G.M.Gavrilenko

SECOND QUANTIZATION METHOD
IN THE THEORY OF SURFACE LAYERS

1987

In the present paper the consistent microsoopic approaoh is developed to be applied for a self-consistent description of wide speotrum of properties of the submonolayer surfaoe ooverages[1 , 2] . It bases both on the microscopic pioture developed by Bogolubov in the polar metal [3] and the generalization of the usual second quantization procedure [4] to the impurity problems with nonfixed configuration of admixtures [5]. Further for definiteness we shall oonsider the chemisorption of hydrogen-like atoms on a surface of a simple metal. Following [3] we shall oonsider this problem as a many-body problem.

So, the adsorbent, a crystal of metal having a free surface, will be desoribed by a oertain relief of the potential energy $u(\vec{x}) = \sum_{f \in R_+} u_f(\vec{x})$ oreated by positive charged metal ions and a system of N_e interaoting electrons in this potential field. The metal ions are fixed at the nodes f of the orystal lattice occupying in a regular way the halfspace R_+ . The total system is electrically neutral and invariant under transformations $f \to f + \vec{G}$, where $\vec{G} = \{n_x d_x, n_y d_y, 0\}$ is any lattioe veotor in the surface plane. Numbers n_x , n_y are integers. Values d_x , d_y are the simple translations in the direotions X and y , respeotively. (We ohoose coordinates so that Z is perpendioular to the surfaoe and $\vec{R} = (x, y)$ lies in the surfaoe. The plane $(R_x, R_y, 0)$ coinoides with the first surfaoe layer of the metal ions. Here we negleot distortions near the surface).

The adsorbat is the impurity atoms whioh contain positive oharge oore and one valence electron in the ground state per atom.
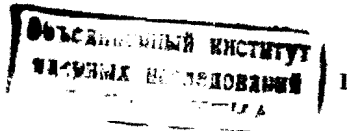
There are certain points on the surface $\vec{R}_d = \{R''_d, h\}$ called
the adsorption centres. They can be occupied by impurity atoms
or adatoms. In the case of crystal substrates the adsorption
centres are described by the points of high symmetry of the
crystal surface $\{R''_d\}$ and the parameter h which is the
equilibrium position of the adatom ions over the surface. The
adatom ions can make the vibrations on the adsorption centres and
jumps from one positions to another.

When an adatom occupies the adsorption centre the wave
function of its valence electron mixes with those of the sub-
strate electron band. As a result, all electrons (valence and
substrate electrons) are collectivized. Thus, we have to study
the problem of N interacting electrons and M interacting
ions in the external field of fixed ions of metal. The Hamiltonian
of such a system can easily be written:

$$H = H_A + H_\Sigma + H_{A\Sigma} \ ,$$

$$(I) \quad H_\Sigma = \sum_{j=1}^{N} \frac{\hat{p}_j^2}{2m} + \frac{1}{2}\sum_{i\neq j}^{N} v(\vec{x}_i - \vec{x}_j) - \sum_{j=1}^{N} u(\vec{x}_j) \ , \quad H_A =$$

$$\sum_{j=1}^{M} \frac{\hat{p}_j^2}{2M} + \frac{1}{2}\sum_{i\neq j}^{M} v(\vec{R}_i - \vec{R}_j) + \sum_{j=1}^{M} u(\vec{R}_j) \ , \quad H_{A\Sigma} = -\sum_{i=1}^{N}\sum_{j=1}^{M} v(\vec{x}_i - \vec{R}_j) \ .$$

Here H_Σ is the Hamiltonian of the electron subsystem. It
involves in an absolutely equivalent way both the substrate band
electrons and the valence adatom electrons, H_A is the Hamil-
tonian of the adatom ion subsystem, $H_{A\Sigma}$ is the interaction
between A and Σ systems, $v(\vec{x} - \vec{y})$ is the Coulomb
interaction of two charges of the same sign.

Further, following Bogolubov [3] one needs to take the
quantization of the model (I). As a single-particle electron
basis we choose the orthonormalized set of functions $\{\theta_d(\vec{x}), \theta_R(\vec{x})\}$
which is constructed of the wave functions of the metal electrons
$\{\psi_R(\vec{x})\}$ and the valence electrons of adatoms $\{\psi_d(\vec{x}) = \psi(\vec{R}_d - \vec{x})\}$
taking into account their involepment: $\langle k|d\rangle \neq 0$, $\langle d|\beta\rangle \neq 0$.

As the single particle ion basis we take the vibration $\psi_{d k}(R)$
states of adatom ions calculated in the effective surface
potential model [7]. We do not describe these spectrum problems
in detail now. We only note that this can be done in self-consis-
tent way [8]. However, the difficulty in applying a standard
procedure of second quantization [4] consists in that the phase
space of states of the electron subsystem depends on the
configuration of the arrangement of the adatom ions over the
adsorption centres $\{\vec{R}_d\}$, which is not fixed. This fact is the
basic specific feature of the problem considered.

Let us pass to a consistent construction of the second
quantization representation for these systems. Introduce the
following functions:

$$(2) \quad \psi_{d6}(X) = \theta_d(\vec{x})\Delta_{x6} \ , \quad \psi_{R6}(X) = \theta_R(\vec{x})\Delta_{x6} \quad \Delta_{x6} = \begin{cases} 1, & x = 6; \\ 0, & x \neq 6 \end{cases}$$

Symbol Δ_{x6} describes the spin state of an electron;
$X = \{\vec{x}, x\} ; 6, x = \pm 1$. Then, we consider the variety of functions
in the form:

$$(3) \quad \psi(X_1,\ldots, X_N; R_1,\ldots, R_M) = \sum_{\substack{\nu_1,\ldots,\nu_N \\ \gamma_1,\ldots,\gamma_M}} \varphi(\nu_1,\ldots,\nu_N; \gamma_1,\ldots,\gamma_M) \prod_{j=1}^{N} \psi_{\nu_j}(X_j) \prod_{i=1}^{M} \psi_{\gamma_i}(R_i)$$

Here index ν_i runs the values from the sets of indices
$\{\vec{k}_i, 6\}$ or $\{d_i, \epsilon_i\}$ and $\gamma_j \in \{d_j, k_j\}$. Index k_j marks
the vibration modes of an adatoms, $\vec{k}_i$ is the quasimomentum
of an electron, and d_i denotes the adsorption centres.

Let G be the linear space of functions of the form (3)
satisfying the requirements:

if P_{ij} is the rank of permutation $(i j)$, then

1) $\varphi(\nu_1,\ldots,\nu_i,\ldots,\nu_j,\ldots,\nu_N; \gamma_1,\ldots,\gamma_M) = (-1)^{P_{ij}}\varphi(\nu_1,\ldots,\nu_j,\ldots,\nu_i,\ldots,\nu_N; \gamma_1,\ldots,\gamma_M)$,

2) $\varphi(\nu_1,\ldots,\nu_N; \gamma_1,\ldots,\gamma_i,\ldots,\gamma_j,\ldots,\gamma_M) = (-1)^{P_{ij}}\varphi(\nu_1,\ldots,\nu_N; \gamma_1,\ldots,\gamma_j,\ldots,\gamma_i,\ldots,\gamma_M)$,

3) $\varphi(\nu_1,\ldots,\nu_N; \gamma_1,\ldots,\gamma_M) = 0$, if $(\nu_1,\ldots,\nu_N, \gamma_1,\ldots,\gamma_M) \bar{\in} G$.

The set $\mathcal{G}$ consists of the sequences of ordered indices

$$\{\vec{k}_1 6_1, ..., \vec{k}_{N^*} 6_{N^*}, \alpha_{N^*+1} 6_{N^*+1}, ..., \alpha_N 6_N ; \alpha_1^* t_1, ..., \alpha_M^* t_M\},$$

where $0 \le N - N^* \le M$ and $\{\alpha_{N^*+1}, ..., \alpha_N\} \subset \{\alpha_1^*, ..., \alpha_M^*\}$.
The space $\mathcal{G}$ has the following sense. It is the physical
space of states of system (1). Indeed, if $\varphi \in \mathcal{G}$, then in
superposition (3) an electron can be found in the localized
state at the α - centre while the adatom ion is absent at the
same centre, which is physically impossible.

Introduce the following operator functions of fields:

$$\Psi^+(x) = \sum_{k6} a_{\vec{k}6}^+ \varphi_{\vec{k}6}^*(x) + \sum_{\alpha 6} N_\alpha b_{\alpha 6}^+ \varphi_{\alpha 6}^*(x),$$

(4) $\quad \Psi(x) = \sum_{k6} a_{\vec{k}6} \varphi_{\vec{k}6}(x) + \sum_{\alpha 6} N_\alpha b_{\alpha 6} \varphi_{\alpha 6}(x),$

$$\Phi^+(R) = \sum_{\alpha t} C_{\alpha t}^+ \varphi_{\alpha t}^*(\vec{R}), \qquad \Phi(R) = \sum_{\alpha t} C_{\alpha t} \varphi_{\alpha t}(\vec{R}),$$

where $a_{\vec{k}6}^+, a_{\vec{k}6}, b_{\alpha 6}^+, b_{\alpha 6}$ are the Fermi operators of the creation
and annihilation of the electrons in the states $(\vec{k},6)$ and $(\alpha,6)$
respectively. $N_\alpha = \sum_t C_{\alpha t}^+ C_{\alpha t}$; $C_{\alpha t}^+, C_{\alpha t}$ have the following
commutation rules:

$$[C_{\alpha t}^+, C_{\alpha' t'}]_+ = \Delta_{\alpha \alpha'} \Delta_{t t'}; \quad [C_{\alpha t}, C_{\alpha' t'}]_+ = [C_{\alpha t}^+, a_{\vec{k}6}]_-$$

(5) $\quad = ... = [C_{\alpha t}, b_{\alpha' 6}]_- = C_{\alpha t} C_{\alpha t'} = C_{\alpha t}^+ C_{\alpha t'} = 0$.

If relations (5) hold, then the operator $N_\alpha = 0, 1$. Relations
(5) mean that any adsorption centre α may simultaneously be
occupied by only one impurity in a state t. It is shown in
ref. [5] how these commutation relations can be realized in an
explicit form. The definition of fields (4) is physically
justified. Indeed, the electronic state $\varphi_{\alpha 6}(x)$ gives a
contribution to the operator electron field $\Psi(x)$ only when the
adsorption centre α is occupied by an adatom ion, i.e. $N_\alpha = 1$.

Further, for any $\varphi \in \mathcal{G}$ let us define the mapping $\varphi \to |C_\varphi\rangle$
of the forms

(6) $\quad |C_\varphi\rangle = \frac{1}{\sqrt{N!M!}} \int dX_{1,N} dR_{1,M} \, \varphi(x_1, ..., x_N; R_1, ..., R_M) \prod_{j=1}^{N} \Psi^+(x_j) \prod_{\ell=1}^{M} \Phi^+(R_\ell) |0\rangle$.

We use the notations: $\int dX_{1,N} = \prod_{j=1}^{N} \int dx_j$, $\int dx_j = \sum_{6=1} \int d\vec{x}$,
$\int dR_{1,M} = \prod_{j=1}^{M} \int d\vec{R}_j$ and $|0\rangle$ is the vacuum vector.

The transformation (6) realizes the desired second
quantization representation. The necessary properties are collec-
ted in Lemmas 1-3.

Lemma 1. Let φ have the form (3), then $|C_\varphi\rangle = |C_{\varphi_\mathcal{G}}\rangle$
where $\varphi_\mathcal{G}$ is the orthogonal projection of φ onto $\mathcal{G}$ ∎.

Lemma 2. Let $\varphi \in \mathcal{G}$ then the following relations hold:

$$N \int dX_{2,N} dR_{1,M} \, \varphi(x_1', x_2, ..., x_N; R_1, ..., R_M) \prod_{j=2}^{N} \Psi^+(x_j) \prod_{\ell=1}^{M} \Phi^+(R_\ell) |0\rangle = \sqrt{N!M!} \, \Psi^+(x_1') \times$$

$$\times |C_\varphi\rangle, \qquad M \int dX_{1,N} dR_{2,M} \, \varphi(x_1, ..., x_N; R_1', R_2, ..., R_M) \prod_{j=1}^{N} \Psi^+(x_j) \prod_{\ell=2}^{M} \Phi^+(R_\ell) |0\rangle$$

$$= \int dX_{1,N} dR_{1,M} \, \varphi(x_1, ..., x_N; R_1, ..., R_M) \prod_{j=1}^{N} \Psi^+(x_j) \Phi^+(R_1') \prod_{\ell=1}^{M} \Phi^+(R_\ell) |0\rangle \; ∎.$$

Lemma 3. Let $\varphi \in \mathcal{G}$ then we have equalities:

$$\int dX_{1,N} \, \varphi(x_1, ..., x_N; R_1, ..., R_M) \prod_{j=1}^{N} \Psi^+(x_j) \, \Phi^+(R) = \int dX_{1,N} \, \varphi(x_1, ..., x_N; R_1, ..., R_M)$$

$$\times \left[\Phi^+(R) \Psi^+(x_1) \Psi^+(x_2) + N B(X, R) \Psi^+(x_2) + \frac{N(N-1)}{2} A(x_1, x_2, R) \right] \times$$

$$\times \prod_{j=3}^{N} \Psi^+(x_j) \; ; \qquad \int dX_{1,N} \, \varphi(x_1, ..., x_N; R_1, ..., R_M) \prod_{j=1}^{N} \Psi^+(x_j) \times$$

$$\times \Phi(R) = \int dX_{1,N} \, \varphi(x_1, ..., x_N; R_1, ..., R_M) \left[\Phi(R) \Psi^+(x_1) \Psi^+(x_2) - \right.$$

$$\left. - N B^*(X_1, R) \Psi^+(x_2) - \frac{N(N-1)}{2} A^*(x_1, x_2, R) \right] \prod_{j=3}^{N} \Psi^+(x_j),$$

where

$$B(X, R) = \sum_{\alpha 6} b_{\alpha 6}^+ C_{\alpha t}^+ \varphi_{\alpha t}^*(R) \varphi_{\alpha 6}^*(X), \quad B^*(X, R) = \sum_{\alpha 6} b_{\alpha 6}^+ C_{\alpha t} \varphi_{\alpha t}(R) \varphi_{\alpha 6}^*(X)$$

$$A(x_1, x_2, R) = \sum_{\alpha 6} b_{\alpha - 6}^+ b_{\alpha 6}^+ C_{\alpha t}^+ \varphi_{\alpha - 6}^*(x_1) \varphi_{\alpha 6}^*(x_2) \varphi_{\alpha t}^*(R),$$

$$A^*(x_1, x_2, R) = \sum_{\alpha 6} b_{\alpha 6}^+ b_{\alpha - 6}^+ C_{\alpha t} \varphi_{\alpha 6}^*(x_1) \varphi_{\alpha 6}^*(x_2) \varphi_{\alpha t}(R).$$

Corollaries of Lemmas 1-3.

(1) $\langle \varphi_\mathcal{G} | \varphi_\mathcal{G}' \rangle = \int dx_{1,N} \int dR_{1,M} \, \varphi_\mathcal{G}^*(x_1, ..., x_N; R_1, ..., R_M) \varphi_\mathcal{G}'(x_1, ..., x_N; R_1, ..., R_M) = \langle C_{\varphi_\mathcal{G}} | C_{\varphi_\mathcal{G}'} \rangle$.

$\langle C_\varphi | = \frac{1}{\sqrt{N!M!}} \langle 0 | \int dX_{1,N} dR_{1,M} \, \varphi^*(x_1, ..., x_N; R_1, ..., R_M) \prod_{j=M} \Phi(R_j) \prod_{\ell=N} \Psi(x_\ell),$

4

(2) $\frac{N!}{K!(N-K)!} \int dx_{K+1,N} dR_{1,M} \, \varphi(x'_1,...,x'_K, x_{K+1},...,x_N; R_1,...,R_M) \prod_{j=K+1}^{N} \psi^+(x_j) \prod_{i=1}^{M} \Phi^+(R_i)|0\rangle$

$= \sqrt{M!\,N!} \prod_{j=K}^{} \psi^+(x_j) |C_\varphi\rangle \, , \qquad \frac{M!}{K!(M-K)!} \int dx_{1,N} dR_{K+1,M} \, \varphi(x_1,..., x_N;$

$R'_1,..., R'_K, R_{K+1},..., R_M) \prod_{j=1}^{N} \psi^+(x_j) \prod_{i=K+1}^{M} \Phi^+(R_i)|0\rangle = \int dx_{1,N} dR_{1,M} \, \varphi(x_1,..., x_N;$

$R_1,...,R_M) \prod_{j=1}^{N} \psi^+(x_j) \prod_{i=1}^{M} \Phi^+(R'_i) \prod_{j=1}^{M} \Phi^+(R_j)|0\rangle$.

(3) If $\varphi \in G$, then $\varphi(x_1,...,x_N; R_1,...,R_M) = \frac{1}{\sqrt{N!\,M!}} \langle 0| \prod_{i=M}^{} \Phi(R_i) \prod_{j=N}^{} \psi(x_j) |C_\varphi\rangle$.

For any operator A acting in the space of the functions G, the second quantization representation $C(A)$ can be defined in a usual way.

(7) $\qquad C(A) |C_\varphi\rangle = |C_{A\varphi}\rangle$.

If the operator A is not closed in the space G in the mapping of $A \to C(A)$, then according to Lemma 1, there occurs a projection onto the space G of the functions $A G$.

Using Lemmas 2,3 and definition (7) we take the quantization of the algebra of observables. Here, we present the results of the quantization of the main types of operators in the model (I):

$C\left(\sum_{j=1}^{N} t(\vec{x}_j)\right) = \int dx \, \psi^+(x) \, t(\vec{x}) \, \psi(x)$,

$C\left(\sum_{i \neq j}^{N} \upsilon(\vec{x}_i \cdot \vec{x}_j)\right) = \int dx\,dx' \, \psi^+(x) \psi^+(x') \psi(x') \psi(x) \, \upsilon(\vec{x} - \vec{x}')$,

$C\left(\sum_{j=1}^{M} t(\vec{R}_j)\right) = \sum_{d,t,t'} C^+_{dt} C_{dt'} \int d\vec{R} \, \varphi^*_{dt}(\vec{R}) \, t(\vec{R}) \, \varphi_{dt'}(\vec{R}) +$

$+ \sum_{d \neq d', t, t'} C^+_{dt} C_{d't'} \int d\vec{R} \, \varphi^*_{dt}(\vec{R}) \, t(\vec{R}) \, \varphi_{d't'}(\vec{R}) \, \hat{\Pi}_{d'}$,

(8) $C\left(\sum_{i \neq j}^{M} \upsilon(\vec{R}_i - \vec{R}_j)\right) = \sum_{d_1 t_1,...,d_4 t_4} \upsilon(d_1 t_1, d_2 t_2; d_3 t_3, d_4 t_4) C^+_{d_1 t_1} C^+_{d_2 t_2} C_{d_3 t_3} C_{d_4 t_4} \times$

$\times \left[\Delta(d_1 \neq d_3 \neq d_4) \hat{\Pi}_{d_3} \hat{\Pi}_{d_4} + \Delta_{d_1 d_3} \Delta_{d_2 d_4} + \Delta_{d_1 d_4} \Delta_{d_2 d_3} + \Delta_{d_1 d_3} \Delta(d_1 \neq d_4) \hat{\Pi}_{d_4} \right.$

$\left. + \Delta_{d_1 d_4} \Delta(d_1 \neq d_3) \hat{\Pi}_{d_3} + \Delta_{d_2 d_3} \Delta(d_1 \neq d_4) \hat{\Pi}_{d_4} + \Delta_{d_2 d_4} \Delta(d_1 \neq d_3) \hat{\Pi}_{d_3} \right]$,

$C\left(\sum_{i=1}^{N} \sum_{j=1}^{M} \upsilon(\vec{x}_i - \vec{R}_j)\right) = \sum_{d_1 d_2 d_3 d_4 \, t_1 t_2 6} \upsilon(d_1 t_1, d_2 | d_3 t_3, d_4) C^+_{d_1 t_1} C_{d_2 t_2} \times$

$\times b^+_{d_3 6} b_{d_4 6} \left[\Delta_{d_1 d_2} N_{d_3} N_{d_3} + \Delta(d_1 \neq d_2) \Delta(d_1 \neq d_3) N_{d_3} N_{d_4} \hat{\Pi}_{d_2} + \Delta(d_1 \neq d_2) \times \right.$

$\times \Delta(d_2 \neq d_3) \Delta_{d_1 d_4} N_{d_3} \hat{R}_{d_3 6} + \Delta(d_1 \neq d_4) \Delta_{d_1 d_3} N_{d_4} \hat{\Pi}_{d_2} + \Delta(d_1 \neq d_2) \Delta_{d_1 d_3} \times$

$\left. \times \Delta_{d_2 d_4} \hat{R}_{d_3 6} \right] + \sum_{d_1 d_2 d_4 6 \, t_1 t_2} \upsilon(d_1 t_1, K / d_2 t_2, d_4) C^+_{d_1 t_1} C_{d_2 t_2} \times$

$\times a^+_{K 6} b_{d_4 6} N_{d_4} \left[\Delta_{d_1 d_2} + \Delta(d_1 \neq d_2) \hat{\Pi}_{d_2} + \Delta(d_1 \neq d_2) \Delta_{d_2 d_4} \hat{R}_{d_3 6} \right]$

$+ \sum_{d_1 d_2 d_3 K 6 \, t_1 t_2} \upsilon(d_1 t_1, d_3; d_2 t_2, K) C^+_{d_1 t_1} C_{d_2 t_2} b^+_{d_3 6} a_{K 6} \left\{ N_{d_3} \left[\Delta(d_1 \neq d_2 \neq d_3) \right. \right.$

$\left. \times \hat{\Pi}_{d_2} + \Delta_{d_1 d_2} \Delta(d_1 \neq d_3) + \Delta_{d_1 d_2} \Delta_{d_2 d_3} \right] + \Delta(d_1 \neq d_2) \Delta_{d_1 d_3} \hat{\Pi}_{d_2} \right\} +$

$+ \sum_{d_1 t_1 d_2 t_2 K_1 K_2 6} \upsilon(d_1 t_1, K_1; d_2 t_2, K_2) C^+_{d_1 t_1} C_{d_2 t_2} a^+_{K_1 6} a_{K_2 6} \left[\Delta_{d_1 d_2} + \Delta(d_1 \neq d_2) \hat{\Pi}_{d_1} \right]$.

Here $\quad t(x) = -\frac{\hbar^2}{2m} \vec{\nabla}^2_x - u(\vec{x})$, $t(\vec{R}) = -\frac{\hbar^2}{2\mu} \vec{\nabla}^2_R + u(\vec{R})$, $\Delta(d_1 \neq d_2) =$

$= 1 - \Delta_{d_1 d_2}$, ... , $\upsilon(d_1 t_1, K; d_2 t_2, d_4) = \int d\vec{R} d\vec{x} \, \varphi^*_{d_1 t_1}(\vec{R}) \, \varphi_{d_2 t_2}(\vec{R}) \, \theta^*_K(\vec{x}) \, \theta_{d_4}(\vec{x}) \upsilon(\vec{R} - \vec{x})$

The order of indices in the matrix element $\upsilon(d_1 t_1, K; d_2 t_2, d_4)$ strongly correlates with the order of the functions $\varphi_{d_1 t_1}, \theta_K, \theta_{d_4}$ in its right-hand side. The rest matrix elements are defined in the same way. $\hat{\Pi}_d = 1 - \sum_6 n_{d6} + n_{d\uparrow} n_{d\downarrow}$ is the projection operator onto the states in which the adsorption centre d is occupied only by the adatom ion (the electrons are absent) . $\hat{R}_{d6} = n_{d6}(1 - n_{d-6})$ is the projection operator onto the states with only one electron having spin (6) at the d adsorption centre. Further, for developing the theory, it is necessary to estimate the matrix elements of relations (8) for model (1) and limit ourselves only to contributions which play the dominating role. As a result, the expressions (8) are very simplified.

The above described approach allows us in the framework of Green function mechinary [9] to develop a self-consistent microscopic theory for describing the thermodynamical, electro- nical, vibrational and migrational properties of chemisorbed

layers. Some results of this approach are presented in refs.[8] and[10],where the connection relation between the pure electron Anderson model and thermodynamical Ising model is discussed. Both models are widely used in the chemisorption theory.

In conclusion the author thanks prof.V.K.Fedyanin for his attention to this work and useful discussions.

References:

1. The Chemical Physics of Solid Surfaces and Heterogeneous Catalis, v.2, Amsterdam, 1983.

2. The Chemical Physics of Solid Surfaces and Heterogeneous Catalis, v.3, Amsterdam ., 1983.

3. N.N.Bogolubov, Lektii po kvantovoi statistike, Razdel 4. Iz.soch.v 3 -h tomah, t.2 "Naukova Dumka",Kiev 1970(Russian).

4. N.N. Bogolubov, N.N.Bogolubov (jr.), Communication JINR, P17-80-239, Dubna 1980.

5. G.M.Gavrilenko, Preprint JINR P17-86-544, Dubna, 1986.

6. J.Zitkova, Rover N., J.Phys.C, v.3, p.L71, 1970.

7. M.Puska, P.M.Niemenen, Surf.Sci., v.157, p.143, 1985.

8. G.M.Gavrilenko, Li Ben Ir, V.K.Fedyanin, Communication JINR P17-86-59, Dubna, 1986.

9. N.N.Bogolubov, S.V.Tjablikov, DAN SSSR, v.126, No. 1, p.53 (1959).

10. G.M.Gavrilenko, JINR Rapid Comm., N 11, p.28, Dubna, 1985.

Гавриленко Г.М.   E17-87-192

Метод вторичного квантования
в теории поверхностных покрытий

Предложен последовательный микроскопический подход для описания свойств субмонослойных атомных покрытий кристаллических поверхностей твердых тел. Основу подхода составляют обобщения: а) микроскопических представлений, используемых Боголюбовым в полярной модели металла; б) стандартной процедуры вторичного квантования, распространенной на системы с неопределенностью части фазовых состояний. Второе характерно для, примесных задач, когда конфигурация примесей не фиксируется.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Gavrilenko G.M.   E17-87-192

Second Quantization Method in the Theory
of Surface Layers

Consistent microscopic approach is developed in the theory of submonoatomic coverages of the crystal surfaces. It bases both on the microscopic picture developed by Bogolubov in the polar model of metal and the generalization of the usual second quantization procedure to the system with stochasticity of some states. This appears in the impurity problems when the configurations of the impurities are not fixed.

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