THE STRUCTURE OF THE GROUND STATE AND LOW-TEMPERATURE THERMODYNAMIC PROPERTIES OF A ONE-DIMENSIONAL ELECTRON LATTICE SYSTEM

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The structure of the ground state and low-temperature thermodynamic properties of a one-dimensional generalized Wigner crystal on a disordered host-lattice are investigated. It is established that the spectrum of elementary excitations has a gapless structure at any finite values of the host-lattice disorder. The instability of the ground state of the system with respect to infinitesimal disturbances of the host-lattice order is discovered. This instability results in the violation of a long-range order in the system. The influence of the long-range action of the interparticle repulsion potential on thermodynamic properties of the system is considered.

1. Introduction

In the last few decades, investigators show the strong interest in low-dimensional and multilayer lattice conductors, where charge carriers (electrons or holes) are essentially separated spatially from impurities. In such conductors, the potential induced by impurity ions in conducting layers slightly differs from a constant value, and the thermodynamic and kinetic properties are determined by the potential of electron-electron (hole-hole) repulsion. Among conductors of such a kind, the systems where the tunneling of charge carriers between sites of a host-lattice (a substrate) is suppressed by their mutual Coulomb repulsion attract a special attention, because charge carriers in these systems turn out to be *self-localized*. The exact criterion of the Coulomb self-localization (CS) is formulated as the smallness of the overlap integral t as compared to the typical variation $\delta\varepsilon \sim (a_0/\bar{l})^2\bar{\varepsilon}$ of the Coulomb energy of a charge carrier as it hops (tunnels) between neighbor sites of the host-lattice (HL). Here, a_0 is the average distance between cites of the HL, $\bar{l}$ is the average distance between particles, and $\bar{\varepsilon}$ is the average Coulomb energy per particle. This condition can be realized in MOSFET structures [1] or in other semiconductor heterostructures. As a typical example of the described systems, one can name MOSFET compounds with an impurity hole zone formed when a part of impurity electrons passes from a semiconductor to a metal (which represents one of the components of a heterostructure) [1, 2]. Another important group of CS compounds is formed by quasi-one-dimensional organic conductors [3]. The latest achievements in nanotechnology allow one to create new types of CS systems, for example, the arrays of quantum dots exchanging electrons [4], networks of metal nanograins with tunnel couplings, whose role is played by organic molecules of various types [5]. In addition, there are all reasons for supposing that the CS criterion ($t < \delta\varepsilon$) can be also realized in multilayer metal-oxides of the type of high-temperature semiconductors under the condition that the concentration of impurities is not too high.

The first theoretical investigation of the structure of the ground state (GS) in CS systems was carried out by Hubbard [3]. He considered a one-dimensional (1D) ensemble of electrons on a *strictly periodic* HL in the limit of strong CS ($t \ll \delta\varepsilon$), when the dynamic effects appearing due to the finiteness of t are negligible and electrons are localized at the sites of the HL to a high accuracy. In the mentioned paper, it was shown that the GS has an incommensurable structure in the general case. This structure depends only on the electron density $n_e = N/N_s$ (N and N_s are the number of electrons and sites of the HL, respectively; $N, N_s \to \infty$), but it doesn't

depend on the form of the potential of electron-electron repulsion $v(r)$ (r is the distance between electrons). The potential $v(r)$ must only satisfy the following limitations obvious from the physical point of view: $v(r) > 0$; $v(r) \to 0$ at $r \to \infty$ more rapidly than $1/r$; $v(r)$ is an everywhere convex function of r. If the above limitations are met, the GS structure is universal. In addition, Hubbard postulated a universal algorithm of constructing the GS [3]. Later on, Hubbard's hypothesis was completely confirmed and validated in [6, 7], and the considered 1D structures were called in the literature as a "generalized Wigner crystal" (GWC). According to the GWC theory, the position of the i-th electron in the GS (x_i) measured in the units of a_0 is described with a simple formula [6]:

$$x_i = [i/n_e + \phi].$$

Here, $[\ldots]$ denotes the integer part of a number, and ϕ is an arbitrary value (the initial phase). As follows from this formula, the distances between each pair of electrons $x_{i+1} - x_i$ can be equal to $[1/n_e]$ or $[1/n_e + 1]$ depending on i and n_e. Hence, even in the case of a regular HL, interelectron distances don't correspond to the minimum of the potential energy of electron-electron interaction (excluding the trivial case where the concentrations are given by $n_e = 1/m, m = 1, 2, 3\ldots$). In particular, this results in a rather specific zero-temperature dependence of n_e on the chemical potential μ which represents a well-developed fractal structure of the "devil staircase" type [7]. Hubbard's results were recently enriched and generalized in [8–10]. The former two works deal with the low-temperature thermodynamics of a 1D GWC, while it was shown in [10] that two-dimensional (2D) systems of this type are characterized with an effective decrease of their dimension. The last circumstance allows one to find the GS structure on the basis of a universal analytical procedure (a 2D generalization of Hubbard's 1D algorithm).

The influence of the HL disorder on the low-temperature behavior and peculiarities of the GS of CS conductors represents an absolutely natural problem, as the majority of real systems of such a kind are disordered. For example, in MOSFET conductors, this disorder is conditioned by a chaotic nature of the distribution of impurities [1,11]. In addition, the disorder in many nanostructures [4,5] is determined by a spread in tunnel couplings. Moreover, there are reasons to suppose that 1D salts of the TCNQ type [3] also belong to this class in view of the imperfection of their chemical structure.

In the case of $n_e \ll 1$ and $t \ll \delta\varepsilon$, the GS configuration of an HL electron system (regardless of its dimension D) represents a slightly distorted Wigner crystal (WC). In such a system, electrons shift from their ideal positions by *discrete* values $\sim a_0$ which are considerably smaller than the lattice constant of the WC $l_{\rm WC} \sim \bar{l}$ ($a_0/l_{\rm WC} \sim n_e^{1/D}$). Here, by "ideal" positions, we understand those of electrons in the WC. If the HL is irregular, the GS configuration becomes disordered in spite of the smallness of shifts of electrons from the WC sites. Such a system can be called a "Wigner glass on a disordered HL" (WGDHL). We'd like to pay attention to the fact that, even in the considered limit of a low electron density, the low-temperature behavior of a WGDHL differs qualitatively from that of an ordinary (*continual*) Wigner crystal subjected to an external periodic or random field. The reason for such a difference lies, first of all, in the fact that all the low-energy excitations in a WGDHL are conditioned by transitions (hops) of electrons by small random but *fixed* distances $\sim a_0$. One of the consequences of such a structure is, for example, the absence of small vibrations in the system, i.e. the absence of acoustic phonons (in the usual meaning of this term).

The basic object of this paper is the construction of a low-temperature thermodynamics and the study of properties of the GS of a 1D WGDHL.

2. Hamiltonian

According to [3, 8], we neglect the tunneling of charge carriers (let's consider electrons for the sake of distinctness) between sites of the HL. In this case, the Hamiltonian of the system under investigation can be given by

$$\mathcal{H} = \frac{1}{2}\sum_{i \neq j} v(|x_i - x_j|) n_i\, n_j.$$

Here, x_i are dimensionless *chaotically* located coordinates of the sites of the 1D HL; the independent variable $n_i = 0\,, 1$ stands for the number of electrons at the i-th site (the occupation number); $v(|x_i - x_j|)$ is the screened Coulomb potential of electron-electron repulsion; the summation is carried out over all the sites of the HL. As the details of the behavior of $v(r)$ are not essential for the further consideration, we extend the class of $v(r)$ under study imposing only those physically obvious restrictions which we pointed out in Introduction. In the Hamiltonian, we omit spin indices, because $n_e \ll 1$, and, hence, the effects associated with the Fermi statistics turn out to be negligible.

In the limit of low temperatures and concentrations, the distances l_n between the neighbor electrons with numbers $n+1$ and n slightly differ from the average interelecron distance $\bar{l} = a_0/n_e$. Representing l_n in the form of $l_n = \bar{l} + \xi_n$, where ξ_n is a small random additive $\sim a_0$, it is convenient to introduce ξ_n as new independent variables (instead of the occupation numbers n_i). The quantities ξ_n can be considered as "dipole lengths" $e\xi_n$ (e is the electron charge), which begin from the "ideal" positions of the WC $n\bar{l}$ ($n = 1, \ldots, N$) and come to the end at one of the HL sites located in a small neighborhood of these "ideal" positions. Without losing generality, one can always choose these neighborhoods in such a way that the number of the HL sites will be the same for all n. We denote this number as ν, and the neighborhoods of the "ideal" WC positions chosen in the indicated way will be called "clusters". Hence, every "cluster" includes one electron. The distances between the "clusters" $\sim \bar{l}$. For the sake of convenience, let's number the HL sites by index k ($k = 1, 2, \ldots, \nu$ for all n). In this case, ν possible positions of electron n are given by $n\bar{l} + \xi_n^k$, where ξ_n^k are random fixed numbers. For the further consideration, it's convenient to renumber the quantities ξ_n^k in each "cluster" in such a way that they form an ascending sequence: $\xi_n^k < \xi_n^{k+1}$ ($\xi_n^{k+1} - \xi_n^k \sim a_0$). The spread in values of ξ_n^k (i.e. $\xi_n^\nu - \xi_n^1$) must be $\ll \bar{l}$, i.e. $\nu a_0 \ll \bar{l}$. The examples of 1D and 2D disordered HLs are depicted in Fig. 1,*a* and Fig. 1,*b*, respectively. It's worth noting that the "dipole lengths" ξ_n^k introduced here can be both positive and negative.

It is convenient to consider the quantities ξ_n^k as eigenvalues of the displacement operator $\hat{\xi}_n$. Depending on the configuration, one of these ν values is realized [1]. Accounting for the smallness of $|\xi_n^k|/\bar{l}$, one can expand the Hamiltonian in powers of $\hat{\xi}_n$ confining to quadratic terms. As a result, we get

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_d + N\varepsilon_{\rm WL},$$

where $\varepsilon_{\rm WL} \sim \bar{\varepsilon}$ represents the WC energy per electron, and the Hamiltonian of the dipole system

$$\hat{\mathcal{H}}_d = \hat{\mathcal{H}}_{dd} + \hat{\mathcal{H}}_{dl}.$$

Here, $\hat{\mathcal{H}}_{dd}$ is the operator of the dipole-dipole interaction, $\hat{\mathcal{H}}_{dl}$ is the operator of the interaction between the dipole system and the WC. The Hamiltonian $\hat{\mathcal{H}}_{dd}$ reads

$$\hat{\mathcal{H}}_{dd} = -e^2 \sum_{n=1}^{N} \sum_{m=1}^{M} b(m) \hat{\xi}_n \hat{\xi}_{n+m},$$

where M is the maximal number of neighbor dipoles, whose interaction is taken into consideration. For example, $M = 1$ corresponds to the approximation of the nearest neighbors. At $M = 2$, we take into account the interaction between the nearest and next nearest neighbors and so on. The function

$$b(m) = \frac{1}{2} \frac{d^2 v(r)}{dr^2}|_{r=m\bar{l}}.$$

The second term

$$\hat{\mathcal{H}}_{dl} = e^2 B \sum_{n=1}^{N} \hat{\xi}_n^2, \quad B = \sum_{m=1}^{M} b(m).$$

Finally, we get

$$\hat{\mathcal{H}}_d = \frac{e^2}{2} \sum_{n=1}^{N} \sum_{m=1}^{M} b(m) (\hat{\xi}_n - \hat{\xi}_{n+n})^2. \tag{1}$$

The Hamiltonian $\hat{\mathcal{H}}_d$ can be represented now in the form

$$\hat{\mathcal{H}}_d = \sum_{n=1}^{N} \hat{\mathcal{H}}_n, \quad \hat{\mathcal{H}}_n = \sum_{m=1}^{M} \hat{\varepsilon}(\hat{\xi}_n, \hat{\xi}_{n+m}), \tag{2}$$

where

$$\hat{\varepsilon}(\hat{\xi}_n, \hat{\xi}_{n+m}) = \frac{e^2}{2} b(m) (\hat{\xi}_n - \hat{\xi}_{n+m})^2. \tag{3}$$

The matrix elements (3) $\varepsilon_m(\xi_n^i, \xi_{n+m}^j)$ stand for the interaction energies of the dipoles located at sites n and $n+m$ and occupying "states" i and j, respectively. Expressions (1) and (3) reflect the constancy of the system energy with respect to a simultaneous shift of all electrons by an arbitrary distance.

Transitions (hops) of electrons from one position to another inside the "clusters" form the low-energy excitation spectrum of the system. Such excitations can be called intracluster ones. Their typical energy $(a_0/\bar{l})^2 \bar{\varepsilon} \ll \bar{\varepsilon}$ ($\bar{\varepsilon}$ is the typical energy of electron transitions from one "cluster" to another). Hence, when constructing the low-temperature thermodynamics of the system under study, one can neglect the transitions of electrons from one "cluster" to another. Several examples of electron configurations are depicted in Fig. 1,*c*.

In the present paper, we consider the case of complete chaos. This means that there are no correlations between

[1] Discreteness of the spectrum of the operator $\hat{\xi}_n$ is conditioned by discreteness of the positions of HL sites ("frozen chaos") and reflects a qualitative difference between a WGDHL and systems of the Wigner glass type, where such a spectrum is always continuous.

both ξ_n^k and $\xi_{n'}^k$ with $n \neq n'$ and ξ_n^k, $\xi_n^{k'}$ with $k \neq k'$. Therefore, the only characteristic of the given "frozen" chaos is the distribution of HL sites in space or, in other words, the distribution ξ_n^k as a function of $k = 1, \ldots \nu$ for all $n = 1, \ldots, N$. In order to describe such a distribution, we introduce the function $W(\xi^1, \ldots, \xi^\nu)$ which is the probability for the "cluster" to be realized by a set of quantities $\xi^1, \ldots, \xi^\nu$. According to what was said above, $W(\xi^1, \ldots, \xi^\nu) \neq 0$ at $\xi^1 < \xi^2 < \ldots < \xi^\nu$ and $|\xi^k| \ll \bar{l}$. $W(\xi^1, \ldots, \xi^\nu)$ is the product

$$W(\xi^1, \ldots, \xi^\nu) = \prod_{k=1}^{\nu} w_k(\xi^k),$$

where $w_k(x)$ $(k = 1, 2, \ldots, \nu)$ differ from one another only in displacements:

$$w_k(x) = w(x + (k-1)a_0 - (\nu-1)a_0/2).$$

The function $w(x)$ stands for the probability for an HL site to be located at a distance x from the origin of coordinates. For computer calculations, $w(x)$ was chosen in such a way that $w(x) = 1/\rho$ if $|x| \leq \rho$ $(\rho \leq a_0)$ and $w(x) = 0$ otherwise. The quantity ρ is interpreted as the disorder parameter of the system. The complete disorder corresponds to $\rho = a_0$. If $\rho \ll a_0$, the quantities ξ_n^k are slightly shifted with respect to the positions $(k-1)a_0 - (\nu-1)a_0/2$, but these displacements don't correlate. The limiting case $\rho \to 0$ corresponds to a periodic HL with a lattice constant a_0 and to the equidistant configuration of the GS with a lattice constant $\bar{l}$.

3. Low-temperature Thermodynamics

The statistical sum of the system under study has a form

$$Z(N,T) = \sum \exp\left(-\frac{\hat{\mathcal{H}}_d}{T}\right). \qquad (4)$$

Here, T denotes the temperature in energy units, and the summation is carried out over all ν^N microscopical configurations. As a matter of principle, the free energy $F(N,T) = -T \ln Z(N,T)$ can be calculated with the help of the replica technique. But in this case, such a technique turns out to be very ineffective as the microscopical variables ξ_n are *random* unlike the *regular* variables s_n in spin glasses. In the considered 1D case, one can overcome this difficulty with the help of the technique which is proposed here and based on the representation of the statistical sum (4) of the system (1) in the form of a product of random non-Hermitian

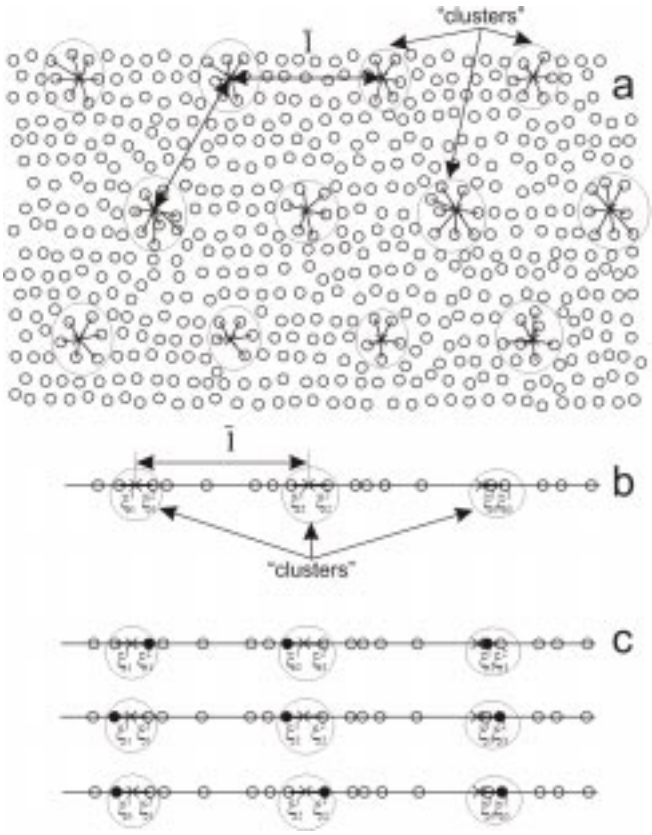

Fig. 1. Examples of disordered 2D (a) and 1D (b) HLs. Symbols $\times$ denote "ideal positions" of the WC, circles denote HL sites; (c) gives some possible configurations of electrons on a 1D HL

modified transfer-matrices $\hat{P}(n)$. Imposing the periodical boundary conditions $\xi_{N+1}^k = \xi_1^k$ $(k = 1, \ldots, \nu)$, one can represent the statistical sum (4) as [13]

$$Z(T,N) = \mathrm{Tr}\left(\prod_{n=1}^{N} \hat{R}(n)\right). \qquad (5)$$

In this case, the symbol Tr stands for the spur of a matrix. It is just the fact that (5) is expressed in terms of the product of matrices $\hat{R}(n)$ allows one to quickly compute the thermodynamic characteristics of a 1D WGDHL. Indeed, if this technique is used, the computation time is proportional to N, while it is proportional to ν^N for expression (4).

In the approximation of the nearest neighbors ($M = 1$), $\hat{R}(n)$ has a form

$$R_{i,j}(n) = \exp\left(-\frac{\varepsilon(\xi_n^i, \xi_{n+1}^j)}{T}\right).$$

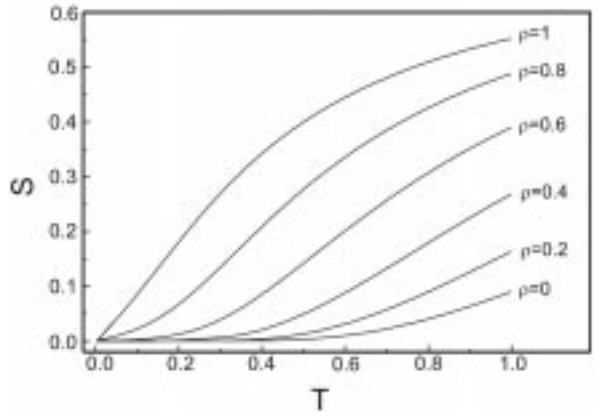

Fig. 2. Dependences $s(T)$ at various values of ρ and $M = 1$

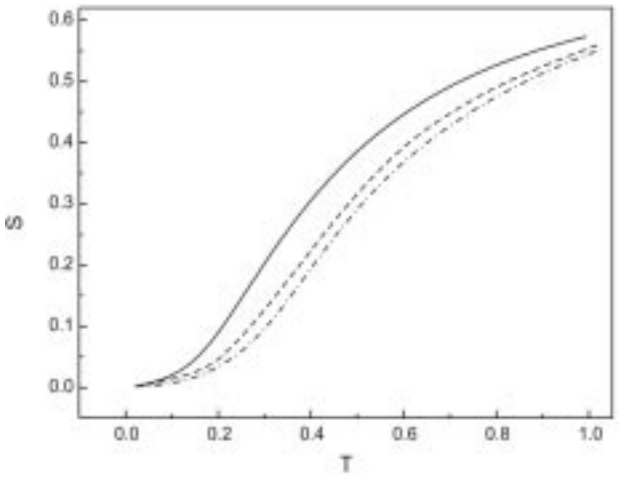

Fig. 3. Dependences $s(T)$ at $\rho = 1/2$, $v(r) = 1/r$, and various M. The continuous curve corresponds to $M = 1$, the dashed one — to $M = 2$, and the dash-dotted line — to $M = 3$

For the interaction between an arbitrary number of neighbors to be taken into account, it is convenient to introduce the matrices $\hat{A}^m(n)$ defined in the following way:

$$A^m_{i,j}(n) = \exp\left(-\frac{\varepsilon(\xi^i_n, \xi^j_{n+m})}{T}\right) \tag{6}$$

It is easy to notice that, in the approximation allowing for the interactions between the nearest and next-nearest neighbors, the matrices $\hat{R}(n)$ take the form

$$R(n)_{i,j,k} = A^1_{i,j}(n)A^2_{i,k}(n).$$

In the general case of the account of M neighbors, the matrices $\hat{R}(n)$ are expressed in terms of $\hat{A}$ as

$$R(n)_{i,k_1,k_2,k_3,\ldots,k_M} =$$

$$= A^1_{i,k_1}(n)A^2_{i,k_2}(n)A^3_{i,k_3}(n)\ldots A^M_{i,k_M}(n), \tag{7}$$

while the multiplication function is defined as

$$(P(n)P(n+1))_{i,k_1,k_2,\ldots,k_M} =$$

$$= \sum_{j=1}^{\nu} P(n)_{i,j,k_1,k_2,\ldots,k_{M-1}} P(n+1)_{j,k_1,k_2,\ldots,k_M}. \tag{8}$$

For example, for $M = 1$,

$$(R(n)\cdot R(n+1))_{i,k} = \sum_{j=1}^{\nu} R(n)_{i,j}R(n+1)_{j,k}.$$

For $M = 2$, we get

$$(R(n)\cdot R(n+1))_{i,k_1,k_2} = (R(n)\cdot R(n+1))_{i,k_1,k_2} =$$

$$= \sum_{j=1}^{\nu} R(n)_{i,j,k_1}R(n+1)_{j,k_1,k_2} =$$

$$= \sum_{j=1}^{\nu} A^1_{i,j}(n)A^2_{i,k_1}(n)A^1_{j,k_1}(n+1)A^2_{j,k_2}(n+1).$$

In computer calculations, the parameters e and a_0 were taken equal to 1, and the disorder parameter $0 \le \rho \le 1$. In the case of $\rho = 1$, the system is completely disordered. For $\rho \ll 1$, there exists a slight disorder, i.e. the quantities ξ^1_n and ξ^2_n take random values within short intervals $[1-\rho, 1]$ and $[-1, -1+\rho]$, respectively. In the case of $\rho = 0$, the system is equivalent to a one-dimensional ferromagnetic chain of spins with $s = 1/2$ and the exchange integral $J = -4b(1)$. The number of electrons in the system amounts to $10^4 - 10^5$ depending on M and ρ. In all the cases, the error of computations was at most 0.1%, i.e. $|1 - f(N,T)/f(2N,T)| < 10^{-3}$, where $f(N,T) = F(N,T)/N$.

A thermodynamic quantity which is mostly sensitive to the degree of disorder of a 1D WGDHL system is the entropy (per particle) as a function of temperature:

$$s(T) = -\frac{\partial}{\partial T} f(N,T). \tag{9}$$

The collections of curves $s(T)$ corresponding to various values of ρ and M obtained with the help of (5)—(8) are depicted in Figs. 2, 3. We'd like to pay attention to the fact that taking into account the long-range interaction results only in a slight modification of the dependences $s(T)$ even in the limit case of the

unscreened Coulomb potential (Fig. 3). As one can see from the figures, the residual value of the entropy $s(0)$ is equal to zero in all the cases (i.e. the Nernst heat theorem *always* holds true). According to Fig. 4, the quantity $s'(T=0)$ is nonzero for all $\rho \neq 0$, which testifies to the gapless character of the excitation spectrum of the considered system at any nonzero values of the disorder parameter. Thereupon, it is natural to study the problem concerning the properties of the excitations realizing such a spectrum. Its complete solving can be reached only after a thorough study of the spatial structure of the ground state.

4. The Structure of the Ground State

All the basic properties of a 1D WGDHL manifest themselves already at $\nu = 2$ and in the nearest neighbor approximation ($M = 1$). That's why for the sake of simplicity, just this case will be considered in the present section. Unlike the frequently used Monte Carlo method, we propose a technique of finding the GS of a 1D WGDHL based on its *accurate* calculation. This technique is grounded on the formalism of modified transfer-matrices (4)—(8). In order to find the GS of the system with Hamiltonian (2), we consider a 1D WGDHL in an external nonuniform electric "field" E. It is assumed that this field is equal to E_0 at the l-th site of the system, and $E = 0$ at all the other sites. The Hamiltonian of such a system has a form

$$\hat{\mathcal{H}}_{d-h} = \hat{\mathcal{H}}_{d-h} = \sum_{n=1}^{N-1} \hat{\varepsilon}(\hat{\xi}_n, \hat{\xi}_{n+1}) - E_0 \hat{\xi}_l, \qquad (10)$$

where $l = 1, 2, \ldots, N$. After substituting (10) in (4), we obtain

$$P(n)_{i,j} = \exp\left(-\frac{\varepsilon(\xi_n^i, \xi_{n+1}^j) + \delta_{i,j}\delta_{n,l}E_0\xi_n^i}{T}\right).$$

Here, $\delta_{k,k'}$ is the Kronecker symbol. As a result, the free energy and the average "polarizability"

$$P(T,E) = P(T,E_0,l) = \frac{\partial}{\partial E}\left(\frac{f(T,E)}{T}\right)$$

can be calculated as functions of E. At $T \to 0$, the basic contribution to (4) is made by configurations close to the GS. In the limit $E \to 0$, the value of the quantity $\langle \xi_l \rangle = P(T \to 0, E_0 \to 0, l)$ is negative if $\xi_l^{\mathrm{GS}} > 0$, and $\langle \xi_l \rangle$ is positive otherwise (ξ_l^{GS} is the "length" of the l-th dipole in the ground state). We'd like to pay attention to a peculiarity concerning the numerical calculation of

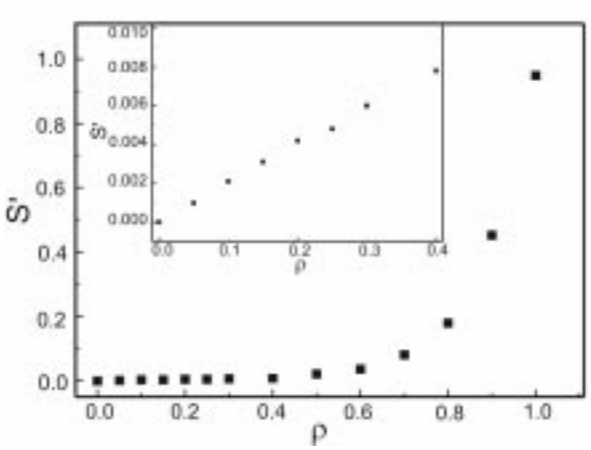

Fig. 4. Dependence of $s'(T=0)$ on the parameter ρ. The inset shows the same dependence in the range of small ρ

the limit $E_0 \to 0$. By virtue of the randomness of the 1D WGDHL structure, energies (3) fluctuate. At certain sites l_0, these energies can take arbitrary small values. In this case, the application of a field E_0 can result in the dipole flip. In order to overcome this difficulty, the polarizability P was calculated at certain small finite values E_0 and $-E_0$. If $< \xi_l(E_0) >$ (the value of $\langle \xi_l \rangle$ corresponding to the field E_0) coincides with $\langle \xi_l(-E_0) \rangle$, then $\xi_l^{\mathrm{GS}} = \langle \xi_{l_0}(E_0) \rangle$. Otherwise, we decrease the field E_0 by a factor of two and repeat the process until the condition $\langle \xi_{l_0}(E_0) \rangle = \langle \xi_{l_0}(-E_0) \rangle$ is satisfied. The system temperature was chosen in such a way that $T \ll E_0$. Calculating $P(T, E_0, l)$ successively for $l = 1, 2, \ldots, N$, one can construct the GS of the 1D WGDHL. Typical structures of the GS of the studied system at various values of the disorder parameter ρ are depicted in Fig. 5.

5. Discussion of the Results

The analysis carried out in Section 4. indicates the domain structure of the GS of a 1D WGDHL at all $\rho \neq 0$. This implies that the GS configuration ξ_l^{GS} must include two types of blocks (domains) alternating with one another: in domains of one kind, all $\xi_l^{\mathrm{GS}} > 0$; in those of another kind, $\xi_l^{\mathrm{GS}} < 0$. At first sight, such a result seems to be doubtful in the case of a slight disorder ($\rho \ll a_0$). Indeed, as was noted above, the considered system is equivalent at $\rho = 0$ to a one-dimensional Ising ferromagnetic. In this case, all ξ_l^{GS} are equal to either -1 or 1 (the two-fold degeneracy of the ground state takes place). At small ρ, the replacement of the dipole ξ_n^{GS} at any site n by the dipole $\approx -\xi_n^{\mathrm{GS}}$ increases the energy

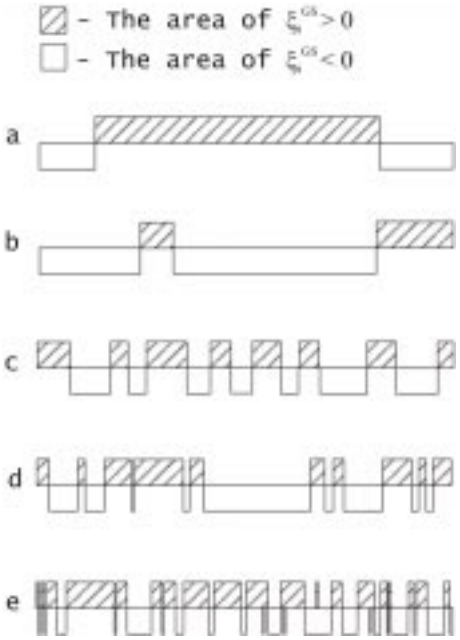

Fig. 5. Examples of the GS configurations of a 1D WGDHL corresponding to the chain including 10^4 sites (a—d) and 400 sites (e) and various values of ρ: a — $\rho = 0.25$, b — 0.3, c — 0.4, d — 0.45, e — 1

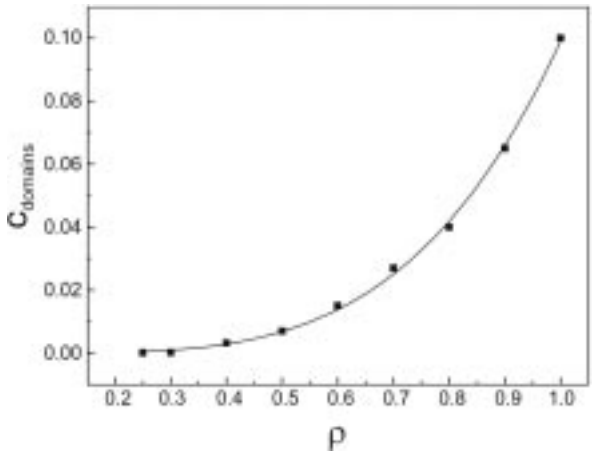

Fig. 6. Concentration of domain walls $c_{\rm domains}$ as a function of ρ. Squares denote the values obtained using the algorithm of constructing the GS of a 1D WGSHL described in Section 4. The continuous line corresponds to the fitting by the function $c_{\rm domains} = c_0\rho^n$ with $c_0 = 0.091$ and $n = 3.95$

of the system by a finite value $\sim 2(ea_0)^2 b(1)$. It would seem that, by this reason, all $\xi_n^{\rm GS}$ must be identical. That is, the long-range ferromagnetic order in the system is preserved, and the spectrum of elementary excitations of a 1D WGDHL with $\rho \ll a_0$ has a gap. By clearly contradicting Fig. 5 and the curves presented in Figs. 2—4, this conclusion would mean that, at a slight disorder, $s'(T)$ exponentially tends to zero with decrease in T. Moreover, at a certain critical ρ, there occurs a phase transition between macroscopic states with the activative and linear dependences of the entropy on temperature. Therefore, we arrive at the conclusion that the ground state of a 1D WGDHL has a domain structure even in the limit $\rho \ll a_0$. In order to understand the nature of its formation, it is necessary to compare the energy of the system with domains $E_{\rm domains}$ with that of the system consisting of dipoles of one kind (E_1 for $\xi_n^{\rm GS} > 0$ or E_2 for $\xi_n^{\rm GS} < 0$). The energy $E_{\rm domains}$ has a form

$$E_{\rm domains} = \sum_{i=1}^{\mathcal{N}} (E_1^i + E_2^i) + (ea_0)^2 \mathcal{N} b(1), \qquad (11)$$

where index i numbers the pairs of domains adjoining each other and having dipoles of unlike signs; $E_{1,2}^i$ are the energies of these domains; $\mathcal{N}$ is the total number of domains in the system; the last term stands for the total energy of domain "walls" (the junctions of domains with $\xi_n^{\rm GS} > 0$ and those with $\xi_n^{\rm GS} < 0$) taken in the zero-order approximation in ρ. The comparison of expression (11), for example, with E_1 gives

$$E_{\rm domain} - E_1 = \sum_{i=1}^{\mathcal{N}} (E_2^i - E_1^i) + (ea_0)^2 \mathcal{N} b(1).$$

In view of the randomness of a 1D WGDHL, the difference between the energies E_1^i and E_2^i fluctuates so that the characteristic energy $|E_2^i - E_1^i| \sim (ea_0\rho)^2 b(1)\sqrt{L}$, where $L = 1/c$ is the characteristic number of sites in a domain, and $c = \mathcal{N}/N$ is the concentration of domain walls. The differences $E_2^i - E_1^i$ can have any signs depending on the positions of the boundaries of domain walls. It is obvious that these boundaries can always be chosen in such a way that all the differences $E_2^i - E_1^i$ were negative. In this case, the difference $E_{\rm domains} - E_1$ stipulated by the loss of energies from domain walls ($E_{\rm domains}$) and the *fluctuation gain* E_1 turns out necessarily to be negative at a sufficiently small value of c, reaching a maximum at $\rho^2/\sqrt{c} \sim 1$, i.e.

$$c_{\rm domains} = c_0\rho^4. \qquad (12)$$

It is worth noting that this estimate agrees completely with the results obtained from the GS structures (Fig. 6). This figure also demonstrates that dependence (c) is universal for all $0 \le \rho \le a_0$. The analysis of the GS structures of a 1D WGDHL shows

that the dependence $c_{\rm domains}(\rho)$ remains qualitatively the same even at $M > 1$, resulting only in a slight decrease of the constant c_0. This is explained by a tougher condition fot the formation of domains and, consequently, by a decrease in their concentration (in the complete accordance with Fig. 3). Thus, we arrive at the conclusion that, in the limit $\rho \ll a_0$, the ground state of the system contains a small but finite concentration of domain walls. This inevitably results in the violation of a long-range order in the system over large spatial intervals, with $L \sim a_0/\rho^4 \gg 1$. That is, a ferromagnetic long-range order existing in the ordered case (at $\rho = 0$, $\xi_n^1 = -\xi_n^2$) turns out to be unstable with respect to an arbitrarily small *random* disturbance of the system.

6. Conclusion

We have investigated the GS structure and the low-temperature thermodynamics of one-dimensional electron systems on disordered HLs. It is shown that the GS structure of these discrete systems contains a small but finite concentration of "domain walls" even in the case of a slight disorder (Figs. 4, 5). As a result, the long-range order is violated. It is established that the entropy $s(T)$ of the 1D WGDHL remains linear in the low-temperature region at all values of the disorder parameter ρ ($0 \le \rho \le 1$) (Figs. 2, 3), which indicates the gapless character of the spectrum of elementary excitations.

New fast numerical methods for the investigation of the GS structures and low-temperature properties of a 1D WGDHL are proposed. They are based on the representation of the statistical sum of a system in terms of modified transfer-matrices. These methods allow one to study the GS configurations of a 1D WGDHL containing $\sim 10^4 - 10^5$ sites (Fig. 5).

The proposed techniques also enable one to calculate thermodynamic functions and to study the GS structure of systems with a long-range potential of interparticle repulsion taking into account the interactions between an arbitrary number of electrons. It is shown that making allowance for the long-range interaction results only in a slight variation of the obtained results (Fig. 3). In particular, this implies that the structure of "domain walls" and the instability of the GS are the properties of the studied system, rather than the peculiarities of the proposed model.

In the nearest future, the author plans to investigate the kinetic properties and the spectrum of low-energy excitations of the system under consideration.

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СТРУКТУРА ОСНОВНОГО СТАНУ І НИЗЬКОТЕМПЕРАТУРНІ ТЕРМОДИНАМІЧНІ ВЛАСТИВОСТІ ОДНОВИМІРНОЇ ЕЛЕКТРОННОЇ ГРАТКОВОЇ СИСТЕМИ

В. В. Славін

Р е з ю м е

Вивчено структуру основного стану і низькотемпературні термодинамічні властивості одновимірного узагальненого вігнерівського кристала на неупорядкованій гратці-матриці. Встановлено, що спектр елементарних збуджень має безщілинну структуру при будь-яких скінченних значеннях разупорядкування гратки-матриці. Виявлено нестійкість основного стану системи стосовно інфінітезимальних порушень упорядкування гратки-матриці. Ця нестійкість приводить до руйнування далекого порядку в системі. Розглянуто вплив дальнодії потенціалу міжчастинкового відштовхування на термодинамічні властивості системи.