YU ISSN 0015—3206
FZKAAA 12 (2) 141 (1980)

MEAN FIELD THEORY TREATMENT OF 3D-ORDERING OF COUPLED CHARGE-DENSITY-WAVES

G. THEODOROU

Institute of Physics of the University, Zagreb, Croatia, Yugoslavia

Department of Physics, University of Crete, Iraklion, Crete, Greece

and

I. BATISTIĆ and S. BARIŠIĆ

Institute of Physics of the University, Zagreb, Croatia, Yugoslavia

Received 30 April 1980

UDC 539.11

Original scientific paper

It is shown that a mean-field theory treatment of coupled incommensurate charge-density-waves (*CDW*'s) provides the correct transition temperature for the 3D-ordering of the average *CDW* but fails to give the correct temperature for the ordering of the soliton lattice. The reasons for the failure are pointed out.

There exist a number of materials which may be viewed as arrays of quasi-one-dimensional (1D) systems[1]. As is well known[2] a strictly one-dimensional system with short-range interactions does not develop long-range order at a finite temperature. However, in the case of coupled linear chains at sufficiently low temperature, the system may undergo a phase transition of a state which has long-range order. In a recent work[3] we examined the phase transition of coupled incommensurate charge density waves (*CDW*'s) in a system of linear chains. The incommensurate state of the *CDW*'s can be described in terms of solitons[4]. Accordingly, in such a system besides the possible ordering of the average discommensuration shift, we may also have ordering of the soliton lattice. In Ref. 3 the problem was treated via perturbation theory. For a coupling between the CDW's of the form $\sum_{n,\delta} \cos(\varphi_n - \varphi_{n+\delta})$, where φ_n is the phase of the CDW at the point x of the n-th chain and the summation over δ refers to all nearest neighbour chains, we found that the soliton lattice is stable at low temperatures and that the average discommensuration shift and all the soliton lattice harmonics order at the same temperature.

In the present Letter we treat the same problem using mean field theory, that is the interchain coupling is approximated by a mean field and the resulting 1D prblem is solved exactly. The Landau free energy density of a system of weakly coupled CDW's is given by

$$f(x) = f_0(x) + f_\lambda(x) \tag{1}$$

where

$$f_0(x) = \sum_n \left\{ \frac{T_0}{2} \left(\frac{\partial \varphi_n}{\partial x} \right)^2 - T_\mu \left(\frac{\partial \varphi_n}{\partial x} \right) + \frac{T_p^2}{16\, T_0} \left[1 + \cos(M \varphi_n)\right] \right\}$$

and

$$f_\lambda = \frac{1}{2} \lambda \sum_{n,\delta} \cos(\varphi_n - \varphi_{n+\delta}).$$

The first term in $f_0(x)$ corresponds to the elastic coupling along the chain, the second term describes the departure from the commensurability, the potential of which is given by the third term. f_λ describes the interchain coupling between the CDW's.

The free energy density in the mean field approximation is given by

$$f_{MF}(x) = f_0(x) - \frac{m\lambda}{4} \sum_n \left(\Delta^*(x)\, e^{i\varphi_n} + \Delta(x)\, e^{-i\varphi_n}\right), \tag{2}$$

where

$$\Delta(x) = \langle e^{i\varphi_n(x)} \rangle .$$

The symbol $\langle\rangle$ denotes thermal average and m is the number of nearest neighbour chains. From Eq. (2) we note that in the mean field approximation the original prblem reduces to that of decoupled CDW's in an external potential. The value of the latter is determined in a self-consistent way. Using the mean field free energy density, Δ can be calculated from the functional integral

$$\Delta(x) = \frac{\int \mathcal{D}\varphi \exp\left[-\beta \int dy\, f_{MF}(y)\right] e^{i\varphi_n(x)}}{\int \mathcal{D}\varphi \exp\left[-\beta \int dy\, f_{MF}(y)\right]}. \tag{3}$$

For $T \cong T_c$, the transition temperature, Δ is small so that we can make the following expansion:

$$\exp\left[-\beta \int dy\, f_{MF}\right] = \exp\left[-\beta \int dy\, f_0\right] \prod_n \left[1 + \frac{\beta m \lambda}{4} \int dy\, \Delta^*(y)\, e^{i\varphi_n(y)} + c.c.\right]. \tag{4}$$

Thus in order to find Δ we have to calculate correlation functions for the decoupled *CDW*'s. This problem has been studied in detail in Ref. 5. Using the results of this work we obtain

$$\Delta(x) = \frac{\beta m \lambda}{4} \int \mathrm{d}y\, K(x-y)\, \Delta(y) \tag{5}$$

with

$$K(x-y) = \langle e^{[i\varphi_n(x) - \varphi_n(y)]} \rangle_0$$

Fourier analyzing Eq. (5) we get

$$\Delta(k) = \Delta(k) \frac{\beta m \lambda}{4} S_k(T), \tag{6}$$

where S_k is the structure factor. It is evident that a non-zero solution of Eq. (6) occurs at the critical temperatuıe T_c, which is the solution of the following equation

$$\beta_c \frac{m \lambda}{4} S_k(T_c) = 1. \tag{7}$$

Eq. (7) implies that we get different transition temperature for different harmonics. The maximum transition temperature occurs for the wave vector which maximizes the structure factor. This corresponds to the transition temperature of the average discommensuration. Using $S_k(T)$ as given by Eq. (21) of Ref. 5, we obtain that the transition temperature for the ordering of the average discommensuration is given by

$$T_C^{(0)} = \sqrt{m \lambda T_0}. \tag{8}$$

The same result has been previously obtained[3] using perturbation theory.

For a wave vector $k = 2k_F \pm \frac{\tau \mu M}{2}$, where $\tau = T/T_0$ and $\mu = \frac{2T_\mu}{MT}$, we have a local maximum of the structure factor which corresponds to the ordering of the first harmonic of the soliton lattice[5]. Evaluation of the corresponding transition temperature gives

$$T_C^{(1)} = T_C^{(0)} \left(\frac{q}{2M\mu^2} \right) \frac{1}{M-1}, \tag{9}$$

where $q = T_p^2/4M^2T^2$. From Eq. (9) we see that, in the context of the mean field theory, the transition temperature of the first soliton lattice harmonic is different than that of the average discommensuration. The same is also true for the higher harmonics of the soliton lattice, whose ordering temperature decreases with the order of the harmonic.

We note that the results of the mean field theory regarding the ordering temperature of the soliton lattice harmonics differ from those obtained via the perturbation expansion[3]. The latter gave that the average discommensuration and all the soliton lattice harmonics order at the same temperature. The failure of the mean field theory to give the correct ordering temperature of the soliton lattice harmonics is due to the fact that it is not capable of accounting for the modification of the ground state caused by the interchain coupling. If in the perturbation approach of Ref. 3 we ignore the modification cf the ground state wave function, we find that the temperature, at which the energy levels of the transfer matrix responsible for the ordering of the first harmonic cross the zero order ground state, is the same with that of Eq. (9).

Summarizing, we have shown that in a system of weakly coupled incommensurate CDWs a mean field theory treatment provides the correct transition temperature for the average CDW while fails to give the correct transition temperature for the ordering of the soliton lattice harmonics.

Acknowledgments

This work has been supported in part by the Greek-Yugoslavian agency for scientific and technological collaboration. One of us (G. T.) is grateful to the Institute of Physics of the University of Zagreb for their hospitality.

References

1) *Proceedings of the Dubrovnik Conference on quasi-one-dimensional conductors*, Lecture Notes in Physics **95** and **96** (Springer-Verlag), 1979;

2) L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, New York, 1969);

3) I. Batistić, G. Theodorou and S. Barišić, Sol. Stat. Comm. (to be published);

4) W. L. McMillan, Phys. Rev. **B15**, 1496 (1976);

5) I. Batistić and S. Barišić, Jour. Physique Lett. **40**, L613 (1979).

TEORIJA SREDNJEG POLJA ZA TRODIMENZIONALNO UREĐENJE VEZANIH VALOVA GUSTOĆE NABOJA

G. THEODOROU

Institut za fiziku Sveučilišta, Zagreb
Odjel za fiziku, Univerzitet na Kreti, Iraklion, Kreta, Grčka

I. BATISTIĆ i S. BARIŠIĆ

Institut za fiziku Sveučilišta, Zagreb

UDK 539.11

Originalni znanstveni rad

Pokazano je da se teorijom srednjeg polja vezanih nesumjerljivih valova gustoće naboja dobiva ispravna vrijednost za temperaturu 3-D uređivanja srednje komponente valova gustoće naboja, ali ne i ispravna temperatura za uređivanje solitonske rešetke. Navedeni su razlozi za ovu poteškoću.