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EQUILIBRIUM AND NONEQUILIBRIUM STATES OF MODEL FRÖHLICH-PEIERLS HAMILTONIAN

РІВНОВАЖНІ ТА НЕРІВНОВАЖНІ СТАНИ МОДЕЛІ ФРЬОЛІХА-ПАЙЕРЛСА

Model Fröhlich-Peierls Hamiltonian for electrons, interacting with phonons only with some infinite discrete modes, is considered. It is shown that in equilibrium case given model is thermodynamically equivalent to model of electrons with periodic potential and free phonons. In the one dimensional case the potential is determined exactly, it is expressed in terms of the Weierstrass elliptic function and eigenvalue problem can be solved exactly. Nonequilibrium states are described by nonlinear Schrödinger and wave equations which have exact soliton solution in the one dimensional case.

Розглянуто модель Фрьоліха—Пайерлса для електронів, що взаємодіють з фононами тільки при певних дискретних модах. Показано, що у рівноважному випадку дана модель термодинамічно еквівалентна моделі електронів з періодичним потенціалом та вільних фононів. В одновимірному випадку потенціал знаходиться точно і виражається через еліптичну функцію Вейерштрасса, а задача на власні значення теж має точний розв'язок. Нерівноважні стани описуються зв'язаними нелінійними рівняннями Шредінгера та хвильовим рівнянням, які в одновимірному випадку мають точні солітонні розв'язки.

Introduction. In given paper we consider the model Fröhlich-Peierls Hamiltonian for electrons interacting with phonons only with some infinite discrete modes.

Equilibrium and nonequilibrium states are investigated.

For equilibrium states the hierarchy of integrodifferential equations for correlation functions are derived. For nonequilibrium states the hierarchy of integrodifferential equations for reduced density matrixes (the quantum BBGKY hierarchy) are derived.

In both chains of equations we are faced with a problem of giving rigorous mathematical meaning to certain integral operators with factor equal to inverse volume of the entire Euclidean space. It was proved that in a functional space of periodic (or quasiperiodic) functions with certain cluster properties a rigorous meaning can be given to these integral operators.

In both cases the hierarchies for infinite sequences of correlation functions or reduced density matrixes are reduced to one- and two-particles correlation functions or reduced density matrixes.

It was proved that equilibrium hierarchy of the model Fröhlich-Peierls Hamiltonian is thermodynamically equivalent to the hierarchy of model with the approximating Hamiltonian for noninteracting electron-phonon system.

Electron subsystem is under influence of an external potential that should be determined from condition of minimum of functional of free energy. In one dimensional case this problem can be solved exactly and external potential is well known one-band potential expressed through the Weierstrass elliptic function. It seems to us that in this respect the model Fröhlich—Peierls Hamiltonian can be useful in theory of semiconductors.

The Hamiltonian of phonon subsystem can be diagonalized to the free system of quasiparticles with a vacuum that is a certain coherent state of phonons.

For two- or three-dimensional Euclidean space the approximating Hamiltonian for electron subsystem is again free system of electrons in periodic (quasiperiodic) external field. Note that in the theory of semiconductors the periodic (quasiperiodic) potential is postulated. We derived such potential from the model Fröhlich-Peierls Hamiltonian.

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It is proved that the nonequilibrium hierarchy in the thermodynamic limit is reduced to two nonlinear equations: the Schrödinger equation for wave function of electron and wave equation for lattice displacement. In the Schrödinger equation the lattice displacement plays the role of potential and in the wave equation the modul of squared wave function of electrons is nonhomogeneous term.

In one-dimensional Euclidean space and for acoustic phonons these nonlinear equations have soliton solution.

We proved the existence of the thermodynamic limit of correlation functions and reduced density matrixes by deriving equations for them and constructing the exact solutions for the obtained equations (in the one dimensional case).

1. Model Fröhlich-Peierls Hamiltonian and approximating Hamiltonian. I.1. Model Fröhlich-Peierls Hamiltonian. Consider a system consisting of electrons and phonons in a cube Λ of 3-dimensional Euclidean space R^3 , with the center at the origin and with the volume $V = V(\Lambda) = L^3$ where L is the length of the edge of the cube Λ .

We consider the periodic boundary condition.

The model Fröhlich-Peierls Hamiltonian for electrons interacting only with phonons having certain distinguished values of momenta, namely $q=mQ=Q_m$ where m belongs to a certain subset Z'=-Z' of the set of integer numbers $m \subset Z' \subset Z$ has the following form [1, 2]

$$H_{\Lambda} = \sum_{k,s} \left(\frac{k^2}{2m} - \mu \right) \psi_{k,s} \psi_{k,s} + \sum_{q} \omega(q) \alpha_q \alpha_q +$$

$$+\frac{1}{V^{\frac{1}{2}}}\sum_{k_1,k_2,q,s}\sum_{m\subset Z'}\delta_{k_1,k_2+q}\delta_{q,Q_m}g(q)\left[\overset{*}{\psi}_{k_1,s}\;\psi_{k_2,s}a_q+\overset{*}{\psi}_{k_2,s}\;\psi_{k_1,s}\overset{*}{a}_q\right], \quad (1.1)$$

where $\delta_{k,k'}$ is the Kronecker symbol, $\omega(q)$, g(q) are some functions that will be fixed later, μ is chemical potential, m is mass of electrons.

We also suppose that the set Z' is invariant with respect to operation $m_0 + Z' = Z'$ for arbitrary $m_0 \subset Z'$.

Here $\overset{*}{\psi}_{k,s}$, $\psi_{k,s}$ are the operators of creation and annihilation of electrons with momenta k and spin $s=\pm 1$, and $\overset{*}{a}_q$, a_q are the operators of creation and annihilation of phonons with momenta q. Momenta k and q are discrete vectors $k=\frac{2\pi}{L}(n_1,n_2,n_3)$, $q=\frac{2\pi}{L}(n_1,n_2,n_3)$ where n_i are integer numbers.

The operators $\psi_{k,s}, \psi_{k,s}$ and a_q , a_q satisfy the canonical anticommutation and respectively commutation relations

$$\{\psi_{k_1,s_1} \overset{*}{\psi}_{k_2,s_2}\} = \delta_{k_1,k_2} \delta_{s_1,s_2}, \quad [a_{q_1}, \overset{*}{a}_{q_2}] = \delta_{q_1,q_2}$$
 (1.2)

and the rest of anticommutators and commutators are equal to zero. Here δ_{s_1,s_2} , δ_{k_1,k_2} are the Kronecker symbols.

We now formally pass to the thermodynamic limit $V \to \infty$ $(L \to \infty)$ using the following relations [2]

$$\frac{(2\pi)^3}{V} \sum_{k} \to \int dk, \qquad \frac{V}{(2\pi)^3} \delta_{k,k'} \to \delta(k-k'), \qquad \frac{V^{\frac{1}{2}}}{(2\pi)^{\frac{3}{2}}} \overset{*}{\psi}_{k,s} \to \overset{*}{\psi}(k,s),
\frac{V^{\frac{1}{2}}}{(2\pi)^{\frac{3}{2}}} \psi_{k,s} \to \psi(k,s), \qquad \frac{V^{\frac{1}{2}}}{(2\pi)^{\frac{3}{2}}} \overset{*}{a}_q \to a(q), \qquad \frac{V^{\frac{1}{2}}}{(2\pi)^{\frac{3}{2}}} a_q \to a(q), \tag{1.3}$$

where $\delta(k)$ is a δ -function and $\tilde{\psi}(k,s)$, $\psi(k,s)$, $\tilde{a}(q)$, a(q) depend on continuous momenta $k \in \mathbb{R}^3$, $q \in \mathbb{R}^3$ and they satisfy the same anticommutation and commutation relations but with δ -functions instead of the Kronecker symbol δ_{k_1,k_2} , δ_{q_1,q_2} . Note that our results also are true for the case \mathbb{R}^{ν} , with $\nu = 1, 2, 3$.

After these substitutions the Hamiltonian (1.1) turns into the model Fröhlich-Peierls Hamiltonian of the infinite systems

$$H = \sum_{s} \int \left(\frac{k^{2}}{2m} - \mu\right) \psi(k, s) \psi(k, s) dk + \int \omega(q) \alpha(q) dq + \frac{(2\pi)^{\frac{3}{2}}}{V} \int \sum_{s,m \in \mathbb{Z}'} \delta(k_{1} - k_{2} - q) \delta(q - Q_{m}) g(q) \times \left[\psi(k_{1}, s) \psi(k_{2}, s) a(q) + \psi(k_{2}, s) \psi(k_{1}, s) \alpha(q)\right] dk_{1} dk_{2} dq,$$
(1.4)

$$\int \dots dk = \int_{\mathbb{R}^3} \dots dk.$$

Performing a formal pass to the thermodynamic limit we fix the ratio $\frac{2\pi}{L}n=mQ$, i.e. together with L vectors n also tend to infinity for all $m \in Z'$. For example, let $Q=Q^{(L)}=\frac{2\pi}{L}(n_1,n_2,n_3)$. Now let $L\to\infty$ in such a way $L^{(1)}=(2l+1)L,\ldots,L^{(l)}=(2l+1)L$ where l are integer. This means that we add to each edge of previous cube the edge with length L on the left and right hand side of it. We have

$$Q^{(lL)} = \frac{2\pi}{(2l+1)L} \Big((2l+1)n_1, (2l+1)n_2, (2l+1)n_3 \Big) =$$

$$= \frac{2\pi}{L} (n_1, n_2, n_3) = Q^{(L)} = Q,$$

$$mQ^{(lL)} = mQ.$$

As it is accepted in Fröhlich-Peierls Hamiltonian, we suppose that $\omega(q) = \omega_0 |q|$, $g(q) = g_0 |q|^{\frac{1}{2}}$, i. e. we consider the case of the acoustic phonons.

The model Hamiltonian (1.4) of the infinite system in the configuration space has the following form

$$H = \sum_{s} \int_{-\infty}^{\infty} \psi(x, s) \left(-\frac{\Delta}{2m} - \mu \right) \psi(x, s) dx + \int_{-\infty}^{\infty} a(y) \Delta^{\frac{1}{2}} a(y) dy +$$

$$+ \frac{1}{V} \sum_{s,m \in Z'} \left[\int e^{-iQ_m x} \stackrel{*}{\psi}(x,s) \psi(x,s) dx \int a(y) e^{iQ_m y} dy g(Q_m) + \right.$$

$$\left. + \int e^{iQ_m x} \stackrel{*}{\psi}(x,s) \psi(x,s) dx \int \stackrel{*}{a}(y) e^{-iQ_m y} dy g(Q_m) \right]. \tag{1.5}$$

By $\Delta^{\frac{1}{2}}$ we denote the operator that in momentum space multiply by $\omega(q) = \omega_0 |q|$.

It is easy to generalize the model Hamiltonian (1.1), (1.4), (1.5) to the case with different $Q_m^{(j)}$ and corresponding subsets Z_i' of integers numbers. Namely, let

$$Q_m^{(j)} = Q^{(j)} \cdot m, \quad m \subset Z_j', \qquad Z_j' = -Z_j',$$

where the set of j is finite or countable one.

We suppose that $Q_{m_1}^{(j_1)} \neq Q_{m_2}^{(j_2)}$ for all $j_1 \neq j_2$ and $m_1 \neq m_2$. In this case instead of (1.1), (1.4), (1.5) one obtains

$$H_{\Lambda} = \sum_{k,s} \left(\frac{k^{2}}{2m} - \mu\right) \overset{*}{\psi}_{k,s} \psi_{k,s} + \sum_{q} \omega(q) \overset{*}{a}_{q} a_{q} + \frac{1}{V^{\frac{1}{2}}} \sum_{k_{1},k_{2},q} \sum_{j} \sum_{s,m \in \mathbb{Z}'_{j}} \delta_{k_{1},k_{2}+q} \delta_{q,Q_{m}^{(j)}} g(q) \left[\overset{*}{\psi}_{k_{1},s} \psi_{k_{2},s} a_{q} + \overset{*}{\psi}_{k_{2},s} \psi_{k_{1},s} \overset{*}{a}_{q} \right],$$

$$(1.1')$$

$$H = \sum_{s} \int \left(\frac{k^{2}}{2m} - \mu\right) \overset{*}{\psi} (k,s) \psi(k,s) dk + \int \omega(q) \overset{*}{a} (q) a(q) dq + \frac{(2\pi)^{\frac{3}{2}}}{V} \int \sum_{j} \sum_{s,m \in \mathbb{Z}'_{j}} \delta(k_{1} - k_{2} - q) \delta(q - Q_{m}^{(j)}) g(q) \times \left[\overset{*}{\psi} (k_{1},s) \psi(k_{2},s) a(q) + \overset{*}{\psi} (k_{2},s) \psi(k_{1},s) \overset{*}{a} (q) \right] dk_{1} dk_{2} dq,$$

$$(1.4')$$

$$H = \sum_{s} \int \overset{*}{\psi} (x,s) \left(-\frac{\Delta}{2m} - \mu\right) \psi(x,s) dx + \int \overset{*}{a} (y) \Delta^{\frac{1}{2}} a(y) dy + \frac{1}{V} \sum_{j} \sum_{s,m \in \mathbb{Z}'_{j}} \left[\int e^{-iQ_{m}^{(j)}x} \overset{*}{\psi} (x,s) \psi(x,s) dx \int a(y) e^{iQ_{m}^{(j)}y} dy g(Q_{m}^{(j)}) + \frac{1}{V} \int e^{iQ_{m}^{(j)}x} \overset{*}{\psi} (x,s) \psi(x,s) dx \int \overset{*}{a} (y) e^{-iQ_{m}^{(j)}y} dy g(Q_{m}^{(j)}) \right].$$

$$(1.5')$$

In what follows for the sake of simplicity we will deal with the case j = 1 because the general case needs only additional summation with respect to j.

One sees that the model Fröhlich-Peierls Hamiltonian contains the factor $\frac{1}{V}$ in the interaction Hamiltonian.

1.2. Heisenberg equations. Introduce the operators of creation and annihilation of electrons and phonons in the Heisenberg representation by the following formulae [2]

$$\psi^{*}(t,x,s) = e^{iHt} \psi^{*}(x,s) e^{-iHt}, \qquad \psi(t,x,s) = e^{iHt} \psi(x,s) e^{-iHt},
a(t,y) = e^{iHt} a(y) e^{-iHt}, \qquad a(t,y) = e^{iHt} a(y) e^{-iHt}$$
(1.6)

where t is time, $-\infty < t < \infty$.

It follows from (1.6) the following Heisenberg equations

$$-i\frac{\partial \mathring{\psi}(t,x,s)}{\partial t} =$$

$$= \left(-\frac{\Delta}{2m} - \mu\right) \mathring{\psi}(t,x,s) + \left[\frac{1}{V} \sum_{s,m \in \mathbb{Z}'} \left(e^{-iQ_m x} \int a(t,y)e^{iQ_m y} dy + e^{iQ_m x} \int \mathring{a}(t,y)e^{-iQ_m y} dy\right) g(Q_m)\right] \mathring{\psi}(t,x,s),$$

$$i\frac{\partial \psi(t,x,s)}{\partial t} = \left(-\frac{\Delta}{2m} - \mu\right) \psi(t,x,s) + \psi(t,x,s) \times$$

$$\times \left[\frac{1}{V} \sum_{m \in \mathbb{Z}'} \left(e^{-iQ_m x} \int a(t,y)e^{iQ_m y} dy + e^{iQ_m x} \int \mathring{a}(t,y)e^{-iQ_m y} dy\right) g(Q_m)\right],$$

$$(1.7)$$

$$i\frac{\partial a(t,y)}{\partial t} = \Delta^{\frac{1}{2}}a(t,y) + \frac{1}{V} \sum_{s,m \in Z'} \int e^{iQ_m x} \psi^*(t,x,s) \psi(t,x,s) dx e^{-iQ_m y} g(Q_m),$$

$$-i\frac{\partial\overset{*}{a}(t,y)}{\partial t} = \Delta^{\frac{1}{2}}\overset{*}{a}(t,y) + \frac{1}{V}\sum_{s,m\subset Z'}\int e^{-iQ_{m}x}\overset{*}{\psi}(t,x,s)\psi(t,x,s)e^{iQ_{m}y}g(Q_{m})dx.$$

1.3. Equations for correlation functions. Define the following correlation functions [1, 2]

$$\langle a(t,y)\rangle = \lim_{V(\Lambda)\to\infty} (\operatorname{Tr} e^{-\beta H_{\Lambda}})^{-1} \operatorname{Tr} (a(t,y)e^{-\beta H_{\Lambda}}),$$

$$\langle \overset{*}{a}(t,y)\rangle = \lim_{V(\Lambda)\to\infty} (\operatorname{Tr} e^{-\beta H_{\Lambda}})^{-1} \operatorname{Tr} (\overset{*}{a}(t,y)e^{-\beta H_{\Lambda}}),$$

$$\left\langle \overset{*}{\psi}(t_{1},x_{1},s)\psi(t_{2},x_{2},s) \overset{\#}{a}(t_{3},y) \right\rangle =$$

$$= \lim_{V(\Lambda)\to\infty} (\operatorname{Tr} e^{-\beta H_{\Lambda}})^{-1} \operatorname{Tr} (\overset{*}{\psi}(t_{1},x_{1},s)\psi(t_{2},x_{2},s) \overset{\#}{a}(t_{3},y)e^{-\beta H_{\Lambda}}), \quad (1.8)$$

where β is the inverse temperature and Tr means trace. We suppose that limiting correlation functions (1.8) exist.

Derive for them equations using the Heisenberg equations. One obtains

$$-i\frac{\partial}{\partial t_{1}}\left\langle \overset{*}{\psi}(t_{1}, x_{1}, s)\psi(t_{2}, x_{2}, s)\right\rangle =$$

$$=\left(-\frac{\Delta_{1}}{2m} - \mu\right)\left\langle \overset{*}{\psi}(t_{1}, x_{1}, s)\psi(t_{2}, x_{2}, s)\right\rangle +$$

$$+\sum_{m\subset Z'}\left[e^{-iQ_{m}x_{1}}g(Q_{m})\frac{1}{V}\int e^{iQ_{m}y}\left\langle \overset{*}{\psi}(t_{1}, x_{1}, s)\psi(t_{2}, x_{2}, s)a(t_{1}, y)\right\rangle dy +$$

$$+e^{iQ_{m}x_{1}}g(Q_{m})\frac{1}{V}\int e^{-iQ_{m}y}\left\langle \overset{*}{\psi}(t_{1}, x_{1}, s)\psi(t_{2}, x_{2}, s)\overset{*}{a}(t_{1}, y)\right\rangle dy\right],$$

$$i\frac{\partial}{\partial t}\left\langle a(t, y)\right\rangle = \Delta^{\frac{1}{2}}\left\langle a(t, y)\right\rangle +$$

$$+\sum_{s,m\subset Z'}g(Q_{m})e^{-iQ_{m}y}\frac{1}{V}\int e^{iQ_{m}x}\left\langle \overset{*}{\psi}(t, x, s)\psi(t, x, s)\right\rangle dx, \qquad (1.9)$$

$$-i\frac{\partial}{\partial t}\left\langle \overset{*}{a}(t, y)\right\rangle = \Delta^{\frac{1}{2}}\left\langle \overset{*}{a}(t, y)\right\rangle +$$

$$+\sum_{s,m\subset Z'}g(Q_{m})e^{iQ_{m}y}\frac{1}{V}\int e^{-iQ_{m}x}\left\langle \overset{*}{\psi}(t, x, s)\psi(t, x, s)\right\rangle dx.$$

Now dwell on equations (1.9). All of them contain integrals over entire three dimensional space divided by the volume of this space. We are faced with problem of giving rigorous meaning to these integrals. To make these expression meaningful we assume that correlation functions (1.8) have the following cluster properties

$$\left\langle \stackrel{*}{\psi}(t_1, x_1, s) \psi(t_2, x_2, s) \stackrel{\#}{a}(t_3, y) \right\rangle = \left\langle \stackrel{*}{\psi}(t_1, x_1, s) \psi(t_2, x_2, s) \right\rangle \left\langle \stackrel{\#}{a}(t_3, y) \right\rangle. \quad (1.10)$$

Further we assume that the functions

$$\langle \dot{\psi}(t, x, s)\psi(t, x, s) \rangle$$
, $\langle a(t, y) \rangle$, $\langle \dot{a}(t, y) \rangle$

do not depend on time t and can be expanded in the following Fourier series .

$$\left\langle \dot{\psi}(t, x, s)\psi(t, x, s)\right\rangle = \left\langle \dot{\psi}(x, s)\psi(x, s)\right\rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_{m \subset Z'} e^{iQ_m x} \left\langle \dot{\psi} \psi\right\rangle (Q_m, s),$$

$$\left\langle \dot{\psi}\psi\right\rangle (Q_m, s) = \sum_{l \subset Z'} \left\langle \dot{\psi}(Q_m + Q_l, s)\psi(Q_l, s)\right\rangle,$$

$$\left\langle a(t, y)\right\rangle = \left\langle a(y)\right\rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_{m \subset Z'} e^{-iQ_m y} \left\langle a(Q_m)\right\rangle,$$

$$\left\langle \dot{a}(t, y)\right\rangle = \left\langle \dot{a}(y)\right\rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_{m \subset Z'} e^{iQ_m y} \left\langle \dot{a}(Q_m)\right\rangle,$$

$$\left\langle \dot{a}(t, y)\right\rangle = \left\langle \dot{a}(y)\right\rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_{m \subset Z'} e^{iQ_m y} \left\langle \dot{a}(Q_m)\right\rangle$$

$$(1.11)$$

where summation is carried out over $m \subset Z'$.

If one substitutes (1.10), (1.11) into (1.9) and emploies the formula

$$\lim_{L \to \infty} \frac{1}{L^3} \int_{-\frac{L}{L} - \frac{L}{L}}^{\frac{L}{L}} \int_{-\frac{L}{L}}^{\frac{L}{L}} e^{i(Q_i - Q_m)x} dx = \delta_{Q_i, Q_m}, \quad V(\Lambda) = L^3,$$

then one obtains

$$-i\frac{\partial}{\partial t_1} \left\langle \stackrel{*}{\psi}(t_1, x_1, s) \psi(t_2, x_2, s) \right\rangle =$$

$$= \left(-\frac{\Delta_1}{2m} - \mu \right) \left\langle \stackrel{*}{\psi}(t_1, x_1, s) \psi(t_2, x_2, s) \right\rangle +$$

$$+ \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_{m \subset \mathbb{Z}'} \left[e^{-iQ_m x_1} g(Q_m) \langle a(Q_m) \rangle +$$

$$+ e^{iQ_m x_1} g(Q_m) \langle \stackrel{*}{a}(Q_m) \rangle \right] \left\langle \stackrel{*}{\psi}(t_1, x_1, s) \psi(t_2, x_2, s) \right\rangle =$$

$$= \left(-\frac{\Delta_1}{2m} - \mu \right) \left\langle \stackrel{*}{\psi}(t_1, x_1, s) \psi(t_2, x_2, s) \right\rangle + 2u(x_1) \left\langle \stackrel{*}{\psi}(t_1, x_1, s) \psi(t_2, x_2, s) \right\rangle, \tag{1.12}$$

where potential u(x) is determined by the formula

$$2u(x) = \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_{m \in \mathbb{Z}'} \left[e^{-iQ_m x} g(Q_m) \langle a(Q_m) \rangle + e^{iQ_m x} g(Q_m) \langle a(Q_m) \rangle \right],$$

and is a real function $u(x)^* = u(x)$.

The last two equations (1.9) reduce to the following ones

$$0 = \Delta^{\frac{1}{2}} \langle \stackrel{*}{a}(y) \rangle + \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_{s,m \in \mathbb{Z}'} e^{iQ_m y} g(Q_m) \langle \stackrel{*}{\psi} \psi \rangle (Q_m, s) = \Delta^{\frac{1}{2}} \langle \stackrel{*}{a}(y) \rangle + w(y),$$

$$0 = \Delta^{\frac{1}{2}} \langle a(y) \rangle + \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_{s,m \in \mathbb{Z}'} e^{-iQ_m y} g(Q_m) \langle \stackrel{*}{\psi} \psi \rangle (-Q_m, s) = \Delta^{\frac{1}{2}} \langle a(y) \rangle + w(-y).$$

$$(1.13)$$

We have

$$w(-y) = \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_{s,m \in Z'} e^{-iQ_m y} g(Q_m) \langle \psi^* \psi \rangle (-Q_m, s) =$$

$$= \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_{s,m \in Z'} e^{iQ_m y} g(Q_m) \langle \psi^* \psi \rangle (Q_m, s) = w(y)$$

because the sets Q_m and $-Q_m$, $m \subset Z'$, coincide and we suppose that $g(Q_m) = g(-Q_m)$.

One can derive equations analogical to ones (1.9) for correlation function with arbitrary numbers of the operators $\overset{*}{\psi}(t,x,s)$, $\psi(t,x,s)$, $\overset{*}{a}(t,y)$, a(t,y). It is easy show that all of them reduce to equations of three correlation functions

$$\langle \dot{\psi}(t_1, x_1, s)\psi(t_2, x_2, s) \rangle$$
, $\langle \dot{a}(t, y) \rangle$, $\langle a(t, y) \rangle$.

1.4. Expression of functions u(x) and w(y). Consider the Fourier transform of (1.13)

$$0 = \omega(Q_m)\langle a(Q_m)\rangle + g(Q_m)\sum_s \langle \psi^* \psi \rangle (-Q_m, s),$$

$$0 = \omega(Q_m) \langle \mathring{a}(Q_m) \rangle + g(Q_m) \sum_{s} \langle \mathring{\psi} \psi \rangle (Q_m, s),$$

or

$$\langle a(Q_m) \rangle = -\frac{g(Q_m)}{\omega(Q_m)} \sum_s \langle \stackrel{*}{\psi} \psi \rangle (-Q_m, s),$$

 $\langle \stackrel{*}{a} (Q_m) \rangle = -\frac{g(Q_m)}{\omega(Q_m)} \sum_s \langle \stackrel{*}{\psi} \psi \rangle (Q_m, s).$
(1.14)

Substitute expressions $\langle a(Q_m) \rangle$, $\langle \stackrel{*}{a}(Q_m) \rangle$ (1.14) in expression (1.12) for u(x)

$$2u(x) = -\frac{1}{(2\pi)^{\frac{3}{2}}} \sum_{m \in Z'} \left[e^{-iQ_m x} \frac{g(Q_m)^2}{\omega(Q_m, s)} \sum_s \langle \psi \psi \rangle (-Q_m, s) + \right.$$

$$\left. + e^{iQ_m x} \frac{g(Q_m)^2}{\omega(Q_m)} \sum_s \langle \psi \psi \rangle (Q_m, s) \right] =$$

$$= -\frac{2}{(2\pi)^{\frac{3}{2}}} \sum_{s,m \in Z'} e^{-iQ_m x} \frac{g(Q_m)^2}{\omega(Q_m)} \langle \psi \psi \rangle (-Q_m, s) =$$

$$= -\frac{2}{(2\pi)^{\frac{3}{2}}} \sum_{s,m \in Z'} e^{iQ_m x} \frac{g(Q_m)^2}{\omega(Q_m)} \langle \psi \psi \rangle (Q_m, s). \tag{1.15}$$

We used again that the sets Q_m and $-Q_m$, $m \subset Z'_i$, coincide and $g(Q_m) =$ $=g(-Q_m), \ \omega(Q_m)=\omega(-Q_m), \ \langle \stackrel{*}{\psi} \ \psi \rangle (Q_m)^*=\langle \stackrel{*}{\psi} \ \psi \rangle (-Q_m)$ (because $\langle \dot{\psi}(x)\psi(x)\rangle^* = \langle \dot{\psi}(x)\psi(x)\rangle$).

It is obvious that $u(x) = u(x)^*$, i.e. the function u(x) is a real one.

Now we are able to express the potential u(x) through $\langle \tilde{\psi}(x,s)\psi(x,s) \rangle$. Suppose, as it is accepted in Fröhlich-Peierls Hamiltonian, that $\omega(q) = \omega_0|q|, \ g(q) = g_0|q|^{\frac{1}{2}},$ i. e. consider the case of acoustic phonons. Then

$$u(x) = -\frac{2}{(2\pi)^{\frac{3}{2}}} \frac{1}{\chi_0} \sum_{s,m \in \mathbb{Z}'} e^{iQ_m x} \langle \psi^* \psi \rangle (Q_m, s) = \frac{1}{\chi} \sum_s \langle \psi^* (x, s) \psi(x, s) \rangle,$$

$$\frac{1}{\chi} = -\frac{2}{(2\pi)^{\frac{3}{2}}} \frac{1}{\chi_0} = -\frac{2}{(2\pi)^{\frac{3}{2}}} \frac{g_0^2}{\omega_0}. \quad (1.16)$$

Let express w(y) through $\langle a(y) \rangle$ or $\langle a(y) \rangle$.

We have from (1.14)

$$\langle a(Q_m) \rangle = -\frac{g(Q_m)}{\omega(Q_m)} \sum_s \langle \psi \psi \rangle (-Q_m, s),$$

$$\langle \tilde{a} (Q_m) \rangle = -\frac{g(Q_m)}{\omega(Q_m)} \sum_s \langle \psi^* \psi \rangle(Q_m, s),$$

$$\langle a(-Q_m)\rangle = \langle \stackrel{*}{a}(Q_m)\rangle.$$

Substituting the last formulae in expression for w(y) one gets

$$w(y) = -\frac{1}{(2\pi)^{\frac{3}{2}}} \sum_{m \in Z'} e^{-iQ_m y} \omega(Q_m) \langle a(Q_m) \rangle = -\Delta^{\frac{1}{2}} \langle a(y) \rangle,$$

$$w(y) = -\frac{1}{(2\pi)^{\frac{3}{2}}} \sum_{m \in Z'} e^{iQ_m y} \omega(Q_m) \langle \overset{*}{a}(Q_m) \rangle = -\Delta^{\frac{1}{2}} \langle \overset{*}{a}(y) \rangle,$$
 (1.17)

$$w(y) = w^{*}(y).$$

The last formulae also follows directly from (1.13).

Thus we express u(x) through $\left\langle \stackrel{*}{\psi}(x,s)\psi(x,s)\right\rangle$ and w(y) through $\left\langle a(y)\right\rangle$ or $\langle \overset{*}{a}(y) \rangle$.

Approximating Hamiltonian. Consider the following approximating Hamiltonian.

$$H_{\text{appr}} = H_a = \sum_{s} \int \overset{\star}{\psi} (x, s) \left(-\frac{\Delta}{2m} - \mu \right) \psi(x, s) dx +$$

$$+ \int \overset{\star}{a} (q) \Delta^{\frac{1}{2}} a(y) dy + \sum_{s} \int \overset{\star}{2} u(x) \overset{\star}{\psi} (x, s) \psi(x, s) dx +$$

$$+ \int (a(y) + a(y))w(y)dq - \chi \int u^{2}(x)dx + \int w(y)\Delta^{-\frac{1}{2}}w(y)dy = H_{ae} + H_{aph},$$
 (1.18)

where H_{ae} is the Hamiltonian of the electron system and H_{aph} is the Hamiltonian of the phonons system.

Define the functions u(x) and w(y) by using the condition of minimum of the free energy as follows

$$u(x) = \frac{1}{\chi} \sum_{s} \left\langle \stackrel{*}{\psi}(x, s) \psi(x, s) \right\rangle_{0},$$

$$(1.19)$$

$$w(y) = -\Delta^{\frac{1}{2}} \langle a(y) \rangle_{0} = -\Delta^{\frac{1}{2}} \langle \stackrel{*}{a}(y) \rangle_{0}.$$

Here $\langle \cdot \rangle_0$ denotes averaging with respect to the approximating Hamiltonian H_a .

Let show that equalities (1.19) indeed follows from condition of minimum of the free energy of the systems with the Hamiltonian H_a . We have the free energy $\lim_{V\to\infty}\frac{1}{V}\ln \operatorname{Tr} e^{-\beta H_a}$. It is easy to see that equalities (1.19) can be obtained differentiating $\lim_{V\to\infty}\frac{1}{V}\ln (\operatorname{Tr} e^{-\beta H_a})$ with respect to u(x) and w(y) and equating derivatives to zero. By direct calculation one can check that the averages $\left\langle \psi(t_1,x_1,s)\psi(t_2,x_2,s)\right\rangle_0$, $\left\langle a(t,y)\right\rangle_0$, $\left\langle a(t,y)\right\rangle_0$, satisfy the same equations (1.12), (1.13) as the corresponding averages (1.11).

We omit the proof that equation for the all averages of the model Hamiltonian H (1.5) coincide in the thermodynamic limit with equations for the all averages of the approximating Hamiltonian H_a .

From (1.18) one sees that the approximating Hamiltonian consists from the Hamiltonian of electrons H_{ae} with potential 2u(x) and the Hamiltonian of phonons without interaction between electron and phonon systems.

Show that the Hamiltonian of phonons can be diagonalized. Represent it in the momentum space

$$H_{aph} = \int \overset{*}{a} (q)\omega(q)a(q)dq + \int \overset{*}{a} (q)w(-q)dq +$$

$$+ \int a(q)w(q)dq + \int w(q)\omega^{-1}(q)w(-q)dq. \tag{1.20}$$

Note that, as usual, we use the same denotation for the Fourier transforms of the operator of creation and annihilation and the function w(q) in the momentum space with momentum q.

Consider the following linear transformation of the operators a(q) and a(q)

$$a(q) = \tilde{a}(q) - w(-q)\omega^{-1}(q), \qquad \overset{*}{a}(q) = \overset{\tilde{*}}{a}(q) - w(q)\omega^{-1}(q).$$
 (1.21)

It is easy to check that the new operators $\tilde{a}(q)$, $\tilde{\tilde{a}}(q)$ satisfy canonical commutation relations and transformation (1.21) are canonical one.

Substituting a(q) and $\overset{*}{a}(q)$ through $\tilde{a}(q)$ and $\overset{*}{a}(q)$ according to (1.21) one obtains

$$H_{aph} = \int \tilde{a}(q)\omega(q)\tilde{a}(q)dq + 2 \int w(q)\omega^{-1}(q)w(-q)dq.$$
 (1.22)

Determine the vacuum state φ_0 for $\tilde{a}(q)$, $\tilde{a}(q)$. It is obtained from equation

$$\tilde{a}(q)\varphi_0 = 0$$

or

$$(a(q) + w(-q)\omega^{-1}(q))\varphi_0 = 0.$$

It is easy to check that φ_0 is the following coherent state

$$\varphi_0 = e^{-\int w(-q)\omega^{-1}(q)\dot{a}(q)dq}|0\rangle \qquad (1.23)$$

where |0 is the Fock vacuum.

Thus H_{aph} describes the system of boson quasiparticles (quasiphonons) with the vacuum that is coherent state (1.23).

The above obtained results can be summarized in the following theorem.

Theorem 1. The model Fröhlich – Peierls Hamiltonian (1.1), (1.4), (1.5) is thermodynamically equivalent to the approximating Hamiltonian (1.18) and sequences of their Green functions coincide in thermodynamic limit.

In given section we follow papers [1] in which analogical results have been obtained in the one-dimensional case and for j = 1, i. e. for a periodic potential u(x).

In the next subsection we will show how to determine the potential u(x) and function w(y).

1.6. Equation for potential u(x) in one-dimensional case. In this subsection we derive an equation for potential u(x) from the self-consistency condition. We will follow papers [1, 3, 4] and book [5]. Namely, we have the following self-consistency condition

$$u(x) = \frac{1}{\chi} \sum_{\sigma} \langle \psi(x, \sigma) \psi(x, \sigma) \rangle$$
 (1.24)

for the acoustic phonons.

Denote by $\varphi(x, E)$ the eigenfunctions of the Schrödinger equation with the potential u(x) and eigenvalue E (in the one-dimensional case)

$$-\frac{\partial^{2}}{\partial x^{2}}\varphi(x,E) + u(x)\varphi(x,E) = E\varphi(x,E). \tag{1.25}$$

Note that for the sake of simplicity we put 2m = 1.

The wave function of equation (1.25) is given by

$$\varphi(x,E) = \left[\left\langle \chi^{-1}(x,E) \right\rangle \chi(x,E) \right]^{-\frac{1}{2}} \exp \left(i \int_{0}^{x} dy \chi(y,E) \right),$$

$$\chi(x,E) = \left[p(E) \right]^{\frac{1}{2}} (E - \gamma(x))^{-1}, \tag{1.26}$$

$$p(E) = (E - E_1)(E - E_2)(E - E_3),$$

$$\gamma(x) = \frac{1}{2} (E_1 + E_2 + E_3 - u(x))$$

where E_1 , E_2 , E_3 are boundaries of the spectrum.

The potential u(x) is a one-band potential.

Represent the operators $\psi(x,\sigma)$ and $\psi(x,\sigma)$ through $\varphi(x,E)$

$$\psi(x,\sigma) = \int a(E,\sigma)\overline{\varphi}(x,E)dE, \quad \psi(x,\sigma) = \int a(E,\sigma)\varphi(x,E)dE, \quad (1.27)$$

where integral is carried out over the spectrum of the Schrödinger equation (1.25).

The operators $a(E,\sigma)$, $a(E,\sigma)$ satisfy the following anticommutation relations

$$\{a(E_1, \sigma_1), a(E_2, \sigma_2)\} = \delta(E_1 - E_2)\delta_{\sigma_1, \sigma_2}$$
 (1.28)

and the rest of anticommutators are equal to zero.

Using representation (1.27) and anticommutation relations (1.28) one obtains from the self-consistency condition (1.24)

$$u(x) = \frac{1}{\chi} \int f(E)|\varphi(x, E)|^2 dE \qquad (1.29)$$

where f(E) is the Fermi distribution function.

From representation (1.29) one can derive an equation for u(x). Namely one can check that the function $|\varphi(x,E)|^2$ as product of solutions of Schrödinger equation (1.25) satisfies the following equation

$$\left(\frac{\partial^3}{\partial x^3} - 4u(x)\frac{\partial}{\partial x} - 2\left(\frac{\partial}{\partial x}u(x)\right)\right)|\varphi(x,E)|^2 = -4E\frac{\partial}{\partial x}|\varphi(x,E)|^2.$$

Now multiply this equation by f(E), integrate over E and use self-consistency condition (1.24). One gets

$$\frac{\partial^3}{\partial x^3}u(x) - 6u(x)\frac{\partial}{\partial x}u(x) = -4\chi^{-1}\frac{\partial}{\partial x}\int Ef(E)|\varphi(x,E)|^2dE. \tag{1.30}$$

The integral in the right hand side of (1.30) is the averaged energy of electrons with spin ± 1 in point x and equilibrium it does not depend on x (otherwise the electrons will move from one point to another). Therefore

$$\frac{\partial^{3}}{\partial x^{3}}u(x) - 6u(x)\frac{\partial}{\partial x}u(x) = 0. \tag{1.31}$$

The last equation is famous Korteveg-de Vries equation. Integrating equation (1.31) twice one gets

$$\left(\frac{\partial}{\partial x}u(x)\right)^2 = 2u^3(x) - 2g_2u(x) - g_3 \tag{1.32}$$

where g_2 and g_3 are constants.

As known the Weierstrass elliptic function P(x) satisfies the following equation

$$\left(\frac{\partial}{\partial z}P(z)\right)^2 = 4P^3(z) - g_2P(z) - g_3. \tag{1.33}$$

Comparing (1.32) and (1.33) one conclude that potential u(x) can be expressed in term of P(z), namely

$$u(x) = -2P(ix + \omega). \tag{1.34}$$

It is well known that potential (1.34) is one-band potential.

The function w(y) can be obtained by using formulae (1.14) and (1.17) in which $\sum_{s} \langle \psi \psi \rangle (\pm Q_{m,s})$ are already known as the Fourier coefficients of known function u(x).

Obtained above results is summarized in the following theorem.

Theorem 2. In the one-dimensional case the self-consistent potential is the one-band one and is expressed through the Weierstrass elliptic function.

2. Hierarchy BBGKY. 2.1. Nonequilibrium reduced density matrixes. Let $\rho(0)$ be nonequilibrium density matrix at time t=0. Introduce the sequence of reduced nonequilibrium density matrixes [2]

$$\langle \psi (t, y_{1}, \sigma_{1}) \cdots \psi (t, y_{s_{1}}, \sigma_{s_{1}}) \psi (t, x_{s_{2}}, \tau_{s_{2}}) \dots \psi (t, x_{1}, \tau_{1}) \times \\
\times \overset{*}{a} (t, z_{1}) \cdots \overset{*}{a} (t, z_{n_{1}}) a(t, z'_{n_{2}}) \dots a(t, z'_{1}) \rangle = \\
= \frac{1}{\Xi} \text{Tr} (\overset{*}{\psi} (t, y_{1}, \sigma_{1}) \cdots \overset{*}{\psi} (t, y_{s_{1}}, \sigma_{s_{1}}) \psi (t, x_{s_{2}}, \tau_{s_{2}}) \dots \psi (t, x_{1}, \tau_{1}) \times \\
\times \overset{*}{a} (t, z_{1}) \cdots \overset{*}{a} (t, z_{n_{1}}) a(t, z'_{n_{2}}) \dots a(t, z'_{1}) \rho(0)) \qquad (2.1)$$

where

$$\Xi = \text{Tr}\rho(0)$$
.

Note that the all operators are in the Heisenberg representation at the same time t. For the sake of simplicity derive equations for the reduced density matrixes with $s_1 = s_2 = 1$, $n_1 = n_2 = 0$, $s_1 = s_2 = 0$, $n_1 = 1$, $n_2 = 0$, and $s_1 = s_2 = 0$, $n_1 = 0$, $n_2 = 1$. The general case will reduce to these three cases.

By using the Heisenberg equations (1.7) one obtains the following equations

$$\begin{split} i\frac{\partial}{\partial t}\langle \overset{\star}{\psi}(t,y,\sigma)\psi(t,x,\tau)\rangle &= \left[-\left(\frac{\Delta x}{2m} + \mu\right) + \left(\frac{\Delta y}{2m} + \mu\right)\right]\langle \overset{\star}{\psi}(t,y,\sigma)\psi(t,x,\tau)\rangle + \\ &+ \left\{\sum_{m} \left[e^{iQ_{m}x}g(Q_{m})\frac{1}{V}\int e^{-iQ_{m}z}\langle \overset{\star}{\psi}(t,y,\sigma)\psi(t,x,\tau)\overset{\star}{a}(t,z)\rangle dz + \right. \\ &+ \left. + e^{-iQ_{m}x}g(Q_{m})\frac{1}{V}\int e^{iQ_{m}z'}\langle \overset{\star}{\psi}(t,y,\sigma)\psi(t,x,\tau)a(t,z')\rangle dz'\right] - \\ &- \sum_{m} \left[e^{iQ_{m}y}g(Q_{m})\frac{1}{V}\int e^{-iQ_{m}z}\langle \overset{\star}{\psi}(t,y,\sigma)\psi(t,x,\tau)\overset{\star}{a}(t,z)\rangle dz + \right] \end{split}$$

(2.2)

$$+ e^{-iQ_m y} g(Q_m) \frac{1}{V} \int e^{iQ_m z'} \langle \stackrel{*}{\psi} (t, y, \sigma) \psi(t, x, \tau) a(t, z') \rangle dz' \bigg] \bigg\},$$

$$-i \frac{\partial}{\partial t} \langle \stackrel{*}{a} (t, z) \rangle = \Delta^{\frac{1}{2}} \langle \stackrel{*}{a} (t, z) \rangle +$$

$$+ \sum_{s,m} e^{+iQ_m z} g(Q_m) \frac{1}{V} \int e^{-iQ_m x} \langle \stackrel{*}{\psi} (t, x, s) \psi(t, x, s) \rangle dx,$$

$$i \frac{\partial}{\partial t} \langle a(t, z') \rangle = \Delta^{\frac{1}{2}} \langle a(t, z') \rangle +$$

$$+ \sum_{s,m} e^{-iQ_m z'} g(Q_m) \frac{1}{V} \int e^{iQ_m x} \langle \stackrel{*}{\psi} (t, x, s) \psi(t, x, s) \rangle dx.$$

We are again faced with a problem of giving a rigorous meaning to the integrals divided by the volume V of the entire space R^3 in the right hand side of (2.2). For this we suppose that the reduced density matrixes (2.1) have the following cluster properties

$$\left\langle \psi(t,x,\sigma)\psi(t,y,\tau)\right\rangle = \left\langle \psi(t,x,\sigma)\right\rangle \langle \psi(t,y,\tau)\rangle,$$

$$\left\langle \psi(t,x,\sigma)\psi(t,y,\tau) \stackrel{*}{a}(t,z)\right\rangle = \left\langle \psi(t,x,\sigma)\right\rangle \langle \psi(t,y,\tau)\rangle \langle \stackrel{*}{a}(t,z)\rangle,$$

$$\left\langle \psi(t,x,\sigma)\psi(t,y,\tau)a(t,z')\right\rangle = \left\langle \psi(t,x,\sigma)\right\rangle \langle \psi(t,y,\tau)\rangle \langle a(t,z')\rangle, \qquad (2.3)$$

$$\left\langle \psi(t,x,\sigma)\right\rangle = \sum_{m} e^{iQ_{m}x} \left\langle \psi(t,Q_{m},\sigma)\right\rangle, \qquad \left\langle \psi(t,y,\tau)\right\rangle = \sum_{m} e^{-iQ_{m}x} \langle \psi(t,Q_{m},\tau),$$

$$\left\langle \stackrel{*}{a}(t,z)\right\rangle = \sum_{m} e^{iQ_{m}z} \langle \stackrel{*}{a}(t,Q_{m})\rangle, \qquad \left\langle a(t,z')\right\rangle = \sum_{m} e^{-iQ_{m}z'} \langle a(t,Q_{m}),$$

for all $t \ge 0$.

Note that, as it is commonly accepted in quantum physics, $\langle \psi(t, Q_m, \sigma) \rangle$, $\langle \psi(t, Q_m, \tau) \rangle$, $\langle \dot{a}(t, Q_m) \rangle$, $\langle a(t, Q_m) \rangle$ means the corresponding Fourier transform with the momentum Q_τ Substituting (2.3) in (2.2) one obtains by analogy with (1.12)

$$\begin{split} i\frac{\partial}{\partial t} \Big(\Big\langle \overset{*}{\psi}(t,y,\sigma) \Big\rangle \langle \psi(t,x,\tau) \rangle \Big) = \\ = \Big[-\Big(\frac{\Delta x}{2m} + \mu \Big) + \Big(\frac{\Delta y}{2m} + \mu \Big) \Big] \Big(\Big\langle \overset{*}{\psi}(t,y,\sigma) \Big\rangle \langle \psi(t,x,\tau) \rangle \Big) + \\ + \sum_{m} \Big[e^{iQ_{m}x} g(Q_{m}) \langle \overset{*}{a}(t,Q_{m}) \rangle + e^{-iQ_{m}x} g(Q_{m}) \langle a(t,Q_{m}) \rangle \Big] \langle \overset{*}{\psi}(t,y,\sigma) \rangle \langle \psi(t,x,\tau) \rangle - \\ \cdot \end{split}$$

(2.4)

$$-\sum_{m} \left[e^{iQ_{m}y} g(Q_{m}) \langle \overset{*}{a}(t,Q_{m}) \rangle + e^{-iQ_{m}y} g(Q_{m}) \langle a(t,Q_{m}) \rangle \right] \langle \overset{*}{\psi}(t,y,\sigma) \rangle \langle \psi(t,x,\tau) \rangle,$$

$$-i \frac{\partial}{\partial t} \langle \overset{*}{a}(t,z) \rangle = \Delta^{\frac{1}{2}} \langle \overset{*}{a}(t,z) \rangle + \sum_{s,m} e^{+iQ_{m}z} g(Q_{m}) \left(\langle \overset{*}{\psi}(t,s) \rangle \langle \psi(t,s) \rangle \right) (-Q_{m}),$$

$$i\frac{\partial}{\partial t}\langle a(t,z')\rangle = \Delta^{\frac{1}{2}}\langle a(t,z')\rangle + \sum_{s,m} e^{-iQ_mz'} g(Q_m) \Big(\Big\langle \overset{*}{\psi}(t,s) \Big\rangle \langle \psi(t,s)\rangle \Big) (Q_m),$$

where by $(\langle \psi(t,s)\rangle \langle \psi(t,s)\rangle)(\pm Q_m)$ is denoted the Fourier transform of $\left(\left\langle \psi(t,x,s)\right\rangle \langle \psi(t,x,s)\right\rangle\right)$ at momentum $\pm Q_m$. By using the method of separation of variables in the first equation one obtains the

following system of nonlinear equations

$$-i\frac{\partial}{\partial t}\langle \stackrel{*}{\psi}(t,x,\sigma)\rangle = \left(-\frac{\Delta}{2m} - \mu\right)\langle \stackrel{*}{\psi}(t,x,\sigma)\rangle +$$

$$+ \left[\Delta^{\frac{1}{4}}\langle \stackrel{*}{a}(t,x)\rangle + \Delta^{\frac{1}{4}}\langle a(t,x)\rangle\right]\langle \stackrel{*}{\psi}(t,x,\sigma)\rangle,$$

$$i\frac{\partial}{\partial t}\langle \psi(t,x,\tau)\rangle = \left(-\frac{\Delta}{2m} - \mu\right)\langle \psi(t,x,\tau)\rangle +$$

$$+ \left[\Delta^{\frac{1}{4}}\langle \stackrel{*}{a}(t,x)\rangle + \Delta^{\frac{1}{4}}\langle a(t,x)\rangle\right]\langle \psi(t,x,\tau)\rangle,$$

$$(2.5)$$

$$-i\frac{\partial}{\partial t}\langle \stackrel{*}{a}(t,x)\rangle = \Delta^{\frac{1}{2}}\langle \stackrel{*}{a}(t,x)\rangle + \sum_{s}\Delta^{\frac{1}{4}}\left(\langle \stackrel{*}{\psi}(t,x,s)\rangle\langle \psi(t,x,s)\rangle\right),$$

$$i\frac{\partial}{\partial t}\langle a(t,x)\rangle = \Delta^{\frac{1}{2}}\langle a(t,x)\rangle + \sum_{s}\Delta^{\frac{1}{4}}\left(\langle \stackrel{*}{\psi}(t,x,s)\rangle\langle \psi(t,x,s)\rangle\right)$$

where by $\Delta^{\frac{1}{2}}$ and $\Delta^{\frac{1}{4}}$ are denoted the operators that correspond to the operators of multiplication by the function $\omega(Q_n)$ and $g(Q_m)$ respectively in the Fourier transform. In the last two equations we again used that the sets $\{Q_m\}$ and $\{-Q_m\}$ coincide.

Now apply the operator $-i\frac{\partial}{\partial t}$ and $i\frac{\partial}{\partial t}$ to the third and fourth equation respectively. One obtains

$$-\frac{\partial^{2}}{\partial t^{2}}\langle \overset{*}{a}(t,x)\rangle = -\omega_{0}^{2} \Delta \langle \overset{*}{a}(t,y)\rangle + \sum_{s} \Delta^{\frac{3}{4}} \left(\langle \overset{*}{\psi}(t,x,s)\rangle \langle \psi(t,x,s)\rangle\right) +$$

$$+ \sum_{s} \Delta^{\frac{1}{4}} \left\{ \left(-\frac{\Delta}{2m} \langle \overset{*}{\psi}(t,x,s)\rangle \right) \langle \psi(t,x,s)\rangle + \langle \overset{*}{\psi}(t,x,s)\rangle \left(\frac{\Delta}{2m} \langle \psi(t,x,s)\rangle \right) \right\}, \tag{2.6}$$

$$\begin{split} -\frac{\partial^2}{\partial t^2}\langle a(t,x)\rangle &= -\omega_0^2 \triangle \langle a(t,x)\rangle + \\ &+ \sum_s \bigg\{ \triangle^{\frac{3}{4}} \big(\langle \overset{\star}{\psi} (t,x,s)\rangle \langle \psi(t,x,s)\rangle \big) + \\ \\ &+ \triangle^{\frac{1}{4}} \bigg[\bigg(\frac{\triangle}{2m} \langle \overset{\star}{\psi} (t,x,s)\rangle \bigg) \langle \psi(t,x,s)\rangle - \langle \overset{\star}{\psi} (t,x,s)\rangle \bigg(\frac{\triangle}{2m} \langle \psi(t,x,s)\rangle \bigg) \bigg] \bigg\}, \\ \\ & \triangle^{\frac{4}{3}} &= \triangle^{\frac{1}{2}} \cdot \triangle^{\frac{1}{4}}. \end{split}$$

Now add the left and right hand sides of (2.6). One obtains

$$-\frac{\partial^{2}}{\partial^{2}t} \left(\langle \overset{\star}{a}(t,x) \rangle + \langle a(t,x) \rangle = -\omega_{0}^{2} \Delta \left(\langle \overset{\star}{a}(t,x) \rangle + \langle a(t,x) \rangle \right) +$$

$$+2 \sum \Delta^{\frac{3}{4}} \left(\langle \overset{\star}{\psi}(t,x,s) \rangle \langle \psi(t,x,s) \rangle \right).$$
(2.7)

Apply to the left and right hand side of (2.7) the operator $\Delta^{\frac{1}{4}}$. One obtains

$$-\frac{\partial^{2}}{\partial t^{2}}\left(\Delta^{\frac{1}{4}}\langle \overset{\bullet}{a}(t,x)\rangle + \Delta^{\frac{1}{4}}\langle a(t,x)\rangle\right) =$$

$$= -\omega_0^2 \Delta \left(\Delta^{\frac{1}{4}} \langle \mathring{a}(t,x) \rangle + \Delta^{\frac{1}{4}} \langle a(t,x) \rangle \right) - 2\alpha \sum_s \Delta \left(\langle \mathring{\psi}(t,x,s) \rangle \langle \psi(t,x,s) \rangle \right), \tag{2.7'}$$

$$\alpha = \omega_0 g_0^2$$
.

Denote by

$$w(t, x) = \Delta^{\frac{1}{4}} \langle a(t, x) \rangle + \Delta^{\frac{1}{4}} \langle a(t, x) \rangle.$$
 (2.8)

Then equation (2.7') looks like the following wave equation for w(y)

$$-\frac{\partial^2}{\partial t^2}w(t,x) + \omega_0^2 \Delta w(t,x) = -2\alpha \sum_s \Delta \left(\langle \psi(t,x,s) \rangle \langle \psi(t,x,s) \rangle \right). \tag{2.9}$$

We have also the equations for $\langle \psi(t,x,s) \rangle$ and $\langle \psi(t,x,s) \rangle$

$$-i\frac{\partial}{\partial t}\langle \dot{\psi}(t,x,s)\rangle = \left(-\frac{\Delta}{2m} - \mu\right)\langle \dot{\psi}(t,x,s)\rangle + w(x)\langle \dot{\psi}(t,x,s)\rangle, \tag{2.10}$$

2.89

$$i\frac{\partial}{\partial t}\langle\psi(t,x,s)\rangle = \left(-\frac{\Delta}{2m} - \mu\right)\langle\psi(t,x,s)\rangle + w(x)\langle\psi(t,x,s)\rangle.$$

It follows from (2.9), (2.10) that and $\langle \psi(t,x,s) \rangle$, $\langle \psi^*(t,x,s) \rangle$ do not depend on spin s

$$\langle \psi(t, x, s) \rangle = \langle \psi(t, x) \rangle, \qquad \langle \psi(t, x, s) \rangle = \langle \psi(t, x) \rangle$$

if initial data do not depend on it.

Thus we have proved the following theorem.

Theorem 3. The equations for nonequilibrium reduced density matrixes (2.4) are equivalent to nonlinear equations (2.9), (2.10) if initial reduced density matrixes satisfy condition (2.3). We consider $\langle \psi(t,x) \rangle$ as the wave function of electron and w(t,x) as lattice displacements.

Equations (2.9), (2.10) have been derived in the one dimensional case by author and Enolskij [6, 7].

Note that in book [5] and paper [8] another, different from (2.9), (2.10), equations have been derived on basis of postulated Hamiltonians with respect to two functions $\psi(t,x)$ and w(t,x). Our equations (2.9), (2.10) follows directly from equation (2.4) for nonequilibrium reduced density matrixes.

2.2. Soliton solution of equation (2.9), (2.10) in one-dimensional case. Consider equations (2.9), (2.10) in one-dimensional case when $\Delta = \frac{\partial^2}{\partial x^2}$, $x \in \mathbb{R}^1$. For the sake of simplicity we will denote $\langle \psi(t,x) \rangle$ by $\psi(t,x)$. Equations (2.9), (2.10) look like those

$$-\frac{\partial^2}{\partial t^2}w(t,x) + \omega_0^2 \frac{\partial^2}{\partial x^2}w(t,x) = -4\alpha \frac{\partial^2}{\partial x^2}|\psi(t,x)|^2, \qquad (2.9')$$

$$i\frac{\partial}{\partial t}\psi(t,x) = \left(-\frac{1}{2m}\frac{\partial^2}{\partial x^2} - \mu\right)\psi(t,x) + w(t,x)\psi(t,x).$$
 (2.10')

Consider solution of (2.9'), (2.10') such that

$$w(t,x) = w(x - Vt - x_0), \qquad |\psi(t,x)|^2 = |\psi(x - Vt - x_0)|^2.$$

From equation (2.9') one obtains

$$\frac{\partial^2}{\partial \zeta^2} w(\zeta) = -\frac{4\alpha}{\omega_0^2 - V^2} \frac{\partial^2}{\partial \zeta^2} |\psi(\zeta)|^2, \quad \zeta = x - Vt - x_0.$$

We suppose that $V^2 < \omega_0^2$.

This equation is satisfied of

$$w(\zeta) = -\frac{4\alpha}{\omega_0^2 - V^2} |\psi(\zeta)|^2.$$

Then the second equation (2.10') is reduced to well known nonlinear Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(t,x) + \left(\frac{1}{2m}\frac{\partial^2}{\partial x^2} + \mu\right)\psi(t,x) + \frac{4\alpha}{\omega_0^2 - V^2}|\psi(t,x)|^2\psi(t,x) = 0.$$

By using the following transformation of the wave function

$$\psi(t,x) = e^{i\mu t}\psi'(t,x) \tag{2.11}$$

and the scaling transformation of the variables

$$t' = \frac{2\alpha}{\omega_0^2 - V^2}t, \quad x' = \sqrt{\frac{4\alpha m}{\omega_0^2 - V^2}x},$$
 (2.12)

one obtains the standard nonlinear Schrödinger equation

$$i\frac{\partial}{\partial t'}\psi'(t',x') + \frac{\partial^2}{\partial x'^2}\psi'(t,x') + 2|\psi'(t',x')|^2\psi'(t',x') = 0.$$
 (2.13)

Equation (2.13) has well known one-soliton solution [9, 10]

$$\psi'(t', x') = 2i\eta \frac{\exp i\left(-2\xi x' - 4(\xi^2 - \eta^2)t' - \varphi_0 + \frac{\pi}{2}\right)}{\cosh 2\eta(x' - 4\xi t' - x_0)}$$
(2.14)

where the constants ξ , η , x_0 , φ_0 are defined by initial data $\psi'(0,x)$. Substituting transformation (2.11), (2.12) into (2.14) one finally obtains

$$\psi(t,x) = 2i\eta \frac{\exp i\left(\frac{1}{2}v2mx - \left(\frac{v^2}{4}2m - \frac{u^2}{4(2m)}\right)t + \mu t - \varphi_0 + \frac{\pi}{2}\right)}{\operatorname{ch}\frac{u}{2}(x - vt - x_0)}$$

where

$$v = -4\xi\sqrt{\frac{\alpha}{(\omega_0^2 - V^2)m}}, \qquad u = 4\eta\sqrt{\frac{4\alpha m}{\omega_0^2 - V^2}}.$$

For the lattice displacements one obtains

$$w(\xi) = \frac{-4\alpha}{\omega_0^2 - V^2} 4\eta^2 \frac{1}{\cosh^2 \frac{u}{2} (x - vt - x_0)}.$$

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