{-\beta(A+B)\} = \exp_\tau\{-\int_0^\beta d\tau\,(A(\tau)+B(\tau))\} \tag{9}$$

for $[A, B] \neq 0$ and the Hubbard-Stratonovitch transformation

$$e^{A^2} = \frac{1}{\sqrt{2\pi}} \int e^{-v_A^2/2 + \sqrt{2} A v_A} dv_A, \tag{10}$$

where A is any bounded operator and v_A a classical field, to transform the two body interaction term $\mathcal{H}_1 = \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}$

in favour of single-particle couplings with classical fields. There are several possibilities to write the interaction term in a quadratic form

$$\mathcal{H}_1 = U \sum_i n_{i\uparrow} n_{i\downarrow} = \frac{1}{2} U \sum_i \hat{n}_i - 2U \sum_i (S_i^z)^2 \quad , \tag{11a}$$

$$= \frac{1}{4} U \sum_i \hat{n}_i^2 - U \sum_i (S_i^z)^2 \quad , \tag{11b}$$

$$= \frac{1}{4} U \sum_i \hat{n}_i^2 - \frac{1}{3} U \sum_i (\vec{S}_i)^2 \quad , \tag{11c}$$

$$= \frac{1}{4} U \sum_i \hat{n}_i^2 - U \sum_i (\vec{e}_i \vec{S}_i)^2 \tag{11d}$$

with $\hat{n}_i = n_{i\downarrow} + n_{i\uparrow}$ and $S_i^z = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$. $\vec{S}_i$ is the total spin of the i-th atom, $\vec{e}_i$ denotes an arbitrary unit vector and one can restore the rotational symmetry by averaging the partition function over all directions of each $\vec{e}_i$.

If we could evaluate the functional integral exactly, then each expression of (11) would give the same result, because an exact evaluation is not possible, the results depend on the writing of interaction term. This is a fundamental ambiguity of the method. Following Moriya and Hasegawa (8) we use the expression (11d), which gives the correct Hartree-Fock equations for the problem at $T = 0$ according to our physical picture and thus admits to compare with the results of the section 2. We make use of the static approximation in which the time fluctuating part of the fields $v_A(r)$ is neglected and functional integral can be written as an ordinary integral. In the notation of Moriya and Hasegawa (MH) we obtain:

$$\Omega = \Omega_0 + \Delta\Omega \tag{12}$$

with

$$e^{-\beta\Omega_0} = \mathrm{sp}\, \sup \{-\beta(\mathcal{H}_0 - \mu \mathcal{N})\}$$

and

$$e^{-\beta\Delta\Omega} = \int \prod_i d\vec{\xi}_i \, d\eta_i \, e^{-\beta\Psi[\vec{\xi},\eta]} \quad ,$$

where the field $\vec{\xi}_i = \xi_i \vec{e}_i$ corresponds to $\vec{S}_i$ and the field η_i to $\hat{n}_i$.

$\Psi[\vec{\xi},\eta]$ is the abreviation for

$$\Psi[\vec{\xi},\eta] = \Psi_0[\vec{\xi},\eta] + \Psi_1[\vec{\xi},\eta] \, , \tag{13}$$

where

$$\Psi_0[\vec{\xi},\eta] = \frac{\pi}{\beta} \sum_j \{(\vec{\xi}_j - \frac{1}{\bar{c}_1}\vec{h})^2 + \eta_j^2\} \tag{14}$$

includes all terms which are related with the first term in eq. (10) and

$$e^{-\beta\Psi_1[\vec{\xi},\eta]} = e^{-\beta\Omega_0} \mathrm{sp}\, \exp\{-\beta[\mathcal{H}_0 - \mu\mathcal{N} - \sum_i (2\bar{c}_1 \vec{\xi}_i \vec{S}_i + \bar{c}_2 \eta_i \hat{n}_i)]\} \tag{15}$$

describes the motion of electrons in a stochastic potential with $\bar{c}_1 = (\frac{\pi U}{\beta})^{1/2}$ and $\bar{c}_2 = (-\frac{\pi U}{\beta})^{1/2}$.

In a more formal way according to Evenson, Schrieffer and Wang /6/ one can write

$$\Psi_1[\vec{\xi},\eta] = -\frac{1}{\beta} \mathrm{sp}\{\ln[1 - gV]\} \, , \tag{16}$$

where $\mathrm{sp} \hat{=} \sum_{\sigma, \ell, n}$ and the matrices g and V are given by

$$g^{\sigma}_{jn,\, \ell n'} = \theta_{nn'} \theta_{\sigma\sigma'} \frac{1}{N} \sum_{\vec{k}} \frac{e^{i\vec{k}(\vec{R}_j - \vec{R}_i)}}{i\omega_n + \mu - \epsilon_{\vec{k}}} \, ,$$

$$V^{\sigma\,\sigma'}_{jn,\, \ell n-m} = \theta_{m0} \theta_{\sigma\sigma'} \theta_{j\ell} V_j$$

with $\omega_n = \frac{(2n+1)\pi}{\beta}$ (n integer) and $V_j = \bar{c}_1 \begin{pmatrix} \xi_j^z & \xi_j^- \\ \xi_j^+ & -\xi_j^z \end{pmatrix} + \bar{c}_2 \eta_j$, $\xi_j^{\pm} = \xi_j^x \pm i\xi_j^y$.

If $\Psi_1[\vec{\xi},\eta]$ is known, the problem is solved, this means, the grand partition function Z is known and we can calculate the static zero-field susceptibility $\chi(\vec{q})$ or the Neel temperature T_N.

The method of MH contains several important steps. Firstly, one introduces the Fourier transformed variables

$$\vec{\xi}_{\vec{q}} = \frac{1}{N} \sum_j \vec{\xi}_j e^{i\vec{q}\vec{R}_j} \quad , \quad \eta_{\vec{q}} = \frac{1}{N} \sum_j \eta_j e^{i\vec{q}\vec{R}_j} \quad . \tag{17}$$

The variable $\eta_{\vec{q}=0} \equiv \eta_0$ we can neglect since it is absorbed by the chemical potential μ. The quantity $\xi_{\vec{q}=0} \equiv \xi_0$ has a special meaning, it is the conjugate variable to the uniform magnetization. Secondary, one defines new variables related with the average squared local amplitudes of spin and charge density fluctuations and their cross term

$$x_\alpha = \frac{1}{N\beta} \sum_{\vec{q} \neq 0, \alpha} \xi_{\vec{q}\alpha}\, \xi_{-\vec{q}\alpha} = \frac{1}{N\beta} \left(\frac{1}{N} \sum_{j\alpha} \xi^2_{j\alpha} - \xi^2_{\vec{q}=0,\alpha} \right), \qquad (\alpha = x, y, z) \tag{18}$$

$$y = \frac{1}{N\beta} \sum_{\vec{q} \neq 0} \eta_{\vec{q}} \eta_{-\vec{q}} \qquad \text{and} \qquad z = \frac{i}{N\beta} \sum_{\vec{q} \neq 0} \xi_{\vec{q}z}\, \eta_{-\vec{q}}.$$

Thirdly, one makes for the functional $\Psi_1[\vec{\xi}, \eta]$ the following ansatz:

$$\Psi_1[\vec{\xi}, \eta] = \frac{\pi}{\beta} \sum_{\vec{q} \neq 0} \{ \sum_{\alpha} X^{\alpha}_{\vec{q}} \xi_{\vec{q}\alpha} \xi_{-\vec{q}\alpha} + 2iZ_{\vec{q}}\, \xi_{\vec{q}z}\, \eta_{-\vec{q}} + Y_{\vec{q}}\, \eta_{\vec{q}} \eta_{-\vec{q}} \} + \pi N L\, [\xi_{\vec{q}=0}, x_\alpha, y, z]. \tag{19}$$

$L, X^{\alpha}_{\vec{q}}, Y_{\vec{q}}$, and $Z_{\vec{q}}$ are functions of ξ_0, x_α, y, and z.

We restrict ourselves to pm, fm and simple afm solutions and solve the integral over ξ_0 (or $\xi_{\vec{q}=\vec{Q}}$) and x_α, y, z in saddle point approximation. The ansatz (19) was justified by MH [8] using coherent potential approximation (CPA). Ψ_1 is expanded as

$$\Psi_1 = \Psi_1^{(1)} + \Psi_1^{(2)} + \dots, \tag{20}$$

where $\Psi_1^{(n)}$ includes all terms which are related with n sites of the lattice. One takes terms up to $n = 2$, only. The local term $\Psi_1^{(1)}$ corresponds to $L[\xi_0, x_\alpha, y, z]$ and $\Psi_1^{(2)}$ gives the $\vec{q}$-dependent terms of $\Psi_1[\vec{\xi}, \eta]$, thus that the functions $L, X^{\alpha}_{\vec{q}}, Y_{\vec{q}}$, and $Z_{\vec{q}}$ are known.

We are interested in the pm phase only. In the pm phase all components x_α in (18) are equal to x and in (19) we can drop α and redefine $X_{\vec{q}}$. (The rotational symmetry of the problem is restored). The quantity x is a measure for the spin fluctuations. In order to simplify the numerical calculations for the Neel temperature T_N

(a) charge fluctuations are neglected, this means, $y = z = 0$, $Y_{\vec{q}} = Z_{\vec{q}} = 0$, and the static zero-field susceptibility $\chi(\vec{q})$ is a function of L and $X_{\vec{q}}$, where for the pair interaction coefficient in the pm phase it is valid

$$X_{\vec{q}} = \sum_i X_{0i}\, e^{i\vec{q}\vec{R}_i}. \tag{21}$$

(b) One restricts itself in (21) to the nearest neighbour overlap, too. It yields

$$X_{\vec{q}} = X_{00} + 2X_{01} (\cos q_x a + \cos q_y a + \cos q_z a) = X_{00} + 12 X_{01} \frac{\epsilon_{\vec{q}}}{W}. \tag{22}$$

(c) We use a semielliptical model density of states for the unperturbed band

$$\rho^\circ(\epsilon) = \frac{2}{\pi} \sqrt{1 - \epsilon^2}\, \Theta(|\epsilon| - 1) \tag{23}$$

instead of the density of states for s.c.l.

For $\vec{q} = \vec{Q} = \pi/a\,(1,1,1)$ we obtain from the instability of the pm susceptibility

$$\chi(\vec{Q}) \propto \frac{\bar{\chi}(\vec{Q})}{1 - 2U\bar{\chi}(\vec{Q})} \tag{24}$$

analogously to (7) a system of equations for the Neel temperature T_N and chemical potential μ, if the parameter n and $\frac{U}{W}$ are fixed

$$\frac{1}{2U} = \bar{\chi}(\vec{Q}; T) \tag{25a}$$

$$n = -\frac{2}{\pi} \int_{-1}^{1} d\epsilon\, f(\epsilon - \mu)\, \mathrm{Im} F(\epsilon + i0), \tag{25b}$$

where $f(\epsilon) = [\exp\{\frac{\epsilon}{k_B T_N}\} + 1]^{-1}$.

Instead of (25a) one can write

$$T_N = \frac{\pi}{3} x_c \frac{U(X_{\vec{Q}} - X_{\vec{q}=0})}{\langle (1 - r_{\vec{q}})^{-1} \rangle_{\vec{q}}} \tag{25c}$$

with

$$\langle A_{\vec{q}} \rangle_{\vec{q}} = \int_{-1}^{1} 3\rho^\circ(3r_{\vec{q}}) A_{\vec{q}} dr_{\vec{q}},$$

where

$$r_{\vec{q}} = \frac{X_{\vec{q}} - \frac{1}{2}(X_{\vec{q}=0} - X_{\vec{Q}})}{\frac{1}{2}(X_{\vec{q}=0} - X_{\vec{Q}})}$$

is a reduced dispersion relation of pair interaction. x_c characterizes the (critical) spin fluctuations at T_N.

$$X_{\vec{q}=0} = \int_{-\infty}^{\infty} d\epsilon \, \frac{1}{2\pi} f(\epsilon-\mu) \, \mathrm{Im}\{\frac{H - F^2}{[1+\Sigma F]^2}\} \tag{26}$$

and

$$X_{\vec{Q}} = \int_{-\infty}^{\infty} d\epsilon \, \frac{1}{2\pi} f(\epsilon-\mu) \, \mathrm{Im}\{[\frac{F}{z-\Sigma} - F^2] \cdot \frac{1}{[1+\Sigma F]^2}\} \tag{27}$$

are obtained from CPA calculations (comp. (20)). F denotes the site-diagonal part of the Green function

$$G = \frac{1}{g^{-1} - 2\bar{c}_1 \vec{\xi}_{\vec{q}=0} \vec{S}_{\vec{q}=0} - \Sigma} \tag{28}$$

which takes into account the random potential

$$H = \frac{\partial F}{\partial \Sigma} = \frac{F^2}{1 - \frac{1}{4}F^2} \quad \text{and} \quad \Sigma = z - \frac{1}{F(z)} - \frac{1}{4}F(z) \, . \tag{29}$$

For the numerical work[10], firstly, one calculates F from the CPA equation

$$\frac{1}{16}F^3 - \frac{1}{2}zF + (z^2 + \frac{1}{4} - b^2)F - z = 0 \tag{30}$$

with $F(z) < 0$ in dependence on $b^2 = U\pi x_c$, and secondly, one has to fulfill the equations (25b) and (25c) by an interaction procedure using (26), (27), and (29).

We remark that for $x = 0$, i.e. without spin fluctuations and therefore at temperature $T = 0$, it follows $\Sigma = 0$, and from (25a) and (25b) one obtains the Hartree-Fock equation like we have expected.

The results for the Neel temperature T_N for different values of the mean occupation number of electrons n as a function of $\frac{U}{W}$ are shown in fig. 7[9].

The broken lines represent the Neel temperature T_N using HFA according to (7) for the semielliptical model density (23) and the solid lines show T_N for the theory of Moriya and Hasegawa according to (25). One sees immediately that these

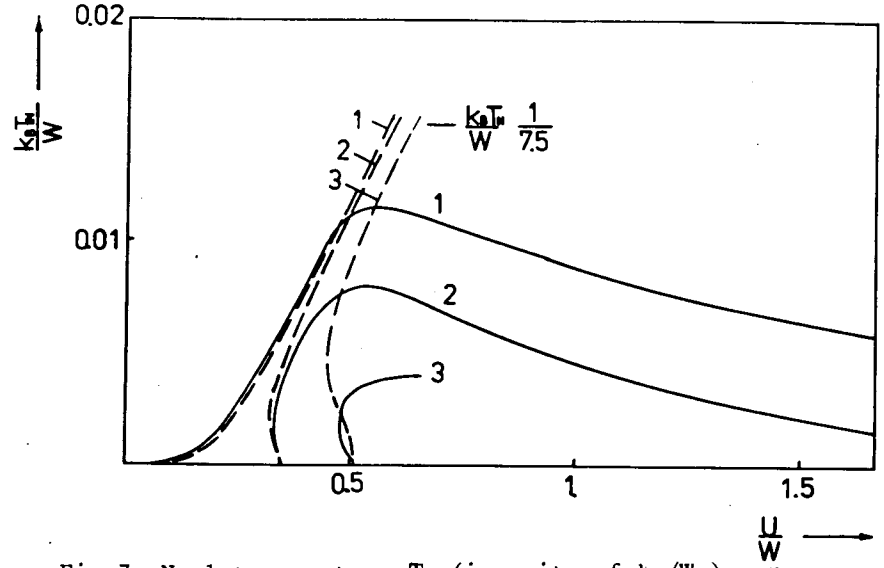

Fig.7. Neel temperature T_N (in units af k_B/W) versus the ratio of the correlation energy U to the band width W for different values of the mean occupation number n. (1) $n = 1$, (2) 1.1 and 0.9; (3) 1.2 and 0.8 (solid lines - MH, broken lines - HFA).

values of T_N are decreased by nearly one order of magnitude compared with those calculated using HFA, as we have expected, and that for non-half-filled band ($n \neq 1$) double solutions of T_N exist. For the intervall Δ in which double solutions appear it yilds: $\Delta/(\frac{U}{W})_0 \approx 5\%$ (comp. fig.8). Moriya and Hasegawa (8) considered the case $n = 1$ only.

Thus we have as answer to our question (ii) that the existence of double solution of the Neel temperature is not an effect of HFA , only.

From the existence of double solutions of the Neel temperature we conclude that incommensurable magnetic phase have to be included in the magnetic phase diagram for the unified theory using functional integral method with HFA as zero-temperature limit, too.

Till now incommensurable magnetic solutions were considered rather scarcely (by Penn[4] for HFA at $T = 0$ and by Kubo for the strong correlation limit). However, we believe that the consideration of incommensurable phases is of fundamental meaning independent of the approximation which is used to the investigation of the magnetic properties.

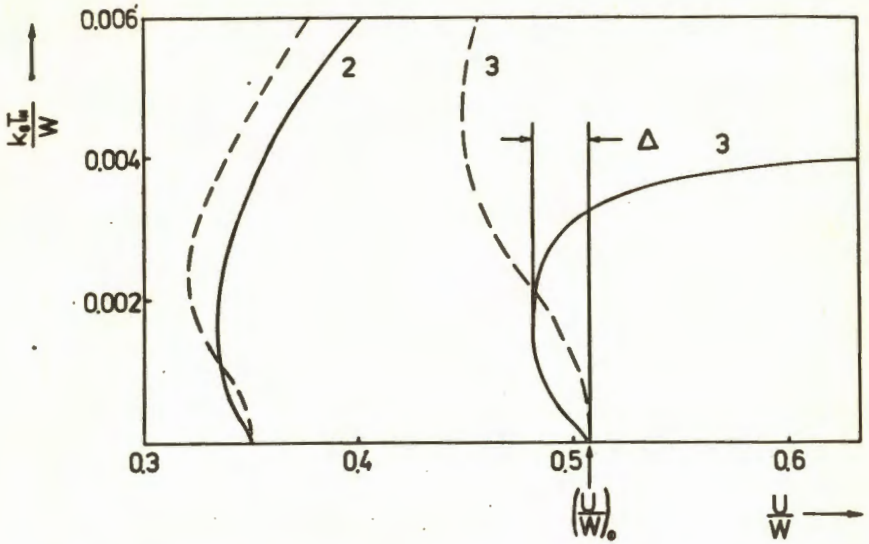

Fig.8. Enlarged cut-out of fig.7, $\Delta/(\frac{U}{W})_0 \approx 5\%$.

REFERENCES

1. Schumacher W., Linder U. R.Jauch, phys.stat.sol. (b), 1978, 86, p. 621.
2. Andriotis A.N., Poulopoulos P.N., Economou E.N. Solid State Comm., 1981, 39, p. 1175.
3. Hubbard J. Electron Correlation and Magnetism in Narrow-Band Systems, ed. by T.Moriya (Springer-Verlag, Berlin, 1981), p. 29.
4. Penn D.R. Phys.Rev., 1966, 142, p. 350.
5. Hubbard J. Phys.Rev., 1981, B23, p. 5974.
6. Wang S.Q., Evenson W.E., Schrieffer J.R. Phys.Rev.Lett., 1969, 23, p. 92; Evenson W.E., Schrieffer J.R., Wang S.A. J.Appl.Phys., 1970, 41, p. 1199; Schrieffer J.R., Evenso Evenson W.E., Wang S.Q. J. de Phys., 1971, 32, C1-1.
7. Cyrot M. Phys.Rev.Lett., 1970, 25, p. 871; Cyrot M. J. de Phys., 1972, 33, p. 125; M. Cyrot Phil.Mag., 1972, 25, p. 1031; Lacour-Gayet P., Cyrot M. J. de Phys., 1974, C7, p. 400.
8. Moriya T., Hasegawa H. J.Phys.Soc.Jpn., 1980, 48, p. 1490.
9. Schumacher W., Lindner U. phys.stat.sol. (b), to be published, 1982.
10. Schumacher W. Thesis, Leipzig, in preparation.
11. Kubo K. Progr.Theor.Phys.Suppl., 1980, 69, p. 290.

Received by Publishing Department
on June 22,1983.

Линднер У., Шумахер В.

E17-83-425

О магнитных решениях модели Хаббарда

Показано, что из существования двойного решения для температуры Нееля в модели Хаббарда для простой кубической решетки с взаимодействием ближайших соседей в рамках приближения Хартри-Фока и в теории Мория и Хазегава следует необходимость учета соизмеримых и несоизмеримых фаз на магнитной фазовой диаграмме. Мы ограничиваемся изучением только магнитного дальнего порядка.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1983

Lindner U., Schumacher W.

E17-83-425

To Magnetic Solutions of the Hubbard Model

From the existence of double solutions of the Neel temperature in the Hubbard model for nearest neighbour overlap and simple cubic lattice in the framework of Hartree-Fock approximation as well as within the unified theory of Moriya and Hasegawa it follows that it is necessary to conclude further magnetic (commensurable and incommensurable) phases in the magnetic phase diagram. We restrict ourself to investigation of magnetic longrange order.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1983