Vol. A52 (1977) ACTA PHYSICA POLONICA No 6

ON ANTIFERROMAGNETISM AND THE PEIERLS INSTABILITY IN THE ONE-DIMENSIONAL HUBBARD MODEL*

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(*Received May 16, 1977*)

Softening of the phonons in the SDW state is considered. A phase stability diagram of the antiferromagnetic state vs the Peierls distorted state is constructed.

1. *Introduction*

Recently an extensive development of experimental and theoretical investigations in quasi-one-dimensional conductors has been observed [1]. Particularly, metal-insulator phase transition phenomena are studied. An insulating state is due to a gap in the electronic band and for a half-filled band the ground state is antiferromagnetic or distorted lattice state [2]. The experimental work [3] shows the existence of the antiferromagnetic ground state in NMP-TCNQ and Bulaevskii et al. [4] suggest that the Peierls distortion occurs below the Néel temperature. A theoretical description of an antiferromagnetism [5] may be done by different orbitals for different spins (DODS) method or by Overhauser spin density wave (SDW), so the mixed state, antiferromagnetic-Peierls distortion state is described in two ways [2, 6, 7]. A criterion for existence of one or the other state is dependent on parameters of the model [2]. In these models the gap in the electronic band is introduced by a parameter of the Hamiltonian.

We are studying a renormalization of a phonon dispersion curve in the SDW state and in the Peierls distorted state. (Recently, Kim [8] considered softening of phonons in magnetic metals.) In Section 2 we describe our model and then we analyse a phonon dispersion curve in the antiferromagnetic and a possibility of the Peierls distortion in this phase.

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* This work was supported by the Polish Academy of Sciences within MR-I.9 project.

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2. The model

We shall be considering a one-dimensional system of electrons in the Hubbard model with phonons interacting with electrons. The Hamiltonian is

$$H = \sum_{k,\sigma} \varepsilon(k) a^{+}_{k\sigma} a_{k\sigma} + \frac{U}{N} \sum_{k,k',q} a^{+}_{k+q+} a_{k+} a^{+}_{k'-q-} a_{k'-} + \sum_{q} \Omega^0(q) b^{+}_{q} b_{q}$$

$$+ \sum_{k,q,\sigma} g(k, q) a^{+}_{k+q\sigma} a_{k\sigma} (b_q + b^{+}_{-q}), \tag{1}$$

where $a_{k,\sigma}$ denotes an annihilation operator for electrons with spin σ, wave vector k and energy in the tight binding approximation $\varepsilon(k) = -t \cos kc$ (c is a lattice constant), U is the Coulomb interaction coupling between electrons, b_q is an annihilation operator for phonons with a wave vector q and energy $\Omega^0(q)$, $g(k, q)$ is the electron-phonon coupling [9]

$$g(k, q) = \left(\frac{\hbar^2}{2M\Omega^0(q)}\right)^{1/2} 2i\tilde{q}_0 t[\sin kc - \sin (k+q)c], \tag{2}$$

where M is the mass of an ion, t is the overlap integral for the nearest neighbours, $\tilde{q}_0$ is of the order of the lattice constant.

Now, we are considering the transverse dynamical susceptibility $\chi_T(q, \omega, T)$ as a response function of a sytem on an external magnetic field. If the function $\chi_T(q, 0, T)$ has a singularity for a given q at a temperature $T_c(q)$, then we have an instability of a system towards formation of a spin density wave. Analogically, if a phonon Green function $D(q, 0, T)$ has a singularity then a sytem is unstable and below a critical temperature there is a lattice distortion with wave vector q. For nonmagnetic state and for the random phase approximation (RPA) the transverse susceptibility and the phonon Green function are

$$\chi_T(q, \omega, T) = \frac{g^2 \mu_B^2}{2N} \frac{\chi_T^0(q, \omega, T)}{1 - \frac{U}{N} \chi_T^0(q, \omega, T)}, \tag{3}$$

$$D(q, \omega, T) = \frac{2\Omega^0(q)}{\omega^2 - \Omega^{02}(q) + 2\Omega^0(q) \Pi^0(q, \omega, T)}, \tag{4}$$

where

$$\chi_T^0(q, \omega, T) = \sum_k \int \frac{d\omega'}{2\pi i} G(k+q, \omega+\omega') G(k, \omega'). \tag{5}$$

In the lowest order with respect to the electron-phonon interaction

$$\Pi^0(q, \omega, T) = \sum_k \int \frac{d\omega'}{2\pi i} |g(k, q)|^2 G(k+q, \omega+\omega') G(k, \omega'), \tag{6}$$

where $G(k, \omega)$ is the Green function of an electron. For a half-filled band the critical temperature satisfies the condition

$$1-\frac{U}{N}\chi_T^0(q_0, 0, T_N) = 0 \tag{7}$$

or

$$1 = \frac{U}{N}\sum_k \frac{n_{k+q_0}(T_N)-n_k(T_N)}{\varepsilon(k)-\varepsilon(k+q_0)}, \tag{8}$$

and

$$\Omega^0(q_0)-2\Pi^0(q_0, 0, T_P) = 0 \tag{9}$$

or

$$1 = \frac{2}{\Omega^0(q_0)}\sum_k |g(k, q_0)|^2 \frac{n_{k+q_0}(T_P)-n_k(T_P)}{\varepsilon(k)-\varepsilon(k+q_0)}, \tag{10}$$

where T_N and T_P denote the Néel temperature and the critical temperature of the Peierls distortion, respectively, $q_0 = \pi/c$ and $n_k(T) = \{\exp[\varepsilon(k)/k_B T]+1\}^{-1}$.

3. *Renormalization of the phonon energy in an antiferromagnetic*

In this section we consider the case when the Néel temperature is higher than the Peierls temperature. (The case of equal temperatures $T_N = T_P$ can only hold for a one special value of the effective electron-phonon coupling parameter.) Below the Néel temperature there is a gap Δ in the electronic band, which satisfies the condition [5]

$$1 = \frac{U}{N}\sum_k \frac{1-2\bar{n}_k(T)}{2\omega_1(k)}, \tag{11}$$

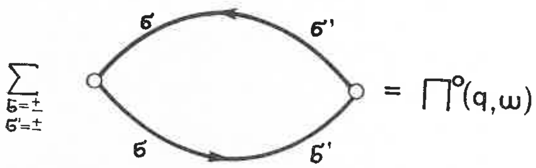

Fig. 1. Graphical representation of $\Pi^0(q, \omega, T)$

where

$$\omega_1(k) = \sqrt{\varepsilon^2(k)+\Delta^2}, \tag{12}$$

and $\bar{n}_k(T) = \{\exp[\omega_1(k)/k_B T]+1\}^{-1}$. For the antiferromagnetic state equation (6) has the diagram form shown in Fig. 1, where the heavy lines correspond to the electron Green functions [5]

$$G_{++}(k,\omega) = \frac{|u(k)|^2}{\omega-\omega_1(k)+i\delta} + \frac{|v(k)|^2}{\omega+\omega_1(k)+i\delta},$$

$$G_{--}(k,\omega) = \frac{|v(k)|^2}{\omega-\omega_1(k)+i\delta} + \frac{|u(k)|^2}{\omega+\omega_1(k)+i\delta},$$

$$G_{+-}(k,\omega) = \frac{\Delta}{2\omega_1(k)}\left[\frac{1}{\omega-\omega_1(k)+i\delta} - \frac{1}{\omega+\omega_1(k)+i\delta}\right],$$

$$G_{-+}(k,\omega) = \frac{\Delta^*}{2\omega_1(k)}\left[\frac{1}{\omega-\omega_1(k)+i\delta} - \frac{1}{\omega+\omega_1(k)+i\delta}\right], \tag{13}$$

and

$$|u(k)|^2 = \tfrac{1}{2}\left(1+\frac{\varepsilon(k)}{\omega_1(k)}\right), \quad |v(k)|^2 = \tfrac{1}{2}\left(1-\frac{\varepsilon(k)}{\omega_1(k)}\right). \tag{14}$$

We calculate explicitly $\Pi^0(q,\omega,T)$ for $T=0$ and for q close to the two interesting points, $q=0$ and $q=\pi/c$

$$\Pi^0(q\simeq 0,\omega,T=0) = \frac{s^2}{v}\,q\,\frac{\Delta^2}{t^2}\,\frac{1}{\sqrt{t^2+\Delta^2}}\left\{F\left(\pi/2,\frac{1}{\sqrt{1+\Delta^2/t^2}}\right)\right.$$

$$\left.+\frac{\omega^2-4\Delta^2}{4t^2+4\Delta^2-\omega^2}\,\Pi\left(\pi/2,\frac{4t^2}{\omega^2-4t^2-4\Delta^2},\frac{1}{\sqrt{1+\Delta^2/t^2}}\right)\right\}, \tag{15}$$

$$\Pi^0(q\simeq\pi/c,\omega,T=0) = 8s_\pi^2\,\frac{1}{t^2}\sqrt{t^2+\Delta^2}\left\{\left(1-\frac{\omega^2}{4(t^2+\Delta^2)}\right)F\left(\pi/2,\frac{1}{\sqrt{1+\Delta^2/t^2}}\right)\right.$$

$$\left.-E\left(\pi/2,\frac{1}{\sqrt{1+\Delta^2/t^2}}\right)+\frac{\omega^2}{4t^2}\,\Pi\left(\pi/2,\frac{4t^2}{\omega^2-4t^2-4\Delta^2},\frac{1}{\sqrt{1+\Delta^2/t^2}}\right)\right\}+0((\pi/c-q)^2). \tag{16}$$

Above F, E, Π denote the first, second, and the third order elliptic integrals, respectively, $s=\sqrt{\hbar^2/2M}\,2\tilde{q}_0t$, $s_\pi=\sqrt{\hbar^2/2M\Omega_\pi^0}\,2\tilde{q}_0t$. In these expressions we restrict ourselves to a linear term in q in $\Pi^0(q,\omega,T=0)$. For $q\simeq 0$ we consider an acoustic phonon branch (with a velocity v) and for $q\simeq\pi/c$ we put $\Omega^0(q\simeq\pi/c)=\Omega_\pi^0+0((\pi/c-q)^2)$, Ω_π^0 being a constant. The phonon dispersion curve may be determined from the equation

$$\Omega^2(q) = \Omega^{02}(q)-2\Omega^0(q)\Pi^0(q,\Omega(q),T=0). \tag{17}$$

Now, we shall analyse a possibility of the lattice distortion in the antiferromagnetic state. We consider the Peierls distortion with a wave vector $q=\pi/c$, thus we have to calculate $\Pi^0(q=\pi/c,\ \omega=0,T)$

$$\Pi^0(\pi/c,0,T) = \sum_k |g(k,\pi/c)|^2\,\frac{1-2\bar{n}_k(T)}{2\omega_1(k)} = 4s_\pi^2\sum_k \sin^2 k\,\frac{1-2\bar{n}_k(T)}{2\omega_1(k)}. \tag{18}$$

If we denote by $J(T)$ and $J_1(T)$ the following integrals

$$J(T) = \frac{1}{2\pi} \int_0^{\pi/2} dk \, \frac{1-2\bar{n}_k(T)}{2\omega_1(k)} \tag{19}$$

and

$$J_1(T) = \frac{1}{2\pi} \int_0^{\pi/2} dk \sin^2 k \, \frac{1-2\bar{n}_k(T)}{2\omega_1(k)}, \tag{20}$$

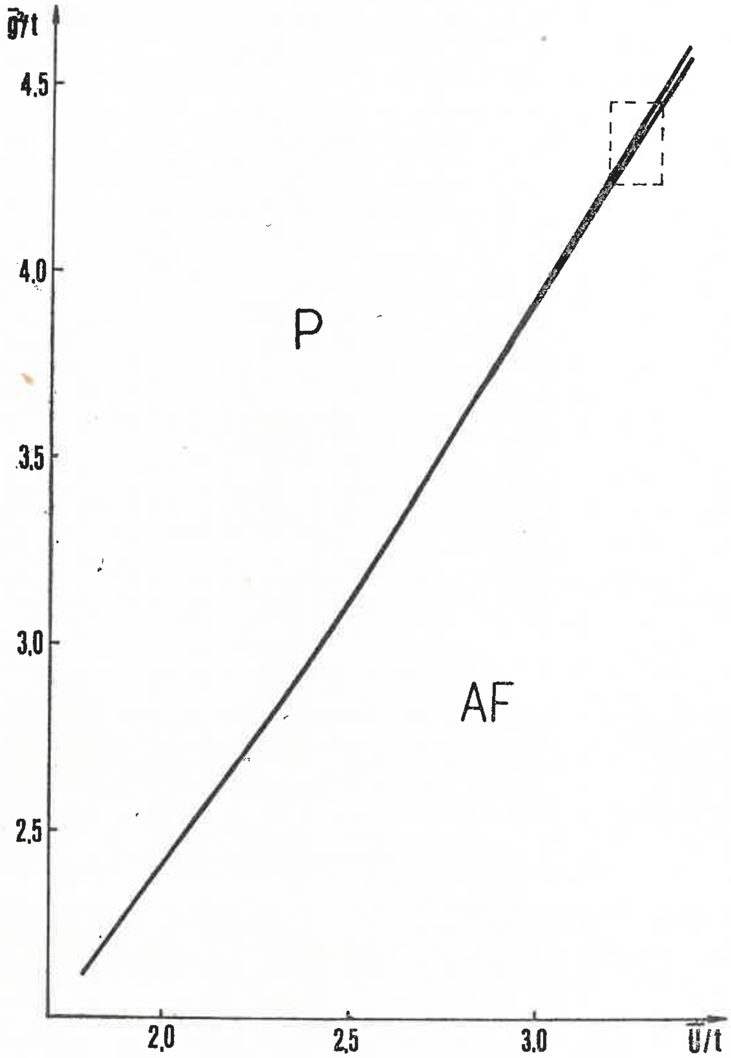

Fig. 2a. The phase stability diagram of the antiferromagnetic state (AF) vs the Peierls distorted state (P)

then the Néel temperature and the Peierls temperature, in the case when T_N is greater than T_P, are determined by the equations

$$\overline{U}J(T_N) = 1 \tag{21}$$

and

$$\overline{g^2}J_1(T_P) = 1, \tag{22}$$

where $\overline{U} = 4U$, $\overline{g^2} = 32s_\pi^2/\Omega_\pi^0$.

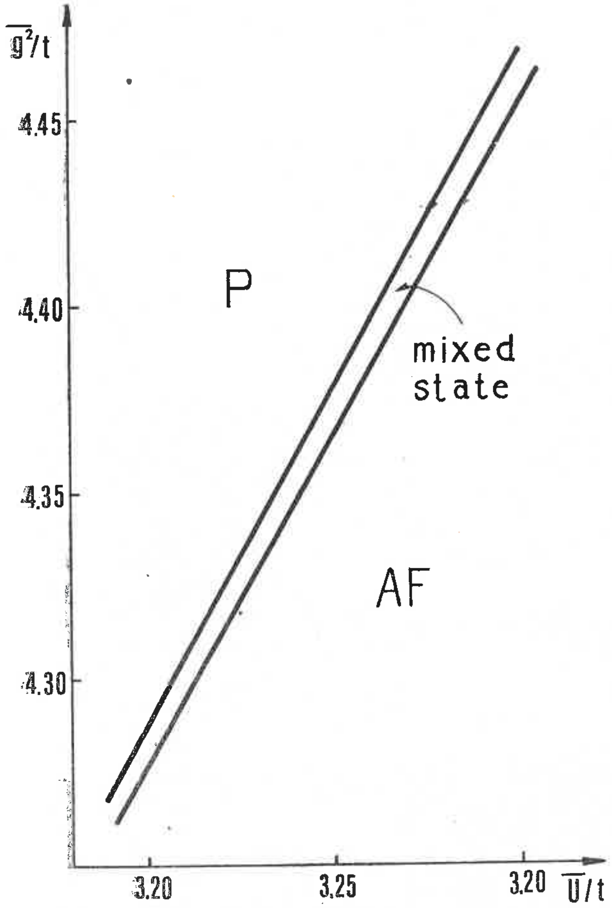

Fig. 2b. The phase stability diagram of the antiferromagnetic state vs the Peierls distorted state (the dashed box in Fig. 2a)

Now, for a given $\overline{U}$, we seek for the parameters $\overline{g^2}$ satisfying equation (22). From equation (11) we find a gap parameter Δ and thereafter $J_1(T_P)$ (for $T_P \leqslant T_N$). From a numerical analysis of the function $J_1(T_P)$ we conclude that the Peierls temperature is a monotonically increasing function of the parameter $\overline{g^2}$. Hence we have an inequality

$\overline{g_0^2} \leqslant \overline{g_N^2}$ (the values $\overline{g_0^2}$, $\overline{g_N^2}$ of the parameter $\overline{g^2}$ are taken at the Peierls temperature T_P equal 0 and T_N, respectively). Thus, the values $\overline{g_0^2}$ and $\overline{g_N^2}$ of the parameter $\overline{g^2}$ bound the region of existence of the Peierls distorted state in the antiferromagnetic state.

If the Peierls temperature T_P is greater than the Néel temperature, then we examine the stability conditions of the antiferromagnetic state in the distorted system. A procedure is completely analogical to that presented above, only we must change suitably parameters and functions describing both states.

Proceeding in this way we have obtained a phase diagram for the antiferromagnetic state and the Peierls distorted state (Fig. 2). For a given $\overline{U}/t$ and for a narrow range of the parameter $\overline{g^2}/t$ there arise a possibility of a mixed state, the antiferromagnetic-Peierls

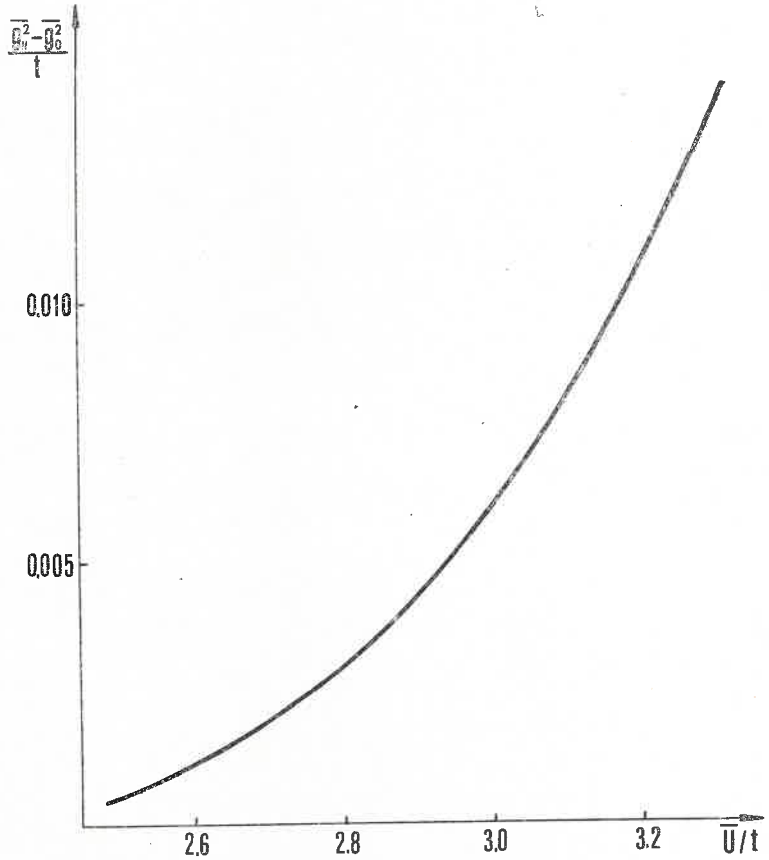

Fig. 3. The width of the region on the phase diagram corresponding to the mixed state

distorted state. A width of the region in the phase diagram corresponding to the mixed state rapidly decreases with decreasing $\overline{U}/t$ (Fig. 3). Our results (cf. Fig. 2b) are different from those given by Mattis [2], who showed that the antiferromagnetic state is stable for $\overline{U} > \overline{g^2}$ and the Peierls distorted state for $\overline{U} < \overline{g^2}$, and the mixed phase exists only at the boundary line $\overline{U} = \overline{g^2}$. Moreover, our phase boundaries (in figure 2) are not straight lines as in [2], where the functions $J(T)$ and $J_1(T)$ were identical, because the electron-phonon coupling was assumed to be independent of the electron momentum.

4. *Summary*

In this paper we investigated the ground state of the one-dimensional system of electrons and phonons. We constructed the phase stability diagram of the antiferromagnetic state vs the Peierls distorted state (Fig. 2). Once more, we would like to emphasize that the mixed state could only exist, for a given $\overline{U}/t$, for a narrow range of the parameter $\overline{g^2}/t$. The preference of coexistence of these two phases is the higher the stronger Coulomb and electron-phonon interactions are. We also considered a behaviour of the phonon dispersion curve near the magnetic Brillouin zone boundaries in the antiferromagnetic state. The results are more important as they can be easily generalized to a non-half-filled electronic band and a three-dimensional model.

The author would like to express his sincere thanks to Professor J. Morkowski for helpful discussions.

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