acta phys. slov. 31. (1981), No. 1

INFLUENCE OF CHEMISORBED ADATOMS ON SURFACE VIBRATIONS

I. KARASOVÁ,* V. K. FEDYANIN,** A. ŠURDA,* Dubna

The surface vibrations of a lattice with chemisorbed adatoms were investigated using the formalism of the occupation number and the correlation functions. The behaviour of the frequency spectrum of a monoatomic quadratic lattice was analysed.

ВЛИЯНИЕ ХЕМИСОРБИРОВАННЫХ АДАТОМОВ НА ПОВЕРХНОСТНЫЕ КОЛЕБАНИЯ

Исходя из формализма чисел заполнения и корреляционных функций, в работе рассматриваются поверхностные колебания решетки с хемисорбированными адатомами. Проведен анализ поведения частотного спектра для одноатомной квадратной решетки.

I. INTRODUCTION

Many physical phenomena can be described with the Ising model. This model was intensively applied in particular to the theory of magnetism. Besides it was used to describe the adsorption in the lattice theory of a liquid, too [1]. In this paper we shall apply the Ising model to the description of a system of atoms adsorbed on a crystal surface. As will be shown, the presence of adatoms on the surface leads to the renormalization of the force constants and frequencies of the surface vibrations by means of adatom correlation functions. The basic idea of our procedure is similar to the one used in the work [2], where the effect of the spin-phonon interaction in the magnetic phase transitions is investigated.

II. MODEL HAMILTONIAN

For simplicity we shall model the adsorbing surface of a solid by a monoatomic two-dimensional lattice. We assume adatoms bound to the surface so strongly that

* Institute of Physics, Slov. Acad. Sci., Dúbravská cesta, CS — 899 30 BRATISLAVA. Present address: Joint Institute for Nuclear Research, Laboratory of Theoretical Physics, SU — DUBNA.
** Joint Inst. for Nucl. Research, SU — DUBNA.

they oscillate together with them (i.e. we shall investigate the chemisorption on an ideal surface).

Using the formalism of the occupation numbers and the correlation functions, the full Hamiltonian of the system surface + adsorbed atoms can be written

$$H=\sum_i \frac{\boldsymbol{P}_i^2}{2M}(1-n_i)+\sum_i \frac{\boldsymbol{P}_i^2}{2(M+m)}n_i+\frac{1}{2}\sum_{i\neq j}S(\boldsymbol{R}_i-\boldsymbol{R}_j)+$$
$$+\nu\sum_i n_i+\frac{1}{2}\sum_{i\neq j}J(\boldsymbol{R}_i-\boldsymbol{R}_j)n_in_j,$$

where M is the mass of an atom of the crystal surface at the lattice site i, m is the mass of an adatom, $\boldsymbol{P}_i$ are their momenta, $\boldsymbol{R}_i$ are their instantaneous position vectors, $S(\boldsymbol{R}_i-\boldsymbol{R}_j)$ is the interaction potential between atoms at the lattice sites i and j; $J(\boldsymbol{R}_i-\boldsymbol{R}_j)$ describes the interaction potential between adatoms at the lattice sites i and j, ν is the effective chemical potential of adatoms and n_i are the occupation numbers having their eigenvalues 0 or 1, where $n_i=1$ corresponds to a surface lattice site occupied by an adsorbed atom, $n_i=0$ corresponds to an unoccupied one. Using relation $n_i^2=n_i$, the Hamiltonian can be written in the more compact form

$$H=\sum_i \frac{\boldsymbol{P}_i^2}{2(M+mn_i)}+\frac{1}{2}\sum_{i\neq j}S(\boldsymbol{R}_i-\boldsymbol{R}_j)+\nu\sum_i n_i+\frac{1}{2}\sum_{i\neq j}J(\boldsymbol{R}_i-\boldsymbol{R}_j)n_in_j. \quad (1)$$

Let us introduce the model Hamiltonian H_0 parameters of which we determine by the Bogolubov variational method:

$$H_0=H_{ph}+H_{ad} \quad (2)$$
$$H_{ph}=\sum_i \frac{\boldsymbol{P}_i^2}{2M_0}+\frac{1}{4}\sum_{\substack{\alpha\beta\\ i\neq j}}A_{ij}^{\alpha\beta}X_{ij}^{\alpha}X_{ij}^{\beta}$$
$$H_{ad}=\frac{1}{2}\varkappa\sum_{i=j}n_in_j+\nu_0\sum_i n_i$$
$$X_{ij}^{\alpha}=u_i^{\alpha}-u_j^{\alpha},$$

where the variational parameters M_0, $A_{ij}^{\alpha\beta}$, ν_0, $\varkappa$ are determined by the minimum of the model free energy

$$F_{mod}=-\beta^{-1}\ln \mathrm{Tr}\, e^{-\beta H_0}+\langle H-H_0\rangle_0 \geqq -\beta^{-1}\ln \mathrm{Tr}\, e^{-\beta H},\ \beta=\frac{1}{kT}.$$

The subscript (0) denotes that we have used the Hamiltonian (2) for calculating the thermodynamical average of the difference $H-H_0$, and u_i^{α} is the α-component of the i-the atom displacement from the equilibrium position (for simplicity we

confine ourselves to the harmonic term). The displacements u_i^{α}, as usually, are determined by the formulas

$$R_i^{\alpha}=\langle R_i^{\alpha}\rangle+u_i^{\alpha}=i^{\alpha}+u_i^{\alpha};\quad \alpha=1,2$$
$$\langle 0\rangle=\frac{\mathrm{Tr}\,[0e^{-\beta H}]}{\mathrm{Tr}\,[e^{-\beta H}]}.$$

The average of the difference $H-H_0$ can be written

$$\langle H-H_0\rangle=\frac{1}{2}\sum_i\langle \boldsymbol{P}_i^2\rangle_{ph}\left[\left\langle\frac{1}{M+mn_i}\right\rangle_{ad}-\frac{1}{M_0}\right]+\frac{1}{2}\left\langle\sum_{i\neq j}S(\boldsymbol{R}_i-\boldsymbol{R}_j)\right\rangle_{ph}-$$
$$-\frac{1}{4}\sum_{\substack{i\neq j\\ \alpha\ \beta}}A_{ij}^{\alpha\beta}\langle X_{ij}^{\alpha}X_{ij}^{\beta}\rangle_{ph}+\frac{1}{2}\sum_{i\neq j}\langle n_in_j\rangle_{ad}[\langle J(\boldsymbol{R}_i-\boldsymbol{R}_j)\rangle_{ph}-\varkappa]+(\nu-\nu_0)\sum_i\langle n_i\rangle_{ad}.$$

It is convenient to express the average of the interaction potentials $S(\boldsymbol{R}_i-\boldsymbol{R}_j)$, $J(\boldsymbol{R}_i-\boldsymbol{R}_j)$ with respect to the model Hamiltonian H_{ph} in the form [2]

$$\langle J(\boldsymbol{R}_i-\boldsymbol{R}_j)\rangle_{ph}\equiv\exp\left[\frac{1}{2}\sum_{\alpha\beta}\langle X_{ij}^{\alpha}X_{ij}^{\beta}\rangle_{ph}\nabla_i^{\alpha}\nabla_i^{\beta}\right]J(i-j)\equiv\bar{J}(i-j). \quad (3)$$
$$\langle S(\boldsymbol{R}_i-\boldsymbol{R}_j)\rangle_{ph}\equiv\exp\left[\frac{1}{2}\sum_{\alpha\beta}\langle X_{ij}^{\alpha}X_{ij}^{\beta}\rangle_{ph}\nabla_i^{\alpha}\nabla_i^{\beta}\right]S(i-j)\equiv\bar{S}(i-j).$$

The condition for a minimum of the free energy

$$\frac{\delta F_{mod}}{\delta M_0}=\frac{\delta F_{mod}}{\delta A_{kl}^{\gamma\delta}}=\frac{\delta F_{mod}}{\delta\varkappa}=\frac{\delta F_{mod}}{\delta\nu_0}=0$$

give the following parameters of H_0:

$$\varkappa=\bar{J}(i-j) \quad (4)$$
$$A_{kl}^{\gamma\delta}=\nabla_k^{\gamma}\nabla_k^{\delta}\bar{S}(k-l)+\langle n_kn_l\rangle\nabla_k^{\gamma}\nabla_k^{\delta}\bar{J}(k-l)$$
$$\frac{1}{M_0}=\left\langle\frac{1}{M+mn_i}\right\rangle_{ad}=\frac{1}{M}+\langle n_i\rangle_{ad}\left(\frac{1}{M+m}-\frac{1}{M}\right)$$
$$\nu_0=\nu+\frac{1}{2}\langle \boldsymbol{P}_i^2\rangle_{ph}\left(\frac{1}{M+m}-\frac{1}{M}\right).$$

The dependence $\langle n_i\rangle_{ad}$ on $1/M_0$ was found by using the property of the projection operators n_i $(n_i^2=n_i)$.

III. THE FREQUENCY SPECTRUM OF A SURFACE WITH ADSORBED ADATOMS

We shall investigate the second equation (4), i.e. the equation

$$A^{\gamma\delta}_{kl} = \nabla^{\gamma}_{k}\nabla^{\delta}_{k}\bar{S}(\boldsymbol{k}-\boldsymbol{l}) + \nabla^{\gamma}_{k}\nabla^{\delta}_{k}\bar{J}(\boldsymbol{k}-\boldsymbol{l})\langle n_k n_l\rangle \tag{5}$$

in which, we remind once more, the equilibrium positions are determined by a choice of the Hamiltonian H_{ph} but no other assumptions have been made. In order to analyse the behaviour of the frequency spectrum, we have to model the surface and the subsystem of adatoms.

We assume that the surface has a structure of the simple square lattice. Let the atoms of the surface interact only with their nearest neighbours by central forces. We assume that the interactions in the subsystem of adatoms have the character of central interactions between pairs of the nearest neighbour adatoms. We assume further that the interaction between the surface and the subsystem of adatoms leads, besides changes of the interaction constants [3], to a change of the lattice parameter, without changing the shape of the cell ($a_0 \to a$). Then equation (5) determines the elements of the force constant matrix $A^{\gamma\delta}_{kl}$ of a simple square lattice. The mass of atoms is now equal to M_0 (see Eq. (4)).

In this case the equation [4]

$$Me^{\alpha}_{qj}\omega^2_{qj} = \sum_{l\beta} e^{\beta}_{qj}\Phi^{2\alpha}_{lo}e^{-iql}$$

for the eigen-mode frequencies ω^2_{qj} and the eigen-mode vectors e_{qj} ($\Phi^{\alpha\beta}_{lo}$ are the elements of a force constant matrix, M is the mass of atoms) can be written as

$$M_0\omega^2_{qj} = -\sum_{l} A^{\alpha\alpha}_{ol}e^{-iql}\,. \tag{6}$$

If the matrix $\|A^{\alpha\beta}_{ol}\|$ has the elements

$$\|A^{\alpha\beta}_{01}\| = \|A^{\alpha\beta}_{03}\| = +\begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}, \quad \|A^{\alpha\beta}_{02}\| = \|A^{\alpha\beta}_{04}\| = +\begin{pmatrix} A_2 & 0 \\ 0 & A_1 \end{pmatrix},$$

where A_1, A_2 are the central and noncentral force constants, then from eq. (6) it follows that

$$M_0\omega^2_{qj=1} = 2A_1(1-\cos q_1 a) + 2A_2(1-\cos q_2 a) \tag{7}$$

$$M_0\omega^2_{qj=2} = 2A_2(1-\cos q_1 a) + 2A_1(1-\cos q_2 a).$$

The displacement correlation function

$$\langle X^{\alpha}_{lm}X^{\prime\prime}_{lm}\rangle_{ph} = \frac{\hbar}{MN}\sum_{qj}\frac{e^{\alpha}_{qj}e^{\beta}_{qj}}{\omega_{qj}}(1-l^{iq(l-m)})\coth\frac{1}{2}\hbar\beta\omega_{qj},$$

with the help of the symmetry properties of the lattice

$$\langle (X^1_{ol})^2\rangle_{ph} = \langle (X^2_{ol})^2\rangle_{ph} \equiv \langle (X)^2\rangle_{ph},$$

can be written as

$$\langle (X)^2\rangle_{ph} = \frac{\hbar}{2M_0N}\sum_{qj}\frac{1-\cos q_1 a}{\omega_{qj}}\,\mathrm{cotgh}\,\frac{1}{2}\hbar\beta\omega_{qj}, \tag{8}$$

where the frequencies ω_{qj} are the solutions of eq. (7). The correlation function $\langle (X)^2\rangle_{ph}$ may be found analytically only in the high-temperature limit. Substituting eq. (7) into eq. (8) and expanding the function $\mathrm{cotgh}\,x$ in the power series, we get

$$\langle (X)^2\rangle_{ph} = \frac{1}{\beta\pi A_1}\left[\mathrm{arc\,tg}\sqrt{\frac{A_1}{A_2}} + \frac{A_1}{A_2}\,\mathrm{arc\,cotg}\sqrt{\frac{A_1}{A_2}}\right]$$

for arbitrary A_1, A_2. If $A_1 \gg A_2$, then

$$\langle (X)^2\rangle_{ph} = \frac{1}{\beta A_1}\left[\frac{1}{2} + \frac{1}{\pi}\sqrt{\frac{A_1}{A_2}}\right]$$

and for the case $A_1 \doteq A_2 = A$

$$\langle (X)^2\rangle_{ph} = \frac{1}{4\beta A_1}\left[1 + \frac{A_1}{A_2}\right] \doteq \frac{1}{2\beta A}\,.$$

From eqs. (4), (5) and (7) it can be seen that the frequencies ω^2_{qj} depend now on the correlation function $\langle n_i n_j\rangle_{ad}$ and on the coverage $\Theta = \langle n_i\rangle$ by means of the lattice parameters A_1, A_2 and M_0. It may be noted that $\langle n_i n_j\rangle_{ad}$ depends on Θ (see below) and the last of them depends on the pressure and the temperature T [1, 3].

In order to solve eq. (7) it is necessary to specify the functions $S(\boldsymbol{R}_i - \boldsymbol{R}_j)$, $J(\boldsymbol{R}_i - \boldsymbol{R}_j)$ and to utilize an approximation for $\langle n_i\rangle_{ad}$ and $\langle n_i n_j\rangle_{ad}$ (i, j — nearest neighbours). Therefore, expanding the functions $S(\boldsymbol{R}_i - \boldsymbol{R}_j)$, $J(\boldsymbol{R}_i - \boldsymbol{R}_j)$ with respect to u^{α}_i, u^{α}_j being the displacements of the surface atoms from the equilibrium positions if the interaction between the clean surface and the adatom subsystem is neglected, we get

$$J(\boldsymbol{R}_i - \boldsymbol{R}_j) = J_0 + \sum_{\alpha} b^{\alpha}_{ij}Y^{\alpha}_{ij} + \frac{1}{2}\Sigma c^{\alpha\alpha}_{ij}Y^{\alpha}_{ij}Y^{\alpha}_{ij}, \tag{9}$$

$$S(\boldsymbol{R}_i - \boldsymbol{R}_j) = S_0 + \frac{1}{2}\Sigma B^{\alpha\alpha}_{ij}Y^{\alpha}_{ij}Y^{\alpha}_{ij}.$$

J_0 is the effective interaction between adatoms on a rigid lattice, $Y^{\alpha}_{ij} = u^{\alpha}_i - u^{\alpha}_j$, ($J_0 > 0$).

If the interaction between the adatoms and the surface atoms is taken into consideration, the atoms vibrate about the new equilibrium positions (without changing the shape of the cell). Substituting now

$$Y_{ij}^{\alpha} = \bar{X}_{ij}^{\alpha} + X_{ij}^{\alpha}$$

into the relation (9), we obtain the expansion of the potentials S and J about the new equilibrium positions

$$J(\boldsymbol{R}_i - \boldsymbol{R}_j) = J_0 + \sum_{\alpha}\left[b_{ij}^{\alpha}\bar{X}_{ij}^{\alpha} + \frac{1}{2}c_{ij}^{\alpha\alpha}(\bar{X}_{ij}^{\alpha})^2\right] + \tag{10}$$

$$+ \sum_{\alpha}[b_{ij}^{\alpha} + c_{ij}^{\alpha\alpha}\bar{X}_{ij}^{\alpha}]X_{ij}^{\alpha} + \frac{1}{2}\sum_{\alpha}c_{ij}(X_{ij}^{\alpha})^2,$$

$$S(\boldsymbol{R}_i - \boldsymbol{R}_j) = S_0 + \frac{1}{2}\sum_{\alpha}B_{ij}^{\alpha\alpha}(\bar{X}_{ij}^{\alpha})^2 + \sum_{\alpha}B_{ij}^{\alpha\alpha}\bar{X}_{ij}^{\alpha}X_{ij}^{\alpha} + \frac{1}{2}\sum_{\alpha}B_{ij}^{\alpha\alpha}(X_{ij}^{\alpha})^2.$$

From (10) it is easy to obtain

$$\langle J(\boldsymbol{R}_i - \boldsymbol{R}_j)\rangle_{ph} = J_0 + \sum_{\alpha}\left[b_{ij}^{\alpha}\bar{X}_{ij}^{\alpha} + \frac{1}{2}c_{ij}^{\alpha\alpha}(\bar{X}_{ij}^{\alpha})^2\right] + \tag{11}$$

$$+ \frac{1}{2}\sum_{\alpha}c_{ij}^{\alpha\alpha}\langle(X_{ij}^{\alpha})^2\rangle_{ph} \equiv \tilde{J}(i-j),$$

where $\langle(X_{ij}^{\alpha})^2\rangle_{ph}$ represents the thermal average with respect to the Hamiltonian (2) where the correlation function is given by (8). The quantity $\bar{X}_{ij}^{\alpha}$ is determined by the external pressure p, which may be expressed by means of averaged forces [5]. In view of our assumption the relation $\bar{X}_{ij}^{\alpha} = \bar{X}_0 \frac{l^{\alpha}}{a}$ has to be satisfied for any pair of nearest neighbours. Taking into consideration the following notation

$$\|B_{01}^{\alpha\beta}\| = \|B_{03}^{\alpha\beta}\| = \begin{pmatrix} B_1 & 0 \\ 0 & B_2 \end{pmatrix} \quad \|C_{01}^{\alpha\beta}\| = \|C_{03}^{\alpha\beta}\| = \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix}$$

$$\|B_{02}^{\alpha\beta}\| = \|B_{04}^{\alpha\beta}\| = \begin{pmatrix} B_2 & 0 \\ 0 & B_1 \end{pmatrix} \quad \|C_{02}^{\alpha\beta}\| = \|C_{04}^{\alpha\beta}\| = \begin{pmatrix} 0 & 0 \\ 0 & C \end{pmatrix}$$

$$\|b_{01}^{\alpha}\| = -\|b_{03}^{\alpha}\| = \begin{pmatrix} b \\ 0 \end{pmatrix} \quad \|b_{02}^{\alpha}\| = -\|b_{04}^{\alpha}\| = \begin{pmatrix} 0 \\ b \end{pmatrix},$$

we have

$$p = -\frac{1}{4v}\sum_{l\alpha}[B_{0l}^{\alpha\alpha}\bar{X}_{l0}^{\alpha} + \langle n_0 n_l\rangle_{ad}(c_{0l}^{\alpha\alpha}\bar{X}_{l0}^{\alpha} - b_{0l}^{\alpha})]l^{\alpha} \tag{12}$$

and $\bar{X}_0$ may be expressed as

$$\bar{X}_0 = \frac{-\frac{vp}{a} + b\Psi}{B_1 + c\Psi} = \frac{-\frac{vp}{a} + b\Psi}{A_1}, \tag{13}$$

where $\Psi = \langle n_i n_j\rangle_{ad}$ is the correlation function of the adatom subsystem. By means of the relation (13) we may rewrite the renormalized interaction between the nearest adatoms in the form

$$\langle J(\boldsymbol{R}_i - \boldsymbol{R}_j)\rangle_{ph} \equiv \tilde{J} = J_0 - b\bar{X}_0 + \frac{c}{2}(\bar{X}_0)^2 + \frac{c}{2}\langle(X)^2\rangle_{ph}. \tag{14}$$

In accordance with eqs. (9—13), eq. (5) for the renormalized force constants may be written as

$$A_1 = B_1 + c\Psi \qquad A_2 = B_2. \tag{15}$$

From relation (15) it can be seen that the knowledge of the correlation function Ψ for an arbitrary pressure, T and for an arbitrary coverage function Θ, is very important in order to analyse the behaviour of the frequency spectrum of surface vibrations.

IV. APPROXIMATIONS OF THE CORRELATION FUNCTIONS OF AN ADATOM SUBSYSTEM

In order to determine the renormalized frequencies and the renormalized force constants from eqs. (7) and (15), it is necessary to take into consideration the approximation of the functions $\langle nn\rangle$ and $\langle n\rangle$:

1) Molecular field approximation

$$\Psi = \langle nn\rangle = \langle n\rangle^2,$$

where $\langle n\rangle = \frac{1}{2}\left\{1 - \mathrm{tgh}\frac{\beta}{2}\left[v' + 4\varkappa\left(\langle n\rangle - \frac{1}{2}\right)\right]\right\}$, $v' = v_0 + 2\varkappa$ and v_0, $\varkappa$ are determined by the formulas (4) and (14).

2) Quasichemical approximation

$$\Psi = \langle nn\rangle = \frac{(1-K)2\langle n\rangle - 1 + \sqrt{4(1-K)\langle n\rangle[\langle n\rangle - 1] + 1}}{2(1-K)}, \quad K = e^{-\beta\varkappa}$$

and $\langle n\rangle$ is determined by the equations

$$r^2 = 4\left(\langle n\rangle - \frac{1}{2}\right)^2 + e^{-\beta\varkappa}\left[1 - 4\left(\langle n\rangle - \frac{1}{2}\right)^2\right]$$

$$e^{\beta v'} = \left[\frac{r + 1 - 2\langle n\rangle}{r - 1 + 2\langle n\rangle}\right]^2\left[\frac{\langle n\rangle}{1 - \langle n\rangle}\right].$$

3) Polynomial decoupling

$$\langle n\rangle=\sum_{k=0}^{4}C_4^k\langle n\rangle^k(1-\langle n\rangle)^{4-k}N_k$$

$$N_k=[1+\exp(\beta(v_0+k\varkappa))]^{-1}$$

$$\Psi=\langle nn\rangle=\sum_{k=0}^{4}\frac{k}{4}C_4^k\langle n\rangle^k(1-\langle n\rangle)^{4-k}N_k.$$

The last two approximations take into account the effects of short range order, the first does not.

4) It can be shown that for the coverage $\langle n\rangle\leqq 0.2$, or for a strong repulsion $\varkappa^{-1}\ll\beta$, $\varkappa>0$ the relation

$$\Psi=\langle nn\rangle=\langle n\rangle^2 e^{-\beta\varkappa},\quad \varkappa\equiv\bar{J} \tag{16}$$

is satisfied for the last two approximations. Then using eqs. (13), (14) we may write the renormalized force constant A_1 (15) as

$$A_1=B_1+c\langle n\rangle^2\exp\left\{-\beta\left[J_0+\frac{bvp}{aB_1}+\frac{c}{2}\left(\frac{vp}{aB_1}\right)^2+\frac{c}{2}\langle(X)^2\rangle_{ph}\right]\right\} \tag{17}$$

if we put Ψ equal to zero in the expression for $\bar{X}_0$.

For a weak repulsion ($\beta\bar{J}\ll 1$) and a small coverage, substituting (16) into (15), we get

$$A_1=B_1+c\langle n\rangle^2\exp\left\{-\beta\left[J_0-b\left(-\frac{vp}{a}+b\Psi\right)(B_1+c\Psi)^{-1}\right]\right\}.$$

Here only the first term in the expansion of the function $\bar{J}$ is taken into account. If we put in the exponent, in accordance with (15), $\langle nn\rangle=(A_1-B_1)/c$, then this expression leads to the equation

$$A_1^2-A_1\left[B_1+\lambda+\bar{\varkappa}\left(-J_0+\frac{b^2}{c}\right)\right]+\bar{\varkappa}b\left(\frac{vp}{a}+\frac{bB_1}{c}\right)=0 \tag{18}$$

$$\lambda=c\langle n\rangle^2,\quad \bar{\varkappa}=c\beta\langle n\rangle^2.$$

If we may assume that $\bar{X}_0=0$, then

$$A_1=B_1+c\langle n\rangle^2\exp\left\{-\beta J_0-\frac{\beta c}{2}\langle(X)^2\rangle_{ph}\right\}. \tag{19}$$

Analysing the behaviour of the frequency spectrum (7) it is necessary to use a computer; in case of a small coverage ($0<\Theta\leqq 0.2$) or a strong repulsion ($\varkappa^{-1}\ll\beta$) the procedure, as it may be seen from eqs. (17—19), is substantially reduced.

REFERENCES

[1] Fedyanin, V. K.: *Method of Correlation Functions in the Ising Model.* Tartu State University, 1971. Particles and Nucleus 9 (1978), 658.

[2] Zagrebnov, V. A., Fedyanin, V. K.: TMF *10* (1972), 127.

[3] Fedyanin, V. K.: *I^st Conf. on Surface Phenomena.* Leningrad State University 1973.

[4] Maradudin, A. A., Montroll, E. W., Weiss, G. H.: *Theory of Lattice Dynamics in the Harmonic Approximation.* Mir, Moscow 1965.

[5] Fedyanin, V. K.: in *Statistical Physics and Quantum Field Theory.* Ed.: N. N. Bogolubov, Nauka, Moscow 1973.

Received November 21st, 1979