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# MAGNETIC SOLUTIONS OF THE HUBBARD MODEL

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# MAGNETIC SOLUTIONS OF THE HUBBARD MODEL

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Магнитные решения модели Хаббарда

Существование и устойчивость антиферромагнитных и ферромагнитных решений модели Хаббарда исследованы в рамках приближения Хартри-Фока. Показано, что модель Хаббарда допускает для простой кубической решетки и определенных параметров в конечной области температур устойчивые магнитные решения, даже в таких случаях, где для этих параметров при T = 0 магнитный порядок не существует.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Magnetic Solutions of the Hubbard Model

Existence and stability of antiferromagnetic and of ferromagnetic solutions of the Hubbard model were investigated in the framework of Hartree-Fock approximation. It was found, the Hubbard model for simple cubic lattice and certain parameters admits stable magnetic solutions in a finite temperature range, even in cases, where for these parameters at T = 0 no magnetic ordering exists (so-called heat magnetization).

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

**Communication of the Joint Institute for Nuclear Research. Dubna** 1978



## 1. Introduction

The aim of this paper is to investigate antiferromagnetic (afm) and ferromagnetic (fm) solutions of the Hubbard model using Hartree-Fock approximation. From the numerous papers on magnetic solutions of the Hubbard model we only refer to the papers /1/, /2/, /3/. We calculated the Néel and Curie temperature, respectively, the temperature dependence of the order parameter, the static zero-field susceptibility and the free energy for a simple cubic lattice and we found among others, that for nearest neighbour overlap and non half-filled bands magnetic ordering can appear in a finite temperature range even if for the temperature T=0 no magnetic ordering exists.

## 2. Hartree-Fock- approximation

In Hartree-Fock - approximation the Hubbard Hamiltonian can be written as

$$\mathcal{H} = -\sum_{i,j,\sigma} t_{ij}\, c_{i\sigma}^{+} c_{j\sigma} + U \sum_{i\sigma} \langle n_{i-\sigma} \rangle\, n_{i\sigma} - \mu \sum_{i\sigma} n_{i\sigma} , \qquad (1)$$

where $c_{i\sigma}^{+}$ and $c_{i\sigma}$ are creation and annihilation

operators for an electron with spin $\sigma$ in a Wannier state of the i-th atom. $t_{ij}$ is the kinetic energy in the band, U is the repulsive interaction between electrons of the same atom and $\mu$ is the chemical potential. In the following we restrict ourselves to a simple cubic lattice.

For the average occupation numbers of electrons with spin $\sigma$ or $-\sigma$ of a Wannier state we use the following ansatz

$$\langle n_{i,\pm\sigma}\rangle = \frac{1}{2}\left(n \pm x\, e^{-i\vec{q}\vec{R}_i}\right), \tag{2}$$

$$n = N^{-1}\sum_i \left(\langle n_{i\sigma}\rangle + \langle n_{i,-\sigma}\rangle\right) \tag{3}$$

being the average occupation number of electrons per atom,

$$x = \left(\langle n_{i\sigma}\rangle - \langle n_{i,-\sigma}\rangle\right) e^{i\vec{q}\vec{R}_i} \tag{4}$$

is the order parameter, $\vec{R}_i$ is the position vector of the i-th atom and N is the number of atoms in the lattice. For $\vec{q} = \vec{g}/2$ ($\vec{g}$ -vector of the reciprocal lattice) we get afm or paramagnetic (pm) solutions and $\mu_B x$ ($\mu_B$ - Bohr magneton) is the sublattice magnetization per lattice point. For $\vec{q} = 0$ we obtain fm or pm solutions and the $\mu_B x$ is the magnetization per lattice point.

Using the retarded Green function

$$G^{\sigma}_{\vec{k}\vec{k}'}(\omega) = \ll c_{\vec{k}\sigma};\, c^{+}_{\vec{k}'\sigma}\gg_{\omega} =$$

$$= \frac{1}{2\sqrt{\varepsilon_{\vec{k}}^2 + \frac{U^2x^2}{4}}}\left\{\delta_{\vec{k}\vec{k}'}\left(\omega - \varepsilon_{\vec{k}} + \mu - \frac{Un}{2}\right) - \delta_{\vec{k},\vec{q},\vec{k}'}\frac{Ux}{2}\right\}\left\{\frac{1}{\omega - E_1(\vec{k})} - \frac{1}{\omega - E_2(\vec{k})}\right\} \tag{5}$$

with

$$E_{1/2}(\vec{k}) = \frac{Un}{2} - \mu \pm \sqrt{\varepsilon_{\vec{k}}^2 + \frac{U^2x^2}{4}} \tag{6}$$



we get in the afm case ($\vec{q} = \vec{g}/2$) the following self-consistent equations for the quantities $n$ and $x$:

$$n = N^{-1}\sum_{\vec{k}}\left\{f(E_1(\vec{k});T) + f(E_2(\vec{k});T)\right\} \tag{7}$$

$$x = N^{-1}\sum_{\vec{k}}\frac{Ux}{2\sqrt{\varepsilon_{\vec{k}}^2 + \frac{U^2x^2}{4}}}\left\{f(E_1(\vec{k});T) - f(E_2(\vec{k});T)\right\} \tag{8}$$

$f(\omega;T)$ denotes the Fermi function

$$f(\omega;T) = \left(1 + e^{\frac{\omega}{k_B T}}\right)^{-1}. \tag{9}$$

(7) and (8) are in accordance with the system given by Langer et al /1/.

For $x \to 0$ the eqs. (7) and (8) become two coupled equations for the Néel temperature $T_N$ and the chemical potential $\mu$:

$$n = N^{-1}\sum_{\vec{k}} f\left(\frac{Un}{2} - \mu - \varepsilon_{\vec{k}};\, T_N\right), \tag{10}$$

$$1 = N^{-1}\sum_{\vec{k}}\frac{U}{2\varepsilon_{\vec{k}}}\left\{f\left(\frac{Un}{2} - \mu - \varepsilon_{\vec{k}};\, T_N\right) - f\left(\frac{Un}{2} - \mu + \varepsilon_{\vec{k}};\, T_N\right)\right\} \tag{11}$$

In the fm case ($\vec{q} = 0$) one obtains from (2)

$$n = N^{-1}\sum_{\vec{k}}\left\{f(E_\uparrow(\vec{k});T) + f(E_\downarrow(\vec{k});T)\right\} \tag{12}$$

$$x = N^{-1}\sum_{\vec{k}}\left\{f(E_\uparrow(\vec{k});T) - f(E_\downarrow(\vec{k});T)\right\} \tag{13}$$

with

$$E_{\uparrow\downarrow}(\vec{k}) = \frac{U}{2}(n \mp x) - \mu - \varepsilon_{\vec{k}} \tag{14}$$

and from these for $x \to 0$ (and therefore $T \to T_C$, where $T_C$ is the Curie temperature) the equations

$$n = N^{-1} \sum_{\vec{k}} 2 f\left(\frac{Un}{2} - \mu - \varepsilon_{\vec{k}}; T_c\right) \tag{15}$$

$$1 = N^{-1} \sum_{\vec{k}} \frac{U}{k_B T_c} f\left(\frac{Un}{2} - \mu - \varepsilon_{\vec{k}}; T_c\right) f\left(-\frac{Un}{2} + \mu + \varepsilon_{\vec{k}}; T_c\right) \tag{16}$$

(For $T_c \to 0$ one gets from (16) the well-known Stoner criterion). Since the self-consistent equations (7), (8) and (12), (13) always admit the solution x=0 (i.e., paramagnetism), one has to discuss the stability of solutions $x \neq 0$, if they exist. To this end we calculate the response of the system to an external static magnetic field of the form $h(\vec{R}_i) = h e^{-i\vec{q}\vec{R}_i}$.

For the static zero-field susceptibility

$$\chi(\vec{q}) = \frac{\partial M(\vec{q})}{\partial h}\Big|_{h=0} \tag{17}$$

with

$$M(\vec{q}) = \mu_B N^{-1} \sum_i (\langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle) e^{i\vec{q}\vec{R}_i} = \mu_B N^{-1} \sum_{\vec{k}\sigma} \sigma \langle c^+_{\vec{k}\sigma} c_{\vec{k}+\vec{q}\sigma}\rangle \tag{18}$$

we get in the afm case ($\vec{q} = \vec{Q}/2$)

$$\chi(\vec{Q}/2) = \frac{2\mu_B^2 N^{-1} \sum_{\vec{k}} \frac{1}{\varepsilon_{\vec{k}}} \left\{ f\left(\frac{Un}{2} - \mu - \varepsilon_{\vec{k}}; T\right) - f\left(\frac{Un}{2} - \mu + \varepsilon_{\vec{k}}; T\right) \right\}}{1 - N^{-1} \sum_{\vec{k}} \frac{U}{\varepsilon_{\vec{k}}} \left\{ f\left(\frac{Un}{2} - \mu - \varepsilon_{\vec{k}}; T\right) - f\left(\frac{Un}{2} - \mu + \varepsilon_{\vec{k}}; T\right) \right\}} \tag{19}$$

and in the fm case ($\vec{q} = 0$)

$$\chi(0) = \frac{\frac{2\mu_B^2}{k_B T} N^{-1} \sum_{\vec{k}} f\left(\frac{Un}{2} - \mu - \varepsilon_{\vec{k}}; T\right) f\left(-\frac{Un}{2} + \mu + \varepsilon_{\vec{k}}; T\right)}{1 - N^{-1} \sum_{\vec{k}} \frac{U}{k_B T} f\left(\frac{Un}{2} - \mu - \varepsilon_{\vec{k}}; T\right) f\left(-\frac{Un}{2} + \mu + \varepsilon_{\vec{k}}; T\right)}. \tag{20}$$



The mean values in (18) are calculated by means of Green functions, which differ from $G^{\sigma}_{\vec{k}\vec{k}'}(\omega)$ according to eq.(5) by the replacement of $\frac{U}{2}x$ by $(\frac{U}{2}x + \mu_B \sigma h)$. Negative values of the function $\chi(\vec{q})$ indicate instability of the pm phase compared with afm ($\vec{q} = \vec{Q}/2$) or fm ($\vec{q} = 0$) spin ordering, respectively. The transition temperatures are obtained by the vanishing of the denominator in (19) and (20). One sees that one gets again the equations (11) and (16) for the Néel and the Curie temperature.

Since among several magnetic phases that of the lowest free energy F is stable, we give the free energy per lattice point for the afm phase $\frac{F_a}{N}$ and for the fm phase $\frac{F_f}{N}$:

$$\frac{F_a}{N} = -k_B T N^{-1} \sum_{\substack{\vec{k} \\ l=1,2}} \ln\left(1 + e^{-\frac{E_l(\vec{k})}{k_B T}}\right) + \mu n - \frac{U}{4}(n^2 - x^2) \tag{21}$$

($E_l(\vec{k})$ according to (6)),

$$\frac{F_f}{N} = -k_B T N^{-1} \sum_{\vec{k}\sigma} \ln\left(1 + e^{-\frac{E_\sigma(\vec{k})}{k_B T}}\right) + \mu n - \frac{U}{4}(n^2 - x^2) \tag{22}$$

($E_\sigma(\vec{k})$ according to (14)).

The chemical potential $\mu$ is determined by $n$. Without external magnetic field the equations (8) and (13) for the order parameter have to result from the condition $\left(\frac{\partial F}{\partial x}\right)_{T,n} = 0$ what is evidently the case. With that is also shown, that in the framework of Hartree-Fock approximation the different methods for determination of the Néel or Curie temperature yield the same result.

3. Discussion

For the numerical evaluation we restricted ourselves for the moment to nearest-neighbour hopping. All the energies are related to the bandwidth W. Fig. 1 shows $k_B T / W$ as a function of $U / W$ for different values of the mean occupation number n. One sees that for non half-filled bands there are double solutions for the Néel temperature in some parameter regions, i.e., to fixed values of n and $U/W$ belong two different values of the Néel temperature. (The values for $T_N=0$ are in accordance with those given by Penn /4/). Furthermore appears, that for nonhalf-filled bands an afm solution only exists above some value of $U/W$. Fig. 2 shows once more that these double solutions for $T_N$ also exist for $U < W$, where one should believe, that the Hartree-Fock approximation is applicable.

The existence of the double solutions is also reflected by the temperature dependence of the order parameter $x$, plotted in Fig.3 for several combinations of the parameters: if for fixed values of $n$ and $\frac{U}{W}$ there are two values of the Néel temperature then afm ordering ( $x \neq 0$) is possible only between these two temperatures. Moreover one sees that with increasing correlation energy $\frac{U}{W}$ the order parameter $x$ increases and the temperature range of afm ordering enlarges.

Fig. 4 shows the static zero-field susceptibility $\chi(\vec{q} = \vec{q}/2)$ for the same parameter values. In the region, for which is $x \neq 0$, is $\chi(\vec{q} = \vec{q}/2) < 0$, i.e., the pm phase is unstable and therefore the afm phase stable. (We remark that for this parameter range no fm phase exists. A numerical evaluation of eqs. (15) and (16) showed that fm ordering for all n is only possible for $\frac{U}{W} \gtrsim 0.57$). Fig. 5 represents the difference of the free energy of the pm and of the afm phase. The free energy of the afm solution is always less than that of the pm solution, i.e., the afm solution is stable and no phase transition of the first kind exists. Besides numerical calculations showed that also in the case of Curie temperature $T_C$ double solutions may exist for certain combination of n and $U / W$ and for nearest-neighbour hopping. Taking into account next-nearest neighbor hopping we get double solutions for $T_N$ and $T_C$ even in the case of an half-filled band (n=1). Moreover, then afm solutions exist only above a certain value of $U / W$ for n=1, too.



Therefore we have concluded, that the Hubbard model for s.c.l., if Hartree-Fock approximation is used, admits magnetic ordering for certain parameters in a finite temperature range, even in the case, that no magnetic ordering exists for these parameters at T=0. Kitano and Trammel /5/ and Berdyshev /6/ found the same phenomenon (so-called heat magnetization) for an effective spin Hamiltonian like we found for the band case.

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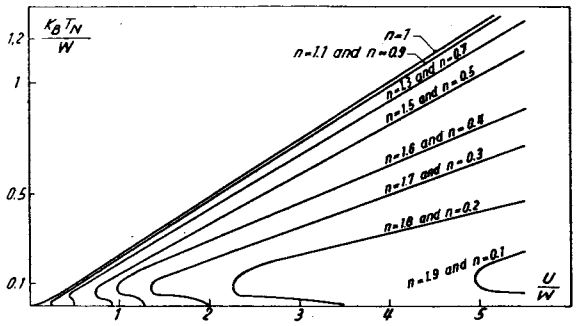


Fig. 1.

Néel temperature in units of $k_B / W$ is plotted against the ratio of the correlation energy U to the band width W for different values of the mean occupation number n.

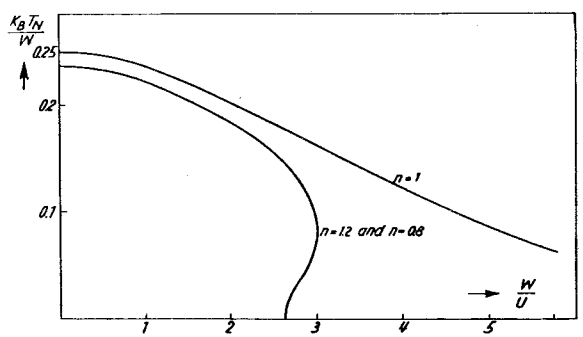


Fig. 2.

Néel temperature in units of $k_B / W$ is plotted as function of $\frac{W}{U}$ for the mean occupation number n=0.8 (or 1.2), where U is the correlation energy and W is the band width.



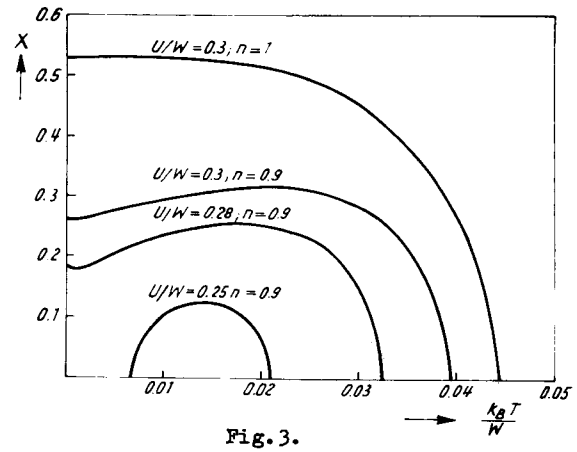


Fig.3.

Ordering parameter x versus temperature T (in units of $k_B / W$ ) for different values of the ratio of correlation energy U to band width W and the mean occupation number n.

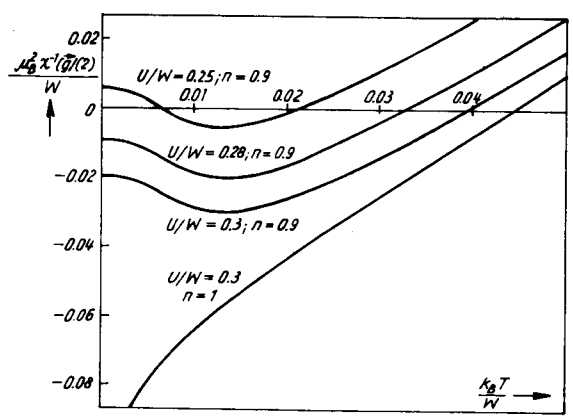


Fig.4.

Temperature dependence of zero-field susceptibility, $\mu_B^2 / W \cdot \chi(\vec{q}/2)$ as function of $k_B T / W$, for the same parameters as the order parameter x in Fig.3.

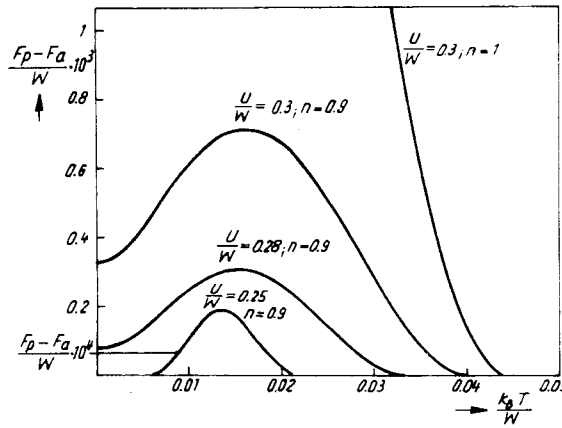


**Fig. 5.**

**Difference of the free energy per lattice point of the pm and of the afm phase versus temperature T in units of $k_B / W$ for the same parameters as the order parameter x in Fig.3.**

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