

# GENERAL QUESTIONS OF THERMODYNAMICS, STATISTICAL PHYSICS, AND QUANTUM MECHANICS

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## ELEMENTARY EXCITATION SPECTRUM AND LOW-TEMPERATURE THERMODYNAMIC PROPERTIES OF A ONE-DIMENSIONAL STRONGLY CORRELATED ELECTRON LATTICE SYSTEM

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The low-energy spectrum and low-temperature thermodynamic properties of a one-dimensional lattice electron system with long-range interelectron repulsion are studied at an arbitrary electron filling factor,  $c_e$ . It is established that the value of the gap in this spectrum is an oscillating function of the inverse filling factor. This value tends to zero at  $c_e = 1/q$  ( $q = 1, 2, \dots$ ) reaching the maximum at  $c_e = 2/(2q + 1)$ . It is shown that the low-energy spectrum of the system under consideration can be described in terms of one-dimensional structures which are analogs of the domains in one-dimensional spin systems. The question about the decay of these “domains” is considered. The method of modified transfer-matrices is proposed for the investigation of thermodynamic properties of such systems. It is shown that increasing the number of interacting electrons leads to the appearance of more and more fine “stairs” in the low-temperature dependence of the chemical potential on the electron density. The influence of a disorder in host-lattice site positions on the thermodynamic characteristics of the system is considered. It is established that the disorder destroys the “stairs”.

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### 1. Introduction

Low-dimensional layered conductors attract researcher’s interest during the last decades. This interest is mainly caused by a number of unusual thermodynamic and kinetic properties revealed by these systems. Among this class, the narrow-band conductors with long-range interparticle repulsion are of special interest. These systems differ qualitatively from metals (including transition metals), semiconductors, and conductors of

the Hubbard type (the latter ones are characterized by the *locality* of their electron-electron interaction). The study of such systems seems to be of special importance, because a lot of high-temperature superconductive metal oxides (even at “metallic” electron densities) and a number of metal oxides belong to this class of conductors.

Ones of the most famous members of this class are quasi-one-dimensional organic conductors (for example, TCNQ salts of different types). These systems got the name “Generalized Wigner Lattices” (GWL) in the literature. As shown in [1, 2], one can neglect, with good accuracy, the influence of dynamic effects on the ground state structure and the low-temperature thermodynamics of such systems. In addition, the adatom systems belong to this class as well, if the interaction of adatoms with a substrate is sufficiently strong [3]. Another interesting group forming this class is the conductors where the tunneling of charge carriers between host-lattice sites is suppressed by their mutual Coulomb repulsion. In such a case, the whole ensemble of charge carriers turns out to be *self-localized* (“frozen”) by the mutual Coulomb interaction [4]. The exact criterion of such Coulomb self-localization is the smallness of the overlapping integral,  $t$ , in contrast with the typical change

$$\delta\varepsilon \sim (a_0/\bar{l})^2 \bar{\varepsilon}$$

in the Coulomb energy of a charge carrier as it hops (tunnels) between host-lattice sites. Here,  $a_0$  is the host-lattice spacing,  $\bar{l}$  is the mean interparticle distance, and  $\bar{\varepsilon}$  is the average Coulomb energy per particle. It should be noted that this Coulomb self-localized electron macroscopic state differs qualitatively from a Wigner crystal due to its dynamic origin [2, 4].

The last achievements of nanotechnologies allow one to create new types of the conducting Coulomb self-localized systems such as the arrays of quantum dots exchanging by electrons [5] and the networks and chains of metallic nano-grains with tunnel junctions between them (organic molecules of different types) [6]. In addition, as mentioned above, there are the strong reasons to suggest that the Coulomb self-localization criterion can be fulfilled in layered metal oxides of the high-temperature superconductor types (if the dopant concentration is not too small).

The ground-state electron configuration of a one-dimensional (1D) GWL in the limiting case  $t = 0$  was considered by Hubbard [1]. He showed that the ground state structure depends only on the electron filling factor for a wide class of the potentials of interparticle repulsion and, thus, has a universal structure. Further, it has been shown in [7, 8] that the ground state structure of such 1D systems is described by simple formula:

$$r(i, c_e) = a_0[i/c_e + \phi]. \quad (1)$$

Here,  $r(i, c_e)$  is the position of a 1D GWL electron with number  $i$ ;  $c_e = N_e/N_h$  is the electron density ( $N_e$  and  $N_h$  are the total number of electrons and host-lattice sites, respectively);  $[\dots]$  denotes the integer part, and  $\phi$  is an arbitrary number (the initial phase). In addition, it is required that the potential of inter-particle repulsion  $u(r)$  ( $r$  is an interelectron distance) fulfill the following restrictions: (i)  $u(r) > 0$ ; (ii)  $u(r) \rightarrow 0$  as  $r \rightarrow \infty$  faster than  $1/r$ ; (iii)  $u(r)$  is an everywhere convex function of  $r$ . Recently, Hubbard's results have been extended to the cases of  $t \neq 0$  [9] and to arbitrary  $u(r)$  with no restrictions mentioned above [10].

At the same time, the spectrum, structure of elementary excitations, and kinetic properties of 1D GWL are not yet investigated. In this connection, it seems to be reasonable to start this work from the limiting case of strong Coulomb self-localization ( $t \ll \delta\varepsilon$ ) and a strictly ordered host-lattice. The main goal of this paper is just to study the low-energy spectral and thermodynamic properties of 1D GWL for arbitrary  $c_e$  and  $u(r)$ .

### 1.1. Hamiltonian

The Hamiltonian of the system under consideration is of the form:

$$\hat{\mathbf{H}} = -t \sum_{i,\sigma} \left( \hat{b}_{i+1,\sigma}^+ \hat{b}_{i,\sigma} + \hat{b}_{i,\sigma}^+ \hat{b}_{i+1,\sigma} \right) + \frac{1}{2} \sum_{i \neq j} u(|r(i, c_e) - r(j, c_e)|) \hat{n}_i \hat{n}_j + \frac{1}{2} \sum_{i,\sigma} V \hat{n}_{i,\sigma} \hat{n}_{i,-\sigma}. \quad (2)$$

Here,  $t$  is the transfer integral;  $\hat{b}_{i,\sigma}$  and  $\hat{b}_{i,\sigma}^+$  the annihilation and creation operators of an electron at site  $i$  and with spin  $\sigma$ ;  $\hat{n}_{i,\sigma} = \hat{b}_{i,\sigma}^+ \hat{b}_{i,\sigma}$  the number of electrons at site  $i$  with spin  $\sigma$ ;  $\hat{n}_i = \sum_{\sigma} \hat{b}_{i,\sigma}^+ \hat{b}_{i,\sigma}$  the total number of electrons at site  $i$ ;  $V$  the interaction energy between two electrons with spins  $\sigma$  and  $-\sigma$  at site  $i$ . In the case of  $c_e \ll 1$ , one can drop spin indices in the Hamiltonian and, hence, neglect the term  $\sum V \hat{n}_{i,\sigma} \hat{n}_{i,-\sigma}$  (the spinless fermion model):

$$\hat{\mathbf{H}} = -t \sum_i \left( \hat{b}_{i+1}^+ \hat{b}_i + \hat{b}_i^+ \hat{b}_{i+1} \right) + \frac{1}{2} \sum_{i \neq j} u(|r(i, c_e) - r(j, c_e)|) \hat{b}_i^+ \hat{b}_i \hat{b}_j^+ \hat{b}_j. \quad (3)$$

### 1.2. The ground state structure and low-energy excitations

The ground state structure of 1D GWL with Hamiltonian (3) was first described by Hubbard [1]. He considered the special case of electron concentrations  $c_e \approx 1/2$  and  $t \rightarrow 0$ . It has been shown that the ground state is a periodic electron structure containing two types of inter-particle distances:  $2a_0$  and  $3a_0$  for  $c_e < 1/2$  and  $2a_0$  and  $a_0$  for  $c_e > 1/2$ . The concentration of electron pairs with a distance of  $3a_0$  (for  $c_e < 1/2$ ) or  $a_0$  (for  $c_e > 1/2$ ) decreases as  $c_e$  tends to  $1/2$ . In the case of  $c_e = 1/2$ , the ground state is a strictly equidistant periodic structure with a period of  $2a_0$ . Hubbard called the pairs of neighboring electrons by "dimers". In a small vicinity of  $c_e = 1/2$ , the distances between the "dimers" with a length of  $3a_0$  for  $c_e < 1/2$  (or  $a_0$  for  $c_e > 1/2$ ) are much more than the average interelectron distance  $\bar{l} = a_0 l_0 \approx 2a_0$  ( $l_0$  is the "inverse concentration",  $l_0 = 1/c_e$ ). One can consider such a structure as the one-dimensional ideal gas of "dimers" with a length of  $3a_0$  (or  $a_0$ ) against the background of an ideal periodic structure of "dimers" with a period of  $2a_0$ .

The structure of elementary excitations of such a system is rather interesting. The typical excitation

energy under the electron hopping at a distance of  $a_0$  is about  $\varepsilon^1$ . It could seem that the spectrum of 1D GWL elementary excitations becomes exhausted by such energies. But this statement is not true. The reason is related to excitations of the “dimers” with a length of  $3a_0$  (or  $a_0$ ). Really, it is easy to see that the hop of a “left” electron of an *isolated* “dimer” to the right (or the hop of a “right” electron to the left) does not change the system energy (see Fig. 1, *a, b, c*). Such hops are equivalent to the “dimer” translation for the period of GWL. Taking into account the finiteness of the overlapping integral  $t$ , the dispersion expression for a “dimer” is  $\varepsilon(k) = -2t \cos(2k)$ , where  $k$  is an electron momentum<sup>2</sup>. Here, it seems to be reasonable to point at a possible mechanism of electric conductivity of 1D GWL. Let us consider the filling factor like  $c_e = 1/q$ . The extraction of *one* electron leads to the creation of  $q$  adjacent “dimers” with a length of  $q + 1$ . Due to the mutual repulsion [1, 2], these “dimers” scatter over the system. One can say that, each “dimer” possesses the electron charge  $e/q$ . In such a case, the dispersion relation has the form

$$\varepsilon(k) = -2t \sum_{i=1}^q \cos(qk_i),$$

where the total electron momentum is

$$k = \sum_{i=1}^q k_i.$$

Here,  $k_i$  is the momentum of the  $i$ -th “dimer”. Thus, the conductivity of 1D GWL is based on the motion of “dimers” with the fractional charge  $e/q$ .

As indicated in Introduction, distribution of electrons of 1D GWL in the ground state is described, in the case of arbitrary  $c_e$ , by formula (1). For our consideration, it is more convenient to work with  $l_0$ , instead of  $c_e$ . Let us rewrite  $l_0$  in the following manner:  $l_0 = m_0 + \delta m$  with the integer  $m_0 = [l_0]$  and the fractional part  $\delta m = l_0 - [l_0]$  ( $0 \leq \delta m < 1$ ). In terms of  $m_0$  and  $\delta m$ , (1) takes the form

$$l_i = a_0(im_0 + [i\delta m]). \quad (4)$$

The electron distribution  $l_i$  is equidistant with a period of  $a_0 m_0$  until  $0 < i\delta m < 1$ . In the position  $i_0 = [1/\delta m]$ , the interelectron distance,  $l_{i_0} - l_{i_0-1}$ , is  $a_0(m_0 + 1)$ . Then the interelectron distances are  $a_0 m_0$  again, until  $1 < i\delta m < 2$ , etc. Thus, one can say about a periodic

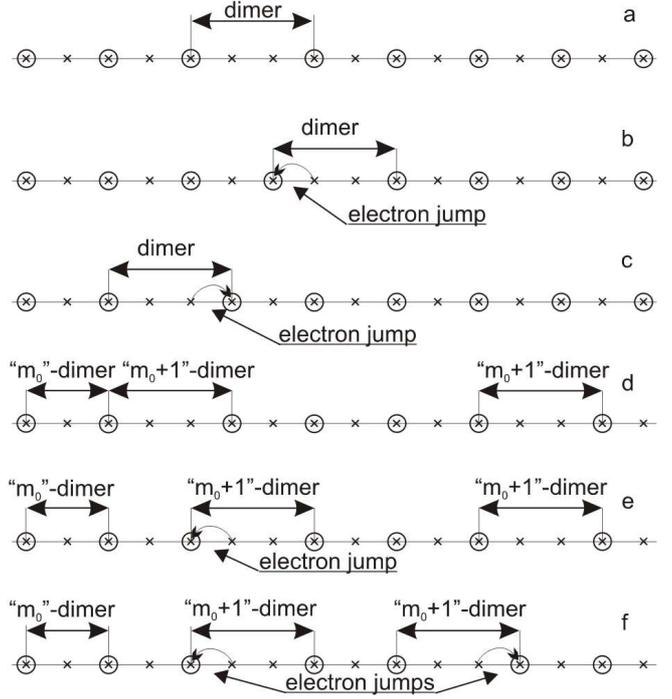


Fig. 1. A fragment of the 1D GWL ground-state structure (*a*); isolated dimer shift to the right (*b*) and left (*c*); the example of “ $m_0$ ”-dimers and “ $m_0 + 1$ ”-dimers (*d*); dimer shift (excitation) (*e*); antiparallel shifts of two “dimers” (*f*)

superstructure of “dimers” with a length of  $a_0(m_0 + 1)$  (we will mark such dimers as “ $m_0 + 1$ ”-dimers) against the background of the ideal “dimer” structure with the interelectron distance equal to  $a_0 m_0$  (“ $m_0$ ”-dimers) (Fig. 1, *d*). According to (4), the concentration of the “ $m_0 + 1$ ”-dimers,  $c_{m+1}$ , is just  $\delta m$ , and the average distance between the “ $m_0 + 1$ ”-dimers is  $\bar{r} = a_0 m_0 / \delta m$  (more exactly,  $\bar{r} = a_0(m_0 / \delta m + 1)$ ). As follows from (1) and (4), the ground-state electron configuration is strictly equidistant with a period of  $m_0$  for integer  $l_0$ , i.e. the concentration of “ $m + 1$ ”-dimers is equal to zero. In the case of  $\delta m = 1/2$ , the concentrations of the “ $m_0$ ”-dimers and “ $m_0 + 1$ ”-dimers are the same, and one can say either about a superstructure of “ $m_0$ ”-dimers against the background of “ $m_0 + 1$ ”-dimers or, vice versa, about that of “ $m_0 + 1$ ”-dimers against the background of “ $m_0$ ”-dimers. At  $\delta m > 1/2$ , the concentration of “ $m_0$ ”-dimers,  $c_m = 1 - c_{m+1}$ , is less than that of “ $m_0 + 1$ ”-dimers, and it is more convenient to consider the system as the superstructure of “ $m_0$ ”-dimers against the background of

<sup>1</sup>A lot of papers is devoted to the investigation of 1D GWL spectral properties produced just by such excitations [9, 13].

<sup>2</sup>The multiplier 2 in the argument of the function  $\cos$  is just related to the above-mentioned fact that the hop of an electron in a “dimer” is equivalent to the “dimer” translation for the period of GWL (which is equal to  $2a_0$  in the case considered by Hubbard).

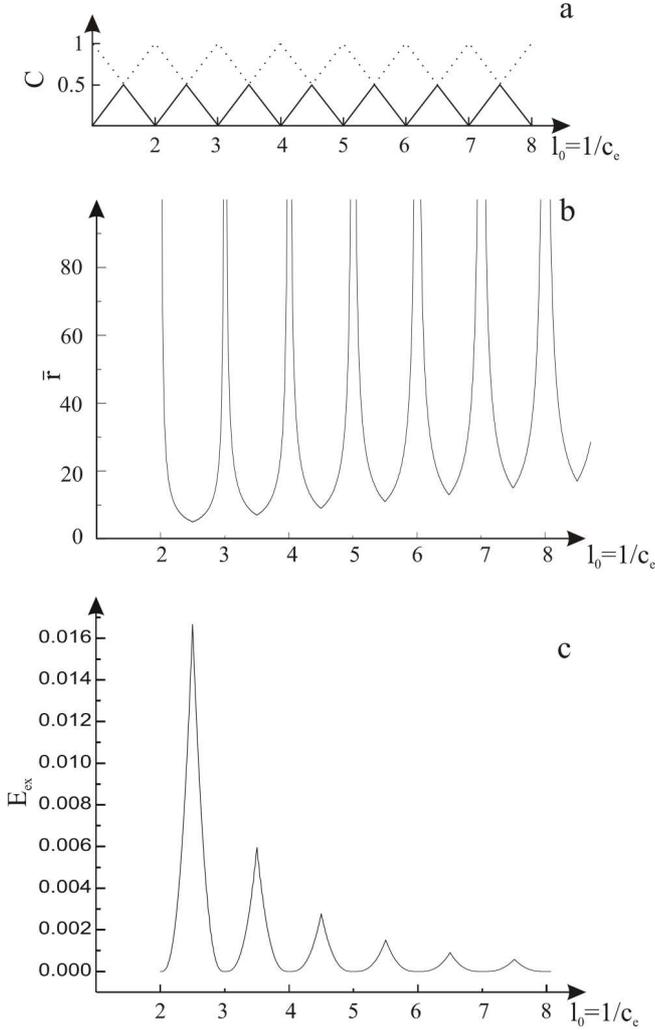


Fig. 2. *a* – Dependences of the “dimer” concentration on the reciprocal electron concentration  $l_0$ : the solid line corresponds to  $c_{\text{dim}}(l_0)$ , dotted lines correspond to  $c_m(l_0)$  and  $c_{m+1}(l_0)$ ; *b* and *c* – the dependences  $\bar{r}(l_0)$  and  $E_{\text{ex}}(l_0)$

“ $m_0 + 1$ ”-dimers. At the limiting point  $\delta m \rightarrow 1$ ,  $c_m = 0$  and the 1D GWL ground state is a superstructure of “ $m_0 + 1$ ”-dimers ( $c_{m+1} = 1$ ), i.e. the strictly periodic structure with a period of  $m_0 + 1$ . It is convenient to define the density of “dimers”,  $c_{\text{dim}}$ , as follows:

$$c_{\text{dim}} = \begin{cases} \delta m = l_0 - [l_0] & \text{for } \delta m \leq 1/2 \\ 1 - \delta m & \text{otherwise} \end{cases}$$

Thus, we come to conclusion that  $c_{\text{dim}}$  (as well as  $c_m$  and  $c_{m+1}$ ) are *periodic functions* of  $1/c_e$  (see Fig. 2,*a*).

Let us consider now the elementary excitation of the “ $m_0 + 1$ ”-dimer. As indicated above, such an excitation is the hop of the “left” electron of the “dimer” to the

right or the hop of the “right” electron to the left. Such electron hops are equivalent to the “dimer” jump for  $m_0 a_0$  steps to the left (for the “left” electron jump) or to the right (for the “right” electron jump) (Fig. 1,*e*). In the near-neighboring approximation, the excitation energy of such a jump is

$$E_{\text{ex}}(\bar{r}) = \delta^2 u(\bar{r}),$$

$$\delta^2 u(x) = u(x + a_0) + u(x - a_0) - 2u(x), \quad (5)$$

$E_{\text{ex}}(\bar{r}) \approx a_0^2 \frac{d^2 u(x)}{dx^2} \Big|_{x=\bar{r}}$  for  $\bar{r} \gg 1$ . Taking into account all the interactions in the system modifies expression (5) as follows:

$$E_{\text{ex}}(\bar{r}) = E(1, \bar{r}) = \sum_{k=1}^{\infty} \delta^2 u(k\bar{r}). \quad (6)$$

The dependences  $\bar{r}(l_0) = a_0(c_{\text{dim}}[l_0] + 1)$  and  $E_{\text{ex}}(l_0)$  are presented in Fig. 2,*b* and Fig. 2,*c*, respectively.

Now, let us consider the excitation energy,  $E(n, \bar{r})$ , of  $n$  successive “ $m_0 + 1$ ”-dimers upon simultaneous parallel electron shifts. One can call such an excitation as a “domain” containing  $n$  “ $m_0 + 1$ ”-dimers. It is easy to see that

$$E(n, \bar{r}) = nE(1, \bar{r}) - \sum_{k=1}^n (n - k) \delta^2 u(k\bar{r}). \quad (7)$$

The distinctive feature of (7) is that the energy of the domain with infinite length,

$$E(\infty, \bar{r}) = \sum_{k=1}^{\infty} k \delta^2 u(k\bar{r}),$$

is finite even in the case of non-screened Coulomb pair potential  $u(r)$ :

$$\delta^2 u(k\bar{r}) \approx (a_0^2/\bar{r}^3) \frac{1}{k^3},$$

$$E(\infty, \bar{r}) \approx (a_0^2/\bar{r}^3) \sum_{k=1}^{\infty} \frac{1}{k^2} = (a_0^2/\bar{r}^3) \frac{\pi^2}{6}.$$

Thus, the spectrum of excitations of a domain has the gap  $E(1, \bar{r})$  and the quasiband with finite width  $\Delta_{\text{band}}$ . The quasiband is a series of lines thickening as the number  $n$  increases:

$$\Delta_{\text{band}} = E(\infty, \bar{r}) - E(1, \bar{r}) = \sum_{k=1}^{\infty} (k - 1) \delta^2 u(k\bar{r}).$$

An example of such excitation spectrum for  $u(r) = 1/r$  is presented in Fig. 3.

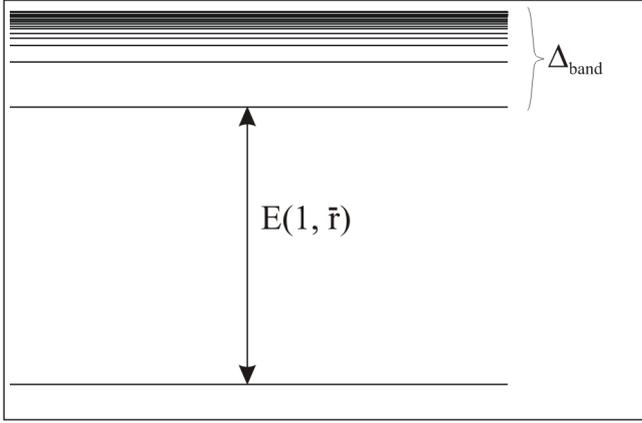


Fig. 3. Spectrum of excitations of a “domain”

Let us consider now the “anti-parallel” electron shift of 2 electrons in the neighboring  $m + 1$  “dimers” (see Fig. 1,f). Such a type of excitations can be associated with oscillations of the density of “dimers”. The excitation energy is

$$\begin{aligned} \tilde{E}_{\text{ex}}(\bar{r}, m_0) &= u(\bar{r}) - 2u(\bar{r} - a_0 m_0) + \\ &+ u(\bar{r} + a_0(m_0 - 1)) \approx 2a_0 m_0 \frac{d}{dx} u(\bar{r}) \sim 2a_0 m_0 / \bar{r}^2, \end{aligned} \quad (8)$$

where  $1 < m_0 < l_0$ . We have

$$\tilde{E}_{\text{ex}}(\bar{r}, m_0) / E_{\text{ex}}(\bar{r}) \sim (m_0 l_0) / a_0^2 \gg 1.$$

This means that the lowest energy excitations in the system under consideration are the “domains”.

### 1.3. Domain decay

Let us consider the destruction of a domain with length  $n$  at the position  $n_0$  ( $1 \leq n_0 \leq n$ ). It is easy to show that the energy of such a process is

$$\begin{aligned} \Delta E(n, n_0, \bar{r}) &= -E(1, \bar{r}) + \sum_{k=1}^{n_0-1} \delta^2 u(k\bar{r}) + \\ &+ \sum_{k=1}^{n-n_0} \delta^2 u(k\bar{r}). \end{aligned} \quad (9)$$

As follows from (9),  $\Delta E(n, n_0, \bar{r})$  is a symmetric function of  $n_0$ , i.e.  $\Delta E(n, n_0, \bar{r}) = \Delta E(n, n + 1 - n_0, \bar{r})$ . In addition,

$$\Delta E(n, 1, \bar{r}) = - \sum_{k=1}^{\infty} \delta^2 u(k\bar{r}) + \sum_{k=1}^{n-1} \delta^2 u(k\bar{r}) =$$

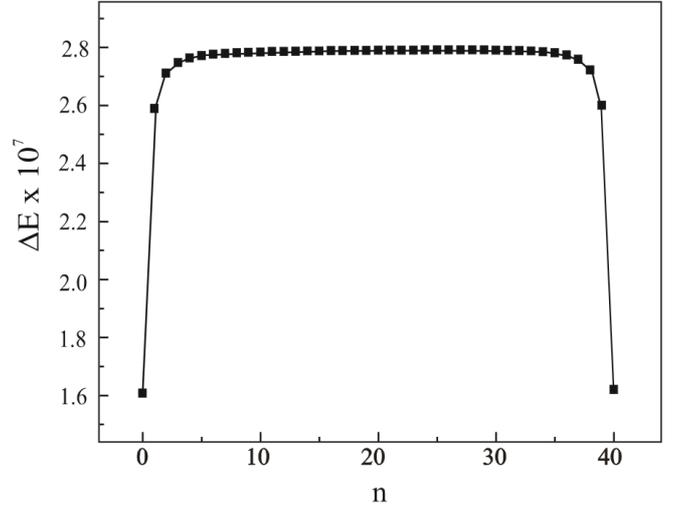


Fig. 4. Excitation energy of a “domain” as a function of  $n_0$  which is obtained by using (9) for  $n = 40$  and for  $u(r) = 1/r$

$$= - \sum_{k=n}^{\infty} \delta^2 u(k\bar{r}), \quad (10)$$

and, hence,  $E(n, \bar{r}) + \Delta E(n, 1, \bar{r}) = E(n - 1, \bar{r})$ . That is,  $-\Delta E(n, 1, \bar{r})$  is just the energy of the detaching of the boundary “dimer” from a “domain” with length  $n$ . The energy  $\Delta E(n, n_0, \bar{r})$  is minimal for  $n_0 = 1$  and  $n_0 = n$ , by reaching the maximum for  $n_0 = [n/2]$  (see Fig. 4). This means that the low-temperature domain decay is realized through the step-by-step detaching of the boundary “dimers” from the domain.

## 2. Low-temperature Thermodynamics

Neglecting the tunneling of charge carriers (for certainty, let us consider electrons) between host sites, Hamiltonian (2) can be written as [1]

$$\mathcal{H} = \frac{1}{2} \sum_{i \neq j} u(|r(i, c_e) - r(j, c_e)|) n_i n_j.$$

The method of construction of low-temperature thermodynamics proposed in [11] can be applied, certainly, also for a 1D electron lattice system on the *strictly ordered* host-lattice, i.e. for 1D GWL. However, in such a case, this method allows us to calculate a lot of thermodynamic characteristics of the system under consideration in *explicit* form.

In the case of low temperatures and low electron densities, the distances  $l_n$  between neighboring electrons with numbers  $n + 1$  and  $n$  deviate slightly from the

mean interelectron distance,  $\bar{l} = a_0/c_e$ . Let us write  $l_n$  as  $l_n = \bar{l} + \xi(n)$ , where  $\xi(n)$  is a small additive  $\sim a_0$ . It is convenient to introduce  $\xi(n)$  as new independent variables, instead of the occupation numbers  $n_i$ . In such a case,  $\xi(n)$  may be considered as the lengths (with corresponding signs) of “dipoles”  $e\xi(n)$  ( $e$  is the electron charge), starting from “ideal” Wigner crystal positions  $n\bar{l}$  ( $n = 1, 2, \dots, N$ ). The endpoints of  $\xi(n)$  are the host-lattice sites located within some region in the vicinity of these “ideal” positions. Without loss of generality, it is always possible to choose these regions so that the number of host-lattice sites should be the same for all the “clusters”. We mark this number by  $\nu$  ( $\nu \geq 2$ ). Thus, the electron with number  $n$  may acquire one of  $\nu$  fixed positions:  $n\bar{l} + \xi(n)_k$ , where  $k = 1, 2, \dots, \nu$ . It is convenient to consider  $\xi(n)_k$  as the eigenvalues of some “shift operator”  $\hat{\xi}(n)$ . Depending on the microscopic configuration,  $\hat{\xi}(n)$  takes on one of these values. The discreteness of  $\hat{\xi}(n)$  spectra is caused by the discreteness of host-lattice positions (“frozen chaos”) and reflects the crucial difference between the system under consideration and a Wigner crystal, where such spectra are continuous. It should be noted that  $\hat{\xi}(n)$  is a function of the electron density  $c_e$ :  $\hat{\xi}(n) = \hat{\xi}(n, c_e)$ . Taking into account the smallness of  $|\xi(n, c_e)_k|/\bar{l}$ , it is possible to expand the Hamiltonian in the degrees of  $\hat{\xi}(n, c_e)$ , restricting oneself by quadratic terms. The details of such a procedure are given in [11]. As a result, we get

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_d + N\bar{\epsilon},$$

$$\hat{\mathcal{H}}_d = \sum_{n=1}^N \sum_{m=1}^M \hat{\epsilon}(\hat{\xi}(n, c_e), \hat{\xi}(n+m, c_e)), \quad (11)$$

where

$$\hat{\epsilon}(\hat{\xi}(n, c_e), \hat{\xi}(n+m, c_e)) =$$

$$= \frac{e^2}{2} b(m, c_e) (\hat{\xi}(n, c_e) - \hat{\xi}(n+m, c_e))^2,$$

$$b(m, c_e) = \frac{1}{2} \frac{d^2 u(r)}{dr^2} \Big|_{r=ma_0/c_e},$$

and  $M$  is the maximum number of neighboring dipoles, whose interactions are taken into account. For example,  $M = 1$  corresponds to the near-neighbor approximation,  $M = 2$  to the near- and next-neighbor approximation, etc.

The partition function of the system under consideration is of the form

$$Z(N, c_e, T) = \sum \exp \left( -\frac{\hat{\mathcal{H}}_d}{T} \right). \quad (12)$$

Here,  $T$  is the temperature, the Boltzmann constant is set to unity, and the summation is carried out over all possible  $\nu^N$  microscopic configurations.

Applying the modified transfer-matrix technique [11], one can represent the partition function (12) in terms of a product of some tensors  $\hat{P}(n, c_e, T)$ . To do this, it is useful to introduce the following auxiliary matrix:

$$\hat{A}(n, m, c_e, T) = \exp \left( -\frac{\hat{\epsilon}(\hat{\xi}(n, c_e), \hat{\xi}(n+m, c_e))}{T} \right), \quad (13)$$

which is a transfer matrix corresponding to the interaction between the dipoles at the positions with numbers  $n$  and  $n+m$ . The matrix elements of  $\hat{A}(n, m, c_e, T)$  have the form

$$A(n, m, c_e, T)_{i,j} = \exp \left( -\frac{\epsilon(\xi(n, c_e)_i, \xi(n+m, c_e)_j)}{T} \right).$$

In the near-neighbor approximation ( $M = 1$ ),  $\hat{P}(n, c_e, T)$  just coincide with  $\hat{A}(n, 1, c_e, T)$ . In the general case of  $M = 1, 2, \dots$  neighbors,  $\hat{P}(n, c_e, T)$  are the tensors of rank  $M+1$  and have the form

$$P(n, c_e, T)_{i,k_1,k_2,\dots,k_M} = A(n, 1, c_e, T)_{i,k_1} \times$$

$$\times A(n, 2, c_e, T)_{i,k_2} A(n, 3, c_e, T)_{i,k_3} \dots A(n, M, c_e, T)_{i,k_M}. \quad (14)$$

The partition function  $Z(N, c_e, T)$  can be written as

$$Z(N, c_e, T) = \Pi(N, c_e, T)_{i_1,i_2,\dots,i_{M+1}} \delta_{i_1,i_2} \delta_{i_1,i_3} \dots \delta_{i_1,i_{M+1}}, \quad (15)$$

where

$$\Pi(N, c_e, T) = \prod_{n=1}^N \hat{P}(n, c_e, T). \quad (16)$$

The tensor product in (16) is defined as

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

$$= \sum_{j=1}^{\nu} P(n, c_e, T)_{i,j,k_1,\dots,k_{M-1}} P(n+1, c_e, T)_{j,k_1,\dots,k_M}. \quad (17)$$

For example, in the near-neighbor approximation ( $M = 1$ ), the partition function (15) is just the trace of  $\Pi(N, c_e, T)$ .

### 3. Results and Discussion

As was shown in [1,7,8], the ground state of GWL with electron density  $c_e = m/l$  ( $m$  and  $l$  are integers such that  $m/l$  is an irreducible fraction) is a periodic structure with period  $la_0$  and  $m$  electrons per cell. This means that product (16) consists of “blocks” with length  $m$  and has the following structure:

$$\begin{aligned} \Pi(N, c_e, T) &= \hat{P}(1, m/l, T) \hat{P}(2, m/l, T) \dots, \\ \hat{P}(m, m/l, T) &\hat{P}(1, m/l, T) \hat{P}(2, m/l, T) \dots \\ \dots \hat{P}(m, m/l, T) &\dots \end{aligned} \quad (18)$$

Introducing

$$\hat{Q}(m, l, T) = \hat{P}(1, m/l, T) \hat{P}(2, m/l, T) \dots \hat{P}(m, m/l, T),$$

we can rewrite (18) as

$$\Pi(N, c_e, T) = \left( \hat{Q}(m, l, T) \right)^{N/m}.$$

Our preliminary calculations have shown that all the features of the system become apparent to the full extent even at  $\nu = 2$ . Hence, all the results presented in the paper lead just to this value of  $\nu$ . In addition, the values of  $\xi(n, c_e)_k$  ( $k = 1, 2$ ) are enumerated for the convenience so that  $\xi(n, c_e)_1 < \xi(n, c_e)_2$  and, hence,  $\xi(n, c_e)_1 = n\bar{l} - r(n, c_e)$ ,  $\xi(n, c_e)_2 = \xi(n, c_e)_1 + a_0$ .

In the near-neighbor approximation ( $M = 1$ ) for the GWL with one particle per cell ( $m = 1$ ), the values  $\xi(n, c_e)_k$  can be chosen so that  $\xi(n, c_e)_1 = -a_0/2$  and  $\xi(n, c_e)_2 = a_0/2$  ( $n = 1, 2, \dots, N$ ). In the case of GWL with two particles per cell ( $m = 2$ ),  $\xi(n, c_e)_k$  can be chosen so that  $\xi(2n, c_e)_1 = 0$ ;  $\xi(2n, c_e)_2 = a_0$  and  $\xi(2n+1, c_e)_1 = -a_0/2$ ;  $\xi(2n+1, c_e)_2 = a_0/2$  ( $n = 1, 2, \dots, N$ ). In both these cases ( $m = 1$  and  $m = 2$ ), the tensors  $\hat{P}(n, c_e, T)$  are the same for all  $n$ , and  $\hat{Q}(m, l, T)$  is of the form

$$\hat{Q}(m, l, T) = \begin{pmatrix} \exp\left(-\frac{\alpha^2 E(c_e)}{T}\right) \exp\left(-\frac{(\alpha+1)^2 E(c_e)}{T}\right) \\ \exp\left(-\frac{(\alpha-1)^2 E(c_e)}{T}\right) \exp\left(-\frac{\alpha^2 E(c_e)}{T}\right) \end{pmatrix}.$$

Here,  $E(c_e) = E(m/l) = \frac{e^2}{2} b(1, m/l)$ . The parameter  $\alpha = |\xi(n, c_e)_1 - \xi(n+1, c_e)_1|$  is equal to zero for  $m = 1$  and  $\alpha = a_0/2$  for  $m = 2$ .

As a result, the free energy per particle,  $f(c_e, T) = F(N, c_e, T)/N$  ( $F(N, c_e, T) = -T \ln(Z(N, c_e, T))$ ) is of the form

$$f(c_e, T) = \alpha^2 E(c_e) - T \ln \left( 1 + \exp\left(-\frac{E(c_e)}{T}\right) \right). \quad (19)$$

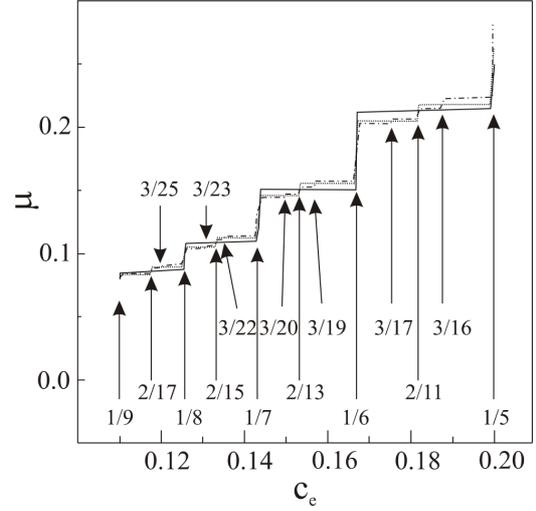


Fig. 5. Dependence  $\mu(c_e)$  obtained with the use of (13)–(17). Solid line corresponds to the near-neighbor approximation ( $M = 1$ ); dotted and dash-dotted lines correspond to  $M = 2$  and  $M = 3$ , accordingly

For the computer calculations, the parameters  $e$  and  $a_0$  were chosen to be equal to 1. The weakly screened Coulomb potential  $u(r) = \exp(-r/r_0)/r$  ( $r_0 = 100a_0 \gg \bar{l} = a_0/c_e$ ) was taken as the potential of interelectron repulsion. It is obvious that this type of pair potential fulfills the restrictions on  $u(r)$  indicated in Introduction. It should be noted that the results of thermodynamic calculations do not depend qualitatively on a specific type of  $u(r)$ . The total number of host-lattice sites was about  $10^2 - 10^3$ , depending on  $M$  and  $c_e$ . At any rate, it was required that the error in the calculations do not exceed 0.1%, i.e.  $|1 - F(N, c_e, T)/F(2N, c_e, T)| < 10^{-3}$ .

One of the important characteristics of the system under consideration is the dependence of the chemical potential  $\mu$  on the electron density  $c_e$ :

$$\begin{aligned} \mu &= \frac{\partial F(N, c_e, T)}{\partial N} \Big|_{T \rightarrow 0} = \\ &= \frac{1}{L} \frac{\partial F(N, c_e, T)}{\partial c_e} \Big|_{T \rightarrow 0} = c_e \frac{\partial f(c_e, T)}{\partial c_e} \Big|_{T \rightarrow 0}. \end{aligned}$$

As was shown in [7], the zero-temperature dependence  $\mu(c_e)$  is a well-developed fractal structure (a “devil staircase”). In this dependence, each rational value of  $c_e$  corresponds to a finite interval of  $\Delta\mu$ , within which  $c_e$  is invariable. Any finite  $T$  completely destroys the “devil staircase” “stairs” with  $\Delta\mu \ll T$ , but the “stairs” with  $\Delta\mu \gg T$  are only slightly modified [2]. The dependence  $\mu(c_e)$  obtained with the use of (15), (16), and (17) is presented in Fig. 5. The temperature is the smallest

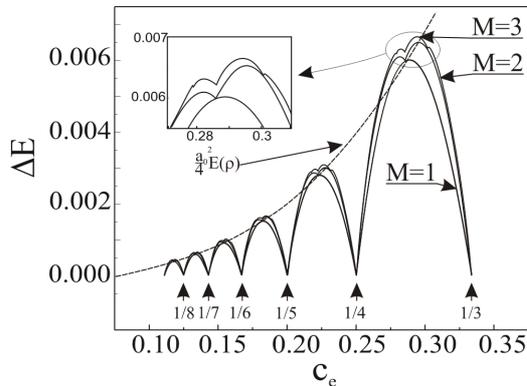


Fig. 6. Dependence  $\Delta E(c_e)$  obtained with the use of (20)

parameter, and it was chosen so that  $T = 10^{-4}\bar{\varepsilon}$ . One can see that only the “stairs” corresponding to  $c_e = 1/l$  are present for  $M = 1$ . For  $M = 2$  and  $M = 3$ , the new series of “stairs” corresponding to  $c_e = 2/l$  and  $c_e = 3/l$  appear.

Another important and informative characteristic of the system is the difference between the energies (per particle) of GWL and an ordinary Wigner crystal as the function of  $c_e$ :

$$\Delta E(c_e) = f(c_e, T \rightarrow 0) - \bar{\varepsilon}(c_e). \tag{20}$$

Here,  $\bar{\varepsilon} = \sum_{i=1}^M u(ia_0/c_e)$ . This dependence calculated with the use of (15) for  $M = 1, 2, 3$  is presented in Fig. 6. As seen, the GWL energy reaches absolute minima for  $c_e = 1/l$  (the energies of GWL and a Wigner crystal coincide). The difference is maximal for  $c_e = 2/l$  and equal to  $\frac{a_0^2}{4}E(c_e)$  (see (19)). Taking into account the interparticle interactions between next-neighbors ( $M = 2$ ) and next-next-neighbors ( $M = 3$ ) leads to the appearance of a series of local minima corresponding to the GWL with two and three particles per cell, respectively.

In small vicinities of  $c_e = 1/l$ , one can see the pronounced linear dependence of  $\Delta E(c_e)$ . This dependence has the following nature. As was mentioned in Introduction, the GWL ground-state structure contains two sorts of dimers: “ $l$ ”-dimers and “ $l + 1$ ”-dimers, where  $l = [1/c_e]$ . At low temperatures, the contributions of the “dimers” with other lengths are exponentially low. In small vicinities of  $c_e = 1/l$ , the ground state of GWL can be described in terms of a gas of “dimers” with a length of  $a_0(l + 1)$  (for  $c_e < 1/l$ ) or  $a_0(l - 1)$  (for  $c_e > 1/l$ ) against the background of a Wigner crystal with a period of  $a_0l$  [1,2,8]. The energy

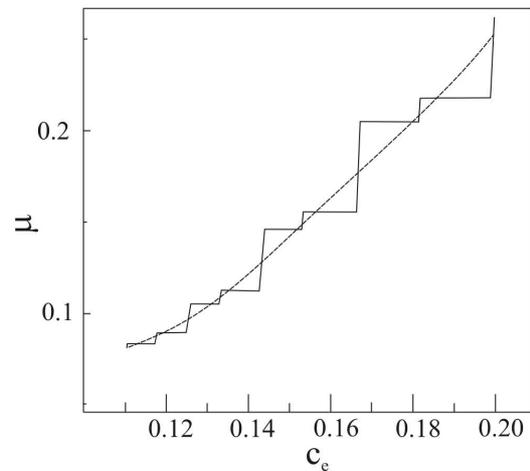


Fig. 7. Dependence  $\mu(c_e)$  for the ordered host-lattice (solid line) and the completely disordered one (dotted line)

of the “ $x$ ”-dimer is just  $u(x)$ , and we get finally that

$$\Delta E(c_e) = \begin{cases} u(a_0(l - 1))(c_e - 1/l) & \text{for } c_e > 1/l, \\ u(a_0(l + 1))(1/l - c_e) & \text{for } c_e < 1/l. \end{cases}$$

The dependences  $\mu(c_e)$  at  $T \rightarrow 0$  in the cases of an ordered host-lattice (GWL) and a completely disordered one are presented in Fig. 7. As seen from the figure, the disorder destroys completely the “stairs”  $\mu(c_e)$  of the “devil staircase”. In some sense, it works like temperature. The reason for such a phenomenon is quite clear: each “stair” of the “devil staircase” corresponds to some periodic electron structure, and a disorder at host-lattice site positions destroys these structures.

#### 4. Conclusions

We have studied the structure of the spectrum of elementary excitations of 1D GWL is studied. The method used is based on the “dimer” description. The structure and properties of the “dimers” are studied in the case of an arbitrary electron density  $c_e$ . It is established that the concentration of such “dimers” is a periodic function of the reciprocal electron concentration  $l_0 = 1/c_e$ . The energy gap in the “dimer” spectrum tends to zero for  $l_0 = 1, 2, \dots$ , reaching the maximum for semiinteger  $l_0$ . It is shown that the low-energy excitations of the system under consideration are the “domains” which are the blocks of adjacent “dimers”. The structure and kinetic properties of the “domains” are studied.

In addition, the low-temperature properties of 1D GWL are studied. The method proposed allows one to study the thermodynamic characteristics of the system

under consideration at arbitrary values of the electron density  $c_e$  and any number of interacting electrons  $M$ . It is shown that an increase in  $M$  leads to the appearance of more and more fine “stairs” in the low-temperature dependence  $\mu(c_e)$ . These “stairs” are remnants of the “devil staircase” which characterizes the zero temperature dependence for such systems. It is established that a disorder in host-lattice site positions destroys “stairs”.

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СПЕКТР  
ЕЛЕМЕНТАРНИХ ЗБУДЖЕНЬ  
ТА НИЗЬКОТЕМПЕРАТУРНІ  
ТЕРМОДИНАМІЧНІ ВЛАСТИВОСТІ  
ОДНОВИМІРНОЇ СИЛЬНОКОРЕЛЬОВАНОЇ  
ЕЛЕКТРОННОЇ ГРАТКОВОЇ СИСТЕМИ

*В.В. Славін*

Р е з ю м е

Вивчено низькоенергетичний спектр та низькотемпературні термодинамічні властивості одновимірної електронної ґраткової системи з дальнодійним потенціалом міжчастинкового відштовхування для довільних значень концентрації електронів  $c_e$ . Показано, що величина щілини в даному спектрі прямує до нуля при  $c_e = 1/q$  ( $q = 1, 2, \dots$ ), досягаючи максимуму при  $c_e = 2/(2q + 1)$ . Показано, що низькоенергетичний спектр досліджуваної системи може бути описаний у термінах одновимірних спінових системах. Розглядається питання про кінетику релаксації “доменів”. Для вивчення термодинамічних властивостей даної системи запропоновано модифікований метод трансфер-матриць. Показано, що врахування більшого числа взаємодіючих електронів (збільшення числа координаційних сфер) приводить до появи усе більшої кількості дрібних сходнок у низькотемпературній залежності хімічного потенціалу від електронної щільності. Вивчено вплив розупорядкування у позиціях вузлів решітки-матриці на термодинамічні характеристики системи. Показано, що розупорядкування усуває згадані сходінки.