

# One-dimensional narrow-band conductors

(Review Article)

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Received March 15, 2021, published online July 26, 2021

We review one-dimensional lattice models and the corresponding results that describe the low-temperature properties of quasi-one-dimensional lattice systems with long-range interaction. A widely known example is narrow-band low-dimensional conductors with long-range interelectron repulsion. The models deal with particles that live on the one-dimensional host lattice (chain), translation invariant or disordered, and interact via the long-range repulsive potential. The results are presented concerning the translation invariant host chain, in particular: the low-temperature thermodynamics incommensurable ground states and related devil-staircase form of various characteristics as functions of pertinent parameters, the self-localization of particles, a new branch of elementary excitations, etc. In the disordered case, where the sites of the host chain fluctuate randomly around the sites of the periodic chain, the low-temperature thermodynamics and the structure of the ground state are discussed in the framework of a certain model, which we call the cluster model and which seems to be a fairly reasonable approximation for low temperatures and small concentration of particles. Using analytical and numerical tools we analyze the thermodynamics and the ground state of the model. The latter proves to be a sequence of random domains and we study in detail their distribution.

Keywords: one-dimensional systems, disordered systems, ground-state structure.

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## 1. Introduction

Low-dimensional and layered conductors are of considerable interest because they possess a number of unusual properties. These are, for instance, the conductors with the combination of narrow-band dynamics and weak Coulomb

screening. In these materials, the effects determined by interelectron (or interholes) repulsion play the dominant role and make them qualitatively different from the compounds described by the Hubbard model where electron-electron interaction is local. These effects are especially pronounced in quasi-one-dimensional systems having the macro-

scopic extent in one direction and the microscopic size in all other directions.

A widely used model that describe these systems consists of  $N$  particles living on the one-dimensional host lattice (host chain)  $\mathcal{L}$  of  $L$  sites (translation invariant or disordered). The pair interaction between particles is described by long-range potential  $V$  that decays polynomially at infinity:

$$V(x) \sim |x|^{-\gamma}, \quad |x| \gg a_0, \quad (1.1)$$

where  $\gamma > 0$  and  $a_0$  is a parameter that determines the basic length scale of the lattice (lattice period in the translation invariant case, the typical distance between the lattice or rather networks sites in the disordered case).

One can broadly classify the  $d$ -dimensional systems with long-range potential (1.1) by writing

$$\gamma = d + \sigma \quad (1.2)$$

and specifying  $\sigma$  (see, e.g., [1]). The systems with  $\sigma < 0$  can be called the “strong” long ranged. In this case, one has either to take into account certain truncations procedures (screening, confining the system to a finite box, etc.), or to be prepared to obtain rather unusual properties, especially if  $V$  is attractive or anisotropic (see, e.g., [2, 3]). The systems with “weak” long-range interaction [ $\sigma > 0$  in (1.1)] admit the traditional statistical mechanics description possessing, however, certain special properties if  $\sigma$  is small (say,  $\sigma < 2$ ).

In this work, we assume that  $d = 1$ ,  $\sigma > 0$  and  $V$  is positive (repulsive) and convex, i.e.,

$$V''(x) > 0. \quad (1.3)$$

The last condition is important [see, e.g., formulas (2.5), (2.6), (2.24), and (3.23)].

The convexity condition is important [see, e.g., formulas (2.5), (2.6), (2.24)] and its violation may change significantly the results (see, e.g., [4]). We will mostly use the model (and the terminology) of narrow-band quasi-one-dimensional conductors with long-range interelectron repulsion. These materials possess a variety of interesting and often counterintuitive properties that not only differ them qualitatively from ordinary metals (including the transition metals) and semiconductors, but also from the conductors described by the conventional Hubbard model, where interaction is local.

Among the conductors of this type those where the charge tunneling between host-lattice sites is suppressed by their mutual repulsion are of special interest. In this case, the whole ensemble of charge carriers turns out to be *self-localized* [5]. The criterion of the self-localization (SL) is the smallness of overlapping integral  $t$  with respect to the typical change

$$\delta V \sim (a_0 / \bar{l})^{\gamma+1} \bar{V} \quad (1.4)$$

in energy of the charge carrier jumping (tunneling) between the lattice sites, where  $\bar{l}$  is the typical interelectron distance and  $\bar{V}$  is the typical energy per electron.

One of the most known examples of the two-dimensional (2D) systems of this type is the so-called MOSFET structure (metal-oxide-semiconductor field-effect transistor) with the hole-impurity band. Note that the systems where the charge carriers are pressed out on the surface by external electric field normal to the surface belong also to this class of conductors (2D lattice electron gas). In this case, the electric field plays the role of a chemical potential  $\mu$ . Changing  $\mu$ , we can vary considerably the electron density  $c_e$ . Besides, there are strong reasons to believe that layered structure, including high-temperature superconductors (HTSC) and a number of metaloxides of other types also possess the long-range interaction.

Another important group consists of one-dimensional (1D) and quasi-1D compounds. These are, for example, quasi-one-dimensional organic conductors [6] and spin valves on the base of narrow-band-gap nonmagnetic metals [7]. Furthermore, a lot of artificially created 1D nanosystems, such as chains of quantum dots [8] and chains of metallic nanograins with tunnel junctions between them [9], also belong to this group.

In view of the above, below we will write an electron instead of a particle.

The question on the influence of disorder of the host-lattice sites on the ground state and low-temperature properties of these systems is of special interest, since the overwhelming majority of SL conductors are essentially disordered. For instance, in semiconductors based on the MOSFET the disorder is due to the random distribution of impurities [10, 11], and in certain nanostructures [8, 9] the disorder is due to fluctuations of tunneling junctions. There are also strong reasons to believe that 1D charge transfer salts of TCNQ, TMTTF, and DCNQI types also belong to this class due to their nonideal chemical structure.

The Hamiltonian of the systems under consideration can be obtained from that of the *extended* Hubbard model [recall that the conventional Hubbard model is given by (1.5), where the last term is absent]

$$H = -t \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle, \sigma} \hat{c}_{\mathbf{r}, \sigma}^+ \hat{c}_{\mathbf{r}', \sigma} + U_0 \sum_{\mathbf{r}} \hat{n}_{\mathbf{r}, \uparrow} \hat{n}_{\mathbf{r}, \downarrow} + \frac{1}{2} \sum_{\mathbf{r} \neq \mathbf{r}'} V(|\mathbf{r} - \mathbf{r}'|) \hat{n}_{\mathbf{r}, \sigma} \hat{n}_{\mathbf{r}', \sigma}, \quad (1.5)$$

in which  $\mathbf{r}, \mathbf{r}' \in \mathcal{L}$  are the coordinates (sites) of the host-lattice  $\mathcal{L}$ , translation invariant or disordered, of  $L$  sites,  $\langle \dots \rangle$  denotes the neighboring sites,  $t$  is the overlap (hopping) integral,  $U_0$  is the strength of the interaction of electrons with opposite spins on the same site,  $V$  is the usual pair interaction,  $\hat{c}_{\mathbf{r}, \sigma}^+$  and  $\hat{c}_{\mathbf{r}, \sigma}$  are creation/annihilation operators of electron on site  $\mathbf{r}$  with spin  $\sigma$ ,  $\hat{n}_{\mathbf{r}, \sigma} = \hat{c}_{\mathbf{r}, \sigma}^+ \hat{c}_{\mathbf{r}, \sigma}$ ,  $\hat{n}_{\mathbf{r}} = \hat{n}_{\mathbf{r}, \uparrow} + \hat{n}_{\mathbf{r}, \downarrow}$  and

$$\sum_{\mathbf{r}} n_{\mathbf{r}} = N$$

is total number of electrons. The electron density is

$$c_e = \frac{N}{L}. \quad (1.6)$$

In a number of 1D narrow-band conductors (for example, charge-transfer salts of a TTF-TCNQ type [6]) and adatom systems (if the adatom interaction with a substrate is sufficiently strong [12]), we have typically  $c_e < 1$  and  $U \gg V(\bar{l})$ . This is why it seems reasonable to neglect the quantum dynamics (first term) and Fermi statistics (second term) effects in (1.5). The obtained system is known as the generalized Wigner crystal (GWC) and is described by the classical Hamiltonian

$$H = \frac{1}{2} \sum_{\mathbf{r} \neq \mathbf{r}'} V(|\mathbf{r} - \mathbf{r}'|) n_{\mathbf{r}} n_{\mathbf{r}'}, \quad (1.7)$$

where  $n_{\mathbf{r}} = 0, 1$  are the classical occupation numbers of electrons on host-lattice site with coordinate  $\mathbf{r}$ .

It is often useful to rewrite Hamiltonian (1.7) in terms of the coordinates of electron  $\{\mathbf{x}_j\}_{j=1}^N$ , instead of occupation numbers  $\{n_{\mathbf{r}}\}_{\mathbf{r} \in \mathcal{L}}$ . Using the condition  $n_{\mathbf{x}_j} = 1$ ,  $j = 1, \dots, N$ , we obtain

$$H = \frac{1}{2} \sum_{j \neq k}^N V(|\mathbf{x}_j - \mathbf{x}_k|). \quad (1.8)$$

## 2. Translation invariant systems

### 2.1. Generalities

The classical lattice gas models with purely repulsive and strictly convex  $V$  of (1.1) were used to study the orderings of electrons in quasi-one-dimensional conductors by Hubbard [6, 13] and the orderings of monolayers of atoms adsorbed on solids by Pokrovsky and Uimin [14]. The periodic ground-state particle configurations of these models have been described exactly in [6, 14]. Namely, it was shown that particles are distributed as far as possible from each other respecting restrictions imposed on their locations by the underlying periodic hostchain. These configurations, the generalized Wigner lattices according to Hubbard [6], are independent of any further details of the interaction potential. Moreover, the ground-state configurations have an interesting property known as the complete devil's staircase [15–17].

One-dimensional systems with  $\gamma = 1$  in (1.1) were considered first by Hubbard [6], who argued that if

$$c_e = N/L = p/q, \quad (2.1)$$

where  $p/q$  is irreducible, then the ground state of (1.7) is the “electron crystal” with cell length  $a_0 q$  and  $p$  particles per cell. Besides, the distance  $l_j$  between the nearest neighboring electrons can assume of the following two values:

$$l_j = x_{j+1} - x_j = a_0 [1/c_e], a_0 ([1/c_e] + 1), \quad (2.2)$$

where [...] denotes the integer part and  $x_j$ ,  $j = 1, 2, \dots$  are the electron positions. More detailed analysis of the ground state of (1.7) was carried out in [16].

The grand canonical ensemble version of the one-dimensional lattice described by (1.7) with potential having an arbitrary  $\gamma > 1$  [see (1.1)] was studied rigorously in [17]. The Hamiltonian in this case is [cf. (1.7)]

$$H = \frac{1}{2} \sum_{\mathbf{r} \neq \mathbf{r}'} V(|\mathbf{r} - \mathbf{r}'|) n_{\mathbf{r}} n_{\mathbf{r}'} - \mu \sum_{\mathbf{r}} n_{\mathbf{r}}, \quad (2.3)$$

where  $\mu$  is the chemical potential. In particular, it follows from [17] that the ground state structure does not depend on  $\gamma$  and can be described by the simple formula

$$x_j = a_0 [j/c_e + \phi], \quad (2.4)$$

valid for any, i.e., not necessarily rational  $c_e$  [the same is true for (2.2)]. Here  $\phi \in [0, 1)$  is an arbitrary (initial) phase determined by the choice of the origin of the host chain. The zero temperature concentration  $c_e$  as a function of  $\mu$  is the devil staircase with the widths of the stairs (stability intervals of electron crystal) equals

$$\Delta\mu(c_e) = \Delta\mu(p, q) = q \sum_{k=1}^{\infty} k \delta^2 V(qk),$$

$$\delta^2 V(x) = V(x+1) - 2V(x) + V(x-1). \quad (2.5)$$

It follows from (2.5) that the widths depend only on the denominator  $q$  of (2.1). Note that the case  $\gamma = 1$  treated in [6, 16] is a bit delicate, since it requires a certain cutoff at a screening radius  $r_0 \gg a_0$  to provide the existence of macroscopic thermodynamics. In this case, the devil-staircase steps with  $\Delta\mu \lesssim V''(r_0)$  vanishes.

### 2.2. Low-temperature thermodynamics.

#### Nearest-neighbor approximation

According to (2.2) and (2.4), the only two interelectron distances are possible in the ground state. This implies that in the low-density region ( $c_e \ll 1$ ) one can assume the quasi-equidistant distribution of particles. Besides, it follows from (2.5) that the only “simple” electron densities like  $c_e = 1/q$  contribute significantly to the low-temperature thermodynamics. Indeed, we have by (2.5)

$$\Delta\mu(c_e = p/q) \sim V''(q).$$

Considering two close electron densities, for example,  $c_e = 1/3$  and  $c_e = 101/300$ , we conclude that

$$\Delta\mu(c_e = 1/3) \sim V''(3) \gg \Delta\mu(c_e = 101/300) \sim V''(300).$$

At any finite temperatures, the devil-staircase steps with  $\Delta\mu(c_e) \ll T$  will be destroyed. According to (2.2), the mean interelectron distance  $\bar{l} \approx x_{j+1} - x_j$  is about  $1/c_e$ , thus  $\Delta\mu \sim V''(1/c_e)$ . Assume that

$$V''(2/c_e) < T < V''(1/c_e). \quad (2.6)$$

These inequalities imply that it suffices to consider only the nearest-neighbor interactions in (1.7), see Sec. 4 for more general case. As a result, we obtain the corresponding approximate Hamiltonian

$$H_{NN} = \sum_{j=1}^{N-1} V(x_{j+1} - x_j),$$

$$1 < x_1 < \dots < x_j < \dots < x_N < a_0 L \quad (2.7)$$

and every  $x_j$ ,  $j = 1, \dots, N$  runs over the set  $\{sa_0\}_{s=1}^L$  of the host-chain sites.

Note that in this approximation we take into account the interaction between the nearest electrons but not the nearest host chain sites. As a result, the only the devil-stair steps corresponding to the structures with  $p = 1$  survive. More detailed explanations of the proposed approximation and its applicability are given at the end of this section.

In order to calculate the corresponding to (2.7) partition function

$$Z(L, N) = \sum_{S_N} \exp\left(-\frac{1}{T} \sum_{j=1}^{N-1} V(x_{j+1} - x_j)\right), \quad (2.8)$$

where  $S_N$  is the domain indicated in (2.7),  $T$  is the temperature and Boltzmann constant is equal to unity here and everywhere below. It is convenient to introduce the partition function  $Q(N, L)$  of  $N$  particles and  $L$  host-chain sites where the last site is occupied. Then we have

$$Z(L, N) = \sum_{l=N}^L Q(l, N). \quad (2.9)$$

It follows from the definition that  $Q(L, N)$  satisfies the recurrent formula

$$Q(L, N) = \sum_{l=N}^{L-1} Q(l, N-1) \exp\left(-\frac{V(L-l)}{T}\right). \quad (2.10)$$

Applying to the formula the discrete Laplace transformation in  $L$ , we obtain

$$\begin{aligned} \tilde{Q}(\alpha, N) &= \sum_{L=N}^{\infty} Q(L, N) \exp(-\alpha L) = \\ &= \sum_{L=N}^{\infty} \exp(-\alpha L) \sum_{l=N}^L Q(l, N-1) \exp\left(-\frac{V(L-l)}{T}\right), \end{aligned} \quad (2.11)$$

hence,

$$\tilde{Q}(\alpha, N) = \tilde{Q}(\alpha, N-1) G(\alpha) = G^N(\alpha) S(0, \alpha), \quad (2.12)$$

where

$$G(\alpha) = \sum_{l=1}^{\infty} \exp\left(-\frac{V(l)}{T} - l\alpha\right) \quad (2.13)$$

and

$$\tilde{Q}(\alpha, 0) = e^{-\alpha} (1 - e^{-\alpha})^{-1}.$$

This and (2.9) imply for the Laplace transform  $\tilde{Z}(P, N)$  of  $Z(L, N)$

$$\tilde{Z}(N, P) = \sum_{L=N}^{\infty} e^{-PL/T} Z(L, N) = e^{-P/T} (1 - e^{-P/T})^{-2} G^N(P/T), \quad (2.14)$$

where we introduced  $P = \alpha T$ ,  $P$  is the pressure.

Note that the introduction of the Laplace transforms  $\tilde{Q}(\alpha, N)$  in (2.11) and  $\tilde{Z}(P, T)$  (2.14) is essentially motivated by the computation need to find the partition function  $Z(L, N)$  (2.8) of the model (1.7) in NN approximation, the discrete analog of the well-known model of hard rods (see, e.g., [18]). On the other hand,  $Z(L, N)$  can be viewed as the partition function of the one-dimensional lattice gas described by the canonical ensemble formalism. The passage from  $Z(L, N)$  to  $\tilde{Z}(P, N)$  can then be interpreted as that from the canonical ensemble description of our lattice gas to the isothermal-isobaric ensemble description used for systems that are in the thermal and mechanical equilibrium with the environment (see, e.g., [19], Sec. 13, 14). The corresponding independent parameters in the ensemble are the temperature, number of particles and pressure and corresponding thermodynamic potential

$$\Phi(N, P, T) = \mu(P, T)N = -T \log \tilde{Z}(P, N). \quad (2.15)$$

which is sometimes called the Gibbs free energy.

Formulas (2.13), (2.14) yield in the thermodynamic limit  $N \rightarrow \infty$ :

$$\mu(P, T) = -T \log \left( \sum_{l=1}^{\infty} \exp\left(-\frac{V(l) + lP}{T}\right) \right). \quad (2.16)$$

Note that the r.h.s. is finite because of the condition  $\gamma > 1$  in (1.1).

### 2.3. The equations of state

According to (2.15) and (2.16), the macroscopic limit of the mean electron concentration as the function of  $P$  and  $T$  is

$$c_e(P, T) = \left( \frac{\partial \mu(P, T)}{\partial P} \right)^{-1} = \frac{\sum_{l=1}^{\infty} \exp\left(-\frac{V(l) + lP}{T}\right)}{\sum_{l=1}^{\infty} l \exp\left(-\frac{V(l) + lP}{T}\right)}. \quad (2.17)$$

We will need below the notion of “ $l$ -pairs”. It is defined as the pairs of the neighboring electrons with the interelectron distance equal  $l$ . According to the above, the mean number of  $l$ -pairs per particle is

$$n(l, P, T) = \frac{\partial \mu(P, T)}{\partial V(l)} = \frac{\exp\left(-\frac{V(l) + lP}{T}\right)}{\sum_{j=1}^{\infty} \exp\left(-\frac{V(j) + jP}{T}\right)}. \quad (2.18)$$

To analyze (2.17) and (2.18), it is convenient to write the exponent of these formulas as  $\alpha\mathcal{F}(l, P)$ , where

$$\mathcal{F}(l, P) = V(l) / P + l, \quad (2.19)$$

$$\alpha = P/T.$$

Consider first the case, where  $\alpha \ll 1$ , i.e., the high-temperature and/or low-pressure region. In this case, the major contribution to the sums over  $l$  in (2.17) is due to the large  $l \sim 1/\alpha$ , hence we can replace  $\mathcal{F}(l, P)$  by  $l$ . This leads to the equation of state of the classical ideal gas

$$PL = NT.$$

The result is quite natural, because in the case  $\alpha \ll 1$  the interelectron interactions can be neglected.

Expanding the sums of (2.17) in powers of  $\alpha$ , we obtain the analogue of the virial expansion. Its first term leads to the van der Waals-like equation of state

$$P(L - B(T)N) = TN, \quad (2.20)$$

where

$$B(T) = \sum_{l=1}^{\infty} \left[ 1 - \exp\left(-\frac{V(l)}{T}\right) \right] > 0$$

(essentially, the second virial coefficient) is the effective deficit of the system volume due to the electron-electron repulsion.

In the opposite limiting case  $\alpha \gg 1$ , the thermodynamics of the system depends essentially on the behavior of  $V(l) + Pl$  as a function of the integer valued argument  $l$ . The function is monotone decreasing for

$$P > P_C = V(1) - V(2), \quad (2.21)$$

while for  $P < P_C$  it has a minimum. Following [6, 16, 17], we will consider a convex  $V$ , thus there is only one minimum at integer  $l_0 = l_0(P) = [x_0 + 1/2] > 1$ , where  $x_0$  is the unique root of the equation (see Fig. 2.1)

$$V'(x) = -P. \quad (2.22)$$

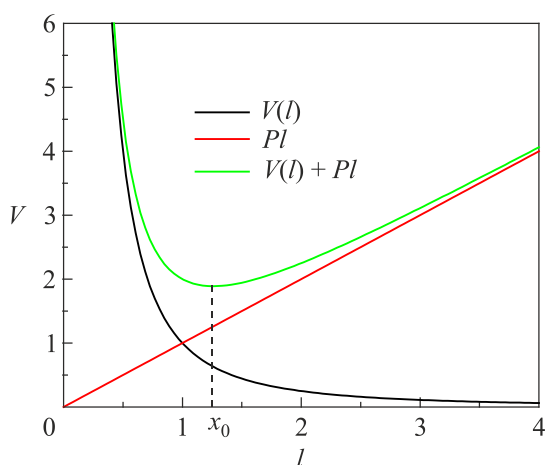


Fig. 2.1. The effective energy  $V(l) + Pl$  as a function of distance  $l$ .

If  $P > P_C$ , the most probable length of  $l$ -pair is  $l = 1$ , while in the opposite case  $P < P_C$  the length is  $l_0(P)$ .

In the first case ( $P < P_C$ ), only the term with  $l = l_0(P)$  contributes to the sums in (2.17). More exactly, this is the case if  $P$  is not too close to the degeneration points  $\{P_q\}$  determined by the expression

$$P_{q+1} = V(q) - V(q+1), \quad q = 1, 2, \dots \quad (2.23)$$

For these values of  $P$ , the contributions of two terms with  $l = [x_0(P_q)] = q$  and  $l = [x_0(P_q) + 1] = q + 1$  coincide [recall that  $x_0(P)$  is the root of equation (2.22)]. The points  $\{P_q\}$  divide the  $P$  axis into intervals  $(P_{q+1}, P_q)$  which form the devil-staircase intervals corresponding to  $p = 1$  of (2.1) in the framework of NN approximation. The width of the  $q$ th interval is

$$\Delta P_q \equiv P_q - P_{q+1} = V(q-1) - 2V(q) + V(q+1). \quad (2.24)$$

Note that the above expression is positive since  $V$  is convex. As was shown in [20], the devil-stairs widths  $\Delta\mu(c_e)$  [see (2.5)] and  $\Delta P(c_e)$  are related as

$$\Delta P(p, q) = p/q \Delta\mu(p, q), \quad (2.25)$$

i.e., (2.24) is just first term of (2.5). Within the  $\Delta P_q$  intervals  $c_e$  is independent of  $P$  with an exponential accuracy in  $\alpha$  and is equal to [cf. (2.1)]

$$c_e = \text{const} = 1/q. \quad (2.26)$$

Thus, for  $P < P_C$ , just as in the parameter region  $\alpha \gg 1$ , the ground state is the complete devil's staircase (see Fig. 2.2).

If  $P$  belongs to the intervals  $(P_{q+1}, P_q)$ , the periodicity of the chain is broken because of the thermal creation of  $l$ -pairs with  $l = q \pm 1$ . According to (2.18) and (2.23), the mean number of  $(q \pm 1)$ -pairs has the exponential form

$$n(q-1, P, T) = N \exp\left(\frac{P - P_q}{T}\right), \quad (2.27)$$

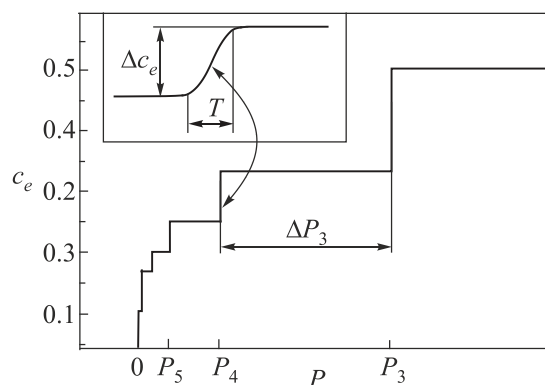


Fig. 2.2. The mean electron density  $c_e$  as a function of pressure  $P$  according to (2.17),  $\Delta c_e = 1/(q-1) - 1/q$ .

$$n(q+1, P, T) = N \exp\left(\frac{P_{q+1} - P}{T}\right). \quad (2.28)$$

As seen from (2.27), the total number of  $l$ -pairs with  $l = q$  and  $l = q-1$  becomes comparable in the regions  $|P - P_q| \lesssim T$ . Similarly, it follows from (2.28) that the numbers of  $l$ -pairs with  $l = q$  and  $l = q+1$  in the regions  $|P - P_{q+1}| \lesssim T$  are comparable. As a result, we have the steps rounding of  $c_e(P)$  (see insert of Fig. 2.2).

Besides, it follows from (2.17) and (2.18) that the presence of  $(q \pm 1)$ -pairs changes the density  $c_e$  by small amount

$$\delta c_e(q, P, T) = \frac{1}{q^2 N} (n(q-1, P, T) - n(q+1, P, T)), \quad (2.29)$$

showing that each  $(q+1)$ -pair *increases* the length of the system from  $L$  to  $L+1$  and, conversely, a  $(q-1)$ -pair *decreases* from  $L$  to  $L-1$ . These pair excitations are the elementary “quanta” of rarefaction [ $(q+1)$ -pairs] or compression [ $(q-1)$ -pairs]. We will call them the rarefaction or compression *defectons*.

In the framework of the NN approximation (2.7), the only  $c_e(P)$  steps corresponding to  $c_e = 1/q$  survive (see Fig. 2.3). This means that the proposed model describes sufficiently well the system under consideration provided that the concentration of  $q$ -pairs is much larger than the concentration of  $l$ -pairs with  $l \neq q$  and that the only term with  $l = q$  gives the major contribution into sums (2.17). This is the case where  $P$  belongs to the neighborhood of the middle points

$$P_q^{\text{mid}} = (P_{q+1} + P_q) / 2$$

of intervals  $(P_{q+1}, P_q)$  of (2.23). In the opposite case of  $P \rightarrow P_{q+1}$ , the number of  $q+1$ -pairs increases exponentially [see (2.28)] and the contributions of two terms with  $l = q$  and  $l = q+1$  into sum (2.17) are comparable. At the same

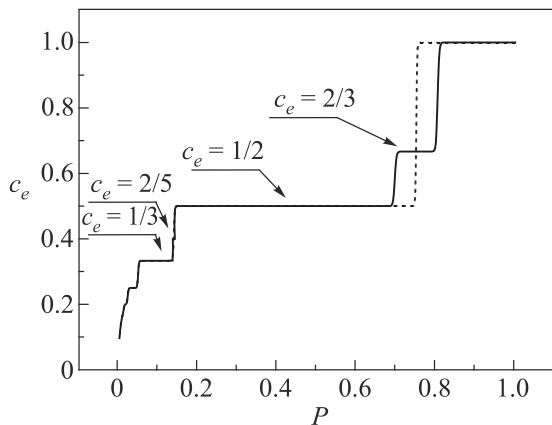


Fig. 2.3. The electron density  $c_e$  as a function of pressure  $P$  for the model that takes into account the nearest and next-nearest neighbors interactions [21]. Dotted line corresponds to the NN approximation.

time, in the framework of the NN model the energy of the system depends on the number of  $l$ -pairs but not on their distribution. Hence, in these  $P$  regions, it is necessary to go beyond the NN approximation.

It was shown in [21] that taking into account the nearest- and next-nearest-neighbor interactions modifies the  $c_e(P)$  dependence (Fig. 2.3). New fine details appear, namely, the steps corresponding to “crystals” with  $c_e = 2/q$ ,  $q = 3, 5, 7, \dots$ . It is important that the step widths are proportional to  $V''(q)$  and, therefore, much less than the step widths of corresponding “crystals” with close  $c_e$ , but belonging to the  $c_e = 1/q$  class. Thus, the long-range interaction for finite temperature leads to a slight modification of  $c_e(P)$  and  $c_e(\mu)$  dependences. It means that in the limiting case  $\alpha \gg 1$  [see (2.19)] the main role play “crystals” with  $c_e = 1/q$ . This result is physically clear. In the nearest-neighbor approximation, the energy of  $l$ -pairs configurations in elementary cell with two or more electrons is the same. For example, if  $c_e = 2/5$ , then the ground-state  $l$ -pairs distributions is  $2-3-2-3-\dots$ . In NN approximation, this configuration is equivalent to  $2-2-3-3-\dots$  one. Next-nearest interaction remove the degeneration. Actually, the energy (per cell) of the configuration  $2-3-2-3-\dots$  is  $V(2)+V(3)+2V(5)$ , whereas this energy is  $V(2)+V(3)+V(4)+V(6)$  for  $2-2-3-3-\dots$  configuration. Due to  $V(x)$  convexity  $2V(5) < V(4)+V(6)$ . Thus, next-nearest interaction stabilizes the “crystals” with two electrons per cell.

On the other hand, the degeneration energy per cell

$$\tilde{E} \sim 2V(5) - V(4) + V(6)$$

is much less than the corresponding energy (per cell) of the “crystals” with close  $c_e$ , but from  $c_e = 1/q$  class ( $c_e = 1/2$  and  $c_e = 1/3$ ). This manifests itself in the graph of  $c_e(P)$  as a short step corresponding to  $c_e = 2/5$  and lying between two wide steps corresponding to  $c_e = 1/2$  and  $c_e = 1/3$  (see Fig. 2.3).

#### 2.4. Elementary excitations, defectons with fractional charge

According to (2.25), the dependence of  $c_e$  on the chemical potential  $\mu$  is devil’s staircase whose widths  $\Delta\mu_q$  are determined by  $\Delta P_q$ . For a given  $\mu$  the deviation  $\delta c$  of (2.29) is due to the change of the particle number  $N$  for a fixed chain length  $L$ . This means that adding or removing an electron in the system increases or decreases by amount  $q$  the total number of the defects. In the limit  $\alpha \ll 1$  [see (2.19)], these defects are in fact free charge carriers with the fractional charge

$$e^* = \pm e / q, \quad (2.30)$$

where  $e$  is the electron charge and the signs “+” and “-” correspond to the rarefaction and the compression, which we call defectons. Formula (2.30) generalizes Hubbard’s result [6], which holds for the special case  $q = 2$ .

It follows from (2.28) and (2.29) that, as  $P$  tends to the endpoints of interval  $(P_{q+1}, P_q)$ , the mean interelectron distances  $n(q-1, P, T)$  or  $n(q+1, P, T)$  rapidly increase by an order of magnitude compared with  $N$ . This means that the number of “ $l$ ”-pairs with  $l = q-1$  or  $l = q+1$  also increases rapidly, and the electron density decreases rapidly from  $c_e = 1/(q-1)$  and  $c_e = 1/q$ .

For the description of these intermediate regions where  $|P - P_q| \ll P_q$  one should take into account the terms with  $l = q-1$  and  $l = q$  in the sums over  $l$  of (2.17). This leads to the simple formula:

$$1/c_e = q - \frac{1}{1 + \exp\left(\frac{P_q - P}{T}\right)}. \quad (2.31)$$

If  $P_q - P \gg T$ , then the r.h.s. of the formula is  $q - (N_{q-1}/N)$ , where  $N_{q-1}$  is given by (2.28). Similarly, in the limit  $P - P_q \gg T$  the r.h.s. of (2.31) is  $q - 1 + (N_q/N)$ . In the intermediate domain  $|P_q - P| \sim T$ , the system is a highly disordered “liquid” since  $N_q$  and  $N_{q-1}$  are of the same order of magnitude.

The case  $P > P_C$  corresponds to  $q = 1$ , thus cannot be treated by the NN approximation (2.6). Nevertheless the results obtained for  $\alpha \gg 1$  are quite reasonable. The “electron crystal” with period  $q = 1$  is formed and the number of the translation symmetry-breaking elementary excitations is

$$n(1, P, T) = N \exp\left(\frac{P_C - P}{T}\right).$$

The excitations are simply the electron vacancies with charge

$$e^* = e.$$

If  $P_C$  coincides with an endpoint  $P_2$  [see (2.21) and (2.23)], the intermediate region between crystals with  $q = 1$  and  $q = 2$  is described by (2.31) with  $q = 1$ .

Thus, the change of the pressure  $P$  for a given  $\alpha \gg 1$  produces a succession of electronic crystals with periods  $q = 1, 2, \dots$  which increases as  $P$  decreases. It should be noted that at  $\alpha \gg 1$  the crystals exist, even if  $P$  is small. In the low-pressure limit the typical value of  $q$  is determined by the equation

$$\left. \frac{dV(x)}{dx} \right|_{x=q} = -P.$$

The thermodynamic behavior of the system in this case is schematically represented in Fig. 2.4.

The discussed above defectons is a rather special and interesting branch of the elementary excitations of the system under consideration. According to (2.2), the ground-state structure of the 1D generalized Wigner crystal consists of two types of  $l$ -pairs, those with  $l = q$  and  $l = q+1$ , where  $q = [1/c_e]$  (except the case  $c_e = 1/q$  where the only distance  $l = q$  is possible). The number of these  $l$ -pairs

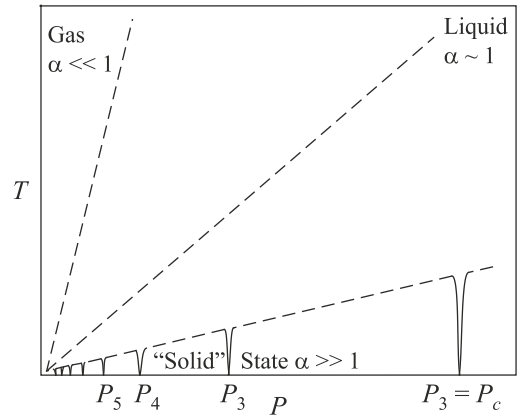


Fig. 2.4. The phase diagram of the system. V-shaped “negative” peaks are boundaries,  $\delta c_e(q, P, T) = 1/q$ ,  $\delta c_e(q+1, P, T) = 1/q$ , between the electronic liquid and the electronic “crystal”.

depends on  $c_e$  [see (2.23), (2.27), (2.28)]. Thus, the ground-state structure can be considered as the superstructure of defectons with  $l = q+1$  on the background of 1D chain with a period  $q$  (or vice versa).

It was shown in [22] that the low-energy excitations of the system form jumps of “left” electron of a defecton to the right or jumps of “right” electron to the left [see Figs. 2.5(a)–(c)]. The jumps are equivalent to the defecton translations by the period of the generalized Wigner crystal. In the quantum case, i.e., if the overlapping integral  $t$  in (1.5) is not zero, defectons acquire the dispersion law

$$\varepsilon(\kappa) = -2t \cos(q\kappa),$$

where  $\kappa$  is an electron quasi-momentum. The factor  $q$  of (2.1) in the argument of the cos is due to the mentioned above fact that the jump of an electron in a defecton is equivalent to the defecton translation to the period of a generalized Wigner crystal.

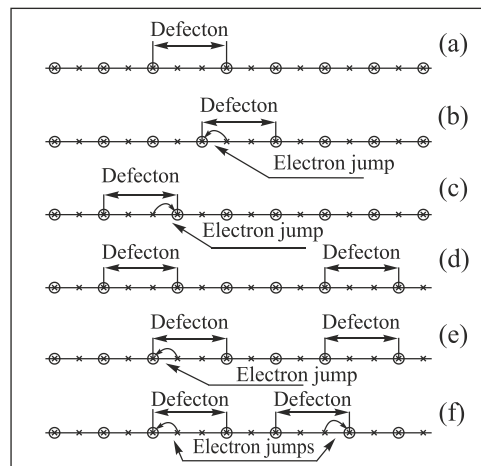


Fig. 2.5. The examples of defectons: (a) a fragment of 1D GWC ground-state structure with  $\delta m \ll 1$ ; (b) and (c) on isolated defecton shifted to the right and to the left; (d) two defectons; (e) a defecton shift (excitation); (f) antiparallel shifts of two defectons.

In what follows, it is more convenient to deal with the mean interelectron distance  $\bar{l} = 1/c_e$  instead of  $c_e$ . Let us write  $\bar{l}$  as  $\bar{l} = m_0 + \delta m$  with integer  $m_0 = [\bar{l}]$  and fractional

$$\delta m = \bar{l} - [\bar{l}], 0 \leq \delta m < 1. \quad (2.32)$$

Then the Hubbard formula (2.4) becomes

$$x_j = a_0(jm_0 + [j\delta m]) \quad (2.33)$$

and we do not write here and below the phase  $\phi$  of (2.4), since it does not contribute to the essential property of the system in view of its translation invariance.

From (2.33) we conclude that the electron coordinates  $\{x_j\}_{j=1}^N$  are equidistant with period  $a_0 m_0$  as long as  $0 < j\delta m < 1$ . For  $j_0 = [1/\delta m]$  the interelectron distance  $x_{j_0} - x_{j_0-1}$  is  $m_0 + 1$ . For  $j > j_0$  the interelectron distances are  $m_0$  again, as long as  $1 < j\delta m < 2$ , etc. Thus, we have here the periodic superstructure of  $(m_0 + 1)$ -pairs (defectons) whose background is the ideal structure of  $m_0$ -pairs [Fig. 2.5(d)]. According to (2.33), the concentration  $c_{m+1}$  of  $(m_0 + 1)$ -pairs is  $\delta m$  and the mean distance between  $(m_0 + 1)$ -pairs is  $\bar{x} = a_0 m_0 / \delta m$  [more exactly,  $\bar{x} = (m_0 / \delta m + 1)$ ]. This and (2.4) imply that the ground-state electron configuration is strictly equidistant with period  $m_0$  for integer  $\bar{l}$ , i.e., the concentration of  $(m + 1)$ -pairs is zero. In the case of  $\delta m = 1/2$ , the concentrations of the  $m_0$ -pairs and  $(m_0 + 1)$ -pairs are the same and we have either superstructure of  $m_0$ -pairs on the background of  $(m_0 + 1)$ -pairs, or, vice versa, that of  $(m_0 + 1)$ -pairs, on the background of  $m_0$ -pairs. For  $\delta m > 1/2$ , the concentration of  $m_0$ -pairs is less than that of  $(m_0 + 1)$ -pairs and it is more convenient to consider the system as the superstructure of  $m_0$ -pairs (defectons) on the background of  $(m_0 + 1)$ -pairs. In the limiting case  $\delta m \rightarrow 1$ , the ground state is the superstructure of  $(m_0 + 1)$ -pairs, i.e., the strictly periodic structure with period  $m_0 + 1$ . It is convenient to define the density of defectons as

$$c_d = \begin{cases} \delta m = \bar{l} - [\bar{l}], & \delta m \leq 1/2, \\ 1 - \delta m, & \text{otherwise.} \end{cases}$$

We conclude that  $c_d$  is *periodic* in  $1/c_e$  [see Fig. 2.6(a)].

The excitation energy of defecton is [22]

$$E_{\text{ex}}(\bar{x}) = E(1, \bar{x}) = \sum_{k=1}^{\infty} \delta^2 V(k\bar{x}), \quad (2.34)$$

where  $\delta^2 V(x)$  is defined in (2.5) and  $\bar{x} = [\bar{l}] / c_{\text{dim}} + 1$ .

The typical forms of  $\bar{x}$  and  $E_{\text{ex}}$  are given by Figs. 2.6(b) and 2.6(c), correspondingly.

Let us consider now the excitation energy  $E(n)$  of  $n$  successive defectons corresponding to parallel electron shifts. We will call such an excitation the “domain” containing  $n$  defectons. It is easy to see that

$$E(n, \bar{x}) = nE(1, \bar{x}) - \sum_{k=1}^n (n-k) \delta^2 V(k\bar{x}). \quad (2.35)$$

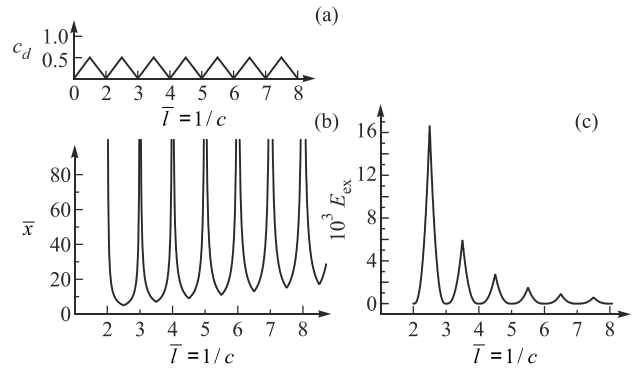


Fig. 2.6. (a) The defecton concentration as a function of the inverse electron concentration  $\bar{l}$ ; (b) and (c) are the typical forms of  $\bar{x}(l_0)$  and  $E_{\text{ex}}(l_0)$ , correspondingly.

It is worth noting that, according to (2.34), (2.35), the energy of the domain of infinite length

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

is finite even in the case of the (nonscreened) Coulomb pair potential:

$$\delta^2 V(k\bar{x}) \approx \frac{\bar{x}^3}{k^3}, \quad E(\infty, \bar{x}) \approx \bar{x}^3 \sum_{k=1}^{\infty} \frac{1}{k^2} = \bar{V} \bar{x}^3 \frac{\pi^2}{6}.$$

Thus, the spectrum of the domain excitations can be viewed as a quasi-band consisting of a series of accumulating levels of width

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

and with the “gap”  $E(1, \bar{x})$  to the ground state.

An example of the domain excitation spectrum is presented in Fig. 2.7.

Let us consider now an “antiparallel” excitation of two neighboring defectons [see Fig. 2.5(f)]. These excitations can be associated with the oscillations of defecton density and have the excitation energy

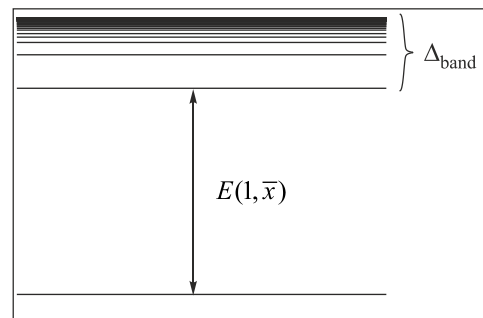


Fig. 2.7. The spectrum of the domain excitations.



$$\begin{aligned}\tilde{E}_{\text{ex}}(\bar{x}, m_0) &= V(\bar{x}) - 2V(\bar{x} - m_0 a_0) + V(\bar{x} + (m_0 - 1) a_0) \approx \\ &\approx 3m_0 a_0 V'(\bar{x}) \sim 2m_0 a_0 \bar{V} / \bar{x}^2,\end{aligned}\quad (2.36)$$

where  $1 < m_0 < l_0$ , and

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

We conclude that the lowest energy excitations in the system under consideration are the “domains”.

### 2.5. Domain decay

Let us consider the process of destruction of domains of length  $n$  centered at  $n_0$  ( $1 \leq n_0 \leq n$ ). It is easy to show that the energy of this process is

$$\Delta E(n, n_0, \bar{x}) = -E(1, \bar{x}) + \sum_{k=1}^{n_0-1} \delta^2 V(k\bar{x}) + \sum_{k=1}^{n-n_0} \delta^2 V(k\bar{x}), \quad (2.37)$$

where  $E(1, \bar{x})$  is defined in (2.34) and  $\delta^2 V$  is defined in (2.5). It follows from (2.37) that  $\Delta E(n, n_0, \bar{x})$  possesses the symmetry property

$$\Delta E(n, n_0, \bar{x}) = \Delta E(n, n+1-n_0, \bar{x}).$$

Besides, we have

$$\Delta E(n, 1, \bar{x}) = -\sum_{k=1}^{\infty} \delta^2 V(k\bar{x}) + \sum_{k=1}^{n-1} \delta^2 V(k\bar{x}) = -\sum_{k=n}^{\infty} \delta^2 V(k\bar{x}), \quad (2.38)$$

and

$$\Delta E(n, 1, \bar{x}) = E(n-1, \bar{x}) - E(n, \bar{x}).$$

Thus,  $-\Delta E(n, 1, \bar{x})$  is the energy of the boundary defecton removed from a “domain” with length  $n$ . The energy  $\Delta E(n, n_0, \bar{x})$  is minimal for  $n_0 = 1$  and  $n_0 = n$  and has a maximum at  $n_0 = [n/2]$  (see Fig. 2.8). It means that the low-temperature domain decay is the step-by-step detaching of the bounded defectons from the domain.

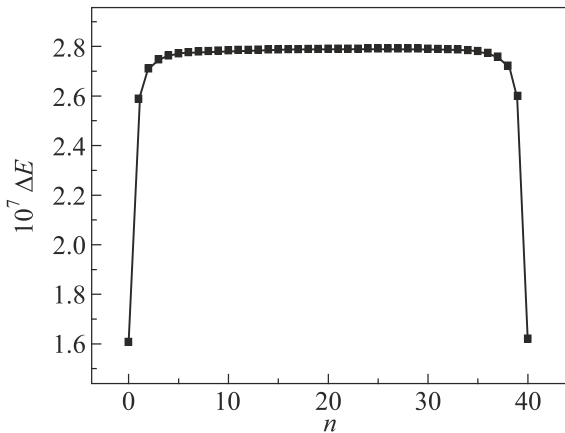


Fig. 2.8. The energy of a “domain” excitation as a function of  $n_0$  obtained using (2.37) for  $n = 40$ .

### 2.6. Quantum effects

Until this paragraph we have neglected the tunneling term in (1.5). As was shown in [6], such an approximation is suitable for the most 1D charge transfer salts. At the same time, for a number of newly artificially-created 1D compounds the tunneling significantly affects on the ground state and low-temperature properties of GWC (see, for example, [23]). Now, we will consider 1D ensemble of fermions with a nonzero overlapping integral  $t$ , interacting via a local repulsion  $U_0$  and a long-ranged repulsive potential  $V$  described by the Hamiltonian (1.5) which we write as

$$H = \hat{T} + \hat{U} + \hat{V}. \quad (2.39)$$

As is indicated in Introduction, the classical limit studied by Hubbard [6] arises in the limit  $t \rightarrow 0$  and  $U_0 \rightarrow \infty$  in (1.5). The ground-state configuration in this case is given by (2.4). For finite  $t$  quantum fluctuations will tend to delocalize the electrons with respect to their classical configuration. Nevertheless, the classical solution is still a good approximation for small  $t$  (see [23]).

In order to study the ground state of (2.39) we will use the variational ansatz

$$\Psi_B(\eta) = e^{-\eta \hat{T}} \Psi_\infty \quad (2.40)$$

introduced previously in the context of the Mott–Hubbard transition [24]. Here  $\eta$  is a variational parameter,  $\hat{T}$  is the kinetic energy operator of (2.39) and  $\Psi_\infty$  is the ground state for  $t = 0$ , i.e., Hubbard’s classical solution.

We first assume that the on-site repulsion is the dominant energy scale, and take the limit  $U_0 \rightarrow \infty$ . This eliminates both double occupancy and mixing of different spin configurations. In the case of Coulomb potential ( $\gamma = 1$ ), we obtain the following simplified model for spinless electrons:

$$\hat{T} + \hat{V} = \sum_{\kappa \in \text{RBZ}} \varepsilon_\kappa \hat{c}_\kappa^+ \hat{c}_\kappa + \frac{1}{2L} \sum_{\kappa \in \text{RBZ}, \kappa \neq 0} V(\kappa) \hat{\rho}_\kappa \hat{\rho}_{-\kappa},$$

where RBZ is the reduced Brillouin zone (the lattice parameter  $a_0$  has been set equal to 1) and

$$\varepsilon_\kappa = -2t \cos \kappa, \quad \hat{\rho}_\kappa = \sum_{\kappa' \in \text{RBZ}} \hat{c}_{\kappa+\kappa'}^+ \hat{c}_{\kappa'},$$

$$V(\kappa) = -V_0 \log(2[1 - \cos \kappa]).$$

The classical solution in the case of  $c_e = 1/2$  corresponds to alternating occupied and empty sites. It should be noted, that half-filling model corresponds to  $c_e = 1$  and quarter-filling model corresponds to  $c_e = 1/2$ . Thus, wave function  $\Psi_\infty$  in (2.40) can be written in the momentum space representation as

$$\Psi_\infty = \prod_{\kappa \in \text{RBZ}} \frac{1}{\sqrt{2}} (\hat{c}_\kappa^+ + \hat{c}_{\kappa+\pi}^+) \Psi_0,$$

where the product runs over the reduced Brillouin zone  $|\kappa| < \pi/2$ , and  $\Psi_0$  is the vacuum for electrons. The opera-

tor  $e^{-\eta\hat{T}}$  is now diagonal and we can write straightforwardly the (normalized) variational wave function (2.40) as

$$\Psi_B(\eta) = \prod_{\kappa \in \text{RBZ}} \frac{1}{N_\kappa} \left( e^{-\eta\epsilon_\kappa} \hat{c}_\kappa^+ + e^{\eta\epsilon_\kappa} \hat{c}_{\kappa+\pi}^+ \right) \Psi_0,$$

where the normalization factor is given by  $N_\kappa^2 = 2 \cosh(2\eta\epsilon_\kappa)$  (we have set  $t = 1$  so that energies are now expressed in units of the hopping parameter). The best variational ground state is obtained by minimising the energy functional

$$E_B(\eta) = (\Psi_B(\eta), \hat{H} \Psi_B(\eta)) \quad (2.41)$$

with respect to the variational parameter.

The structure factor

$$S(\kappa) = (\Psi_B(\eta), \hat{\rho}_\kappa \hat{\rho}_{-\kappa} \Psi_B(\eta))$$

has a regular part

$$S(\kappa) = \frac{1}{4} - \frac{1}{4\pi} \int_{\text{RBZ}} d\kappa' \frac{1 + \sinh(2\eta\epsilon_{\kappa'}) \sinh(2\eta\epsilon_{\kappa-\kappa'})}{\cosh(2\eta\epsilon_{\kappa'}) \cosh(2\eta\epsilon_{\kappa-\kappa'})}$$

and the Bragg peak

$$S(\pi) = \left[ \int_{\text{RBZ}} \frac{d\kappa}{2\pi} \frac{1}{\cosh(2\eta\epsilon_\kappa)} \right]^2$$

at  $q = \pi$  of the amplitude corresponding to the periodic ordering of electrons.

According to (2.4), the charge density at the site  $s$  for electron concentration  $c_e$  [see (2.1)] can be written as

$$n(s) = [sp/q] - [(s-1)p/q].$$

Setting  $n(s) = n + \tilde{n} \cos(\pi s)$ , we see that the intensity of the Bragg peaks in the structure factor is proportional to the square of the order parameter,  $S(\pi) = \tilde{n}^2$ . It is finite for any finite  $\eta$ , so that the wave function  $\Psi_B(\eta)$  always represents a charge-ordered state.

In the limit  $\eta \rightarrow 0$ , one recovers the classical GWC. The kinetic energy vanishes and the structure factor becomes  $S(q) = \delta_{q,\pi} / 4$ . This and (2.41) yield

$$E_B(0) = V(\pi) / 8 = -V_0 / 4 \log 2.$$

The opposite limit  $\eta \rightarrow \infty$  yields the Hartree–Fock energy of the liquid phase, which is equivalent to taking into account the interaction in lowest order in perturbation theory.

### 3. Disordered systems

In the Introduction, it was indicated that the influence of the host lattice disorder on the ground state and low-temperature properties of the system under consideration is important because a lot of these systems are essentially disordered. In this section, we study a disordered version of the translation invariant model considered in previous sections.

#### 3.1. Cluster model and its basic properties

Consider the case, where the sites  $\{r_s\}_{s=1}^L$  of the host chain deviate slightly from those  $\{s\}_{s=1}^L$  of the periodic one-dimensional lattice, more precisely, we assume that the coordinates of the host chain sites are

$$u + \chi_u, \quad u = 1, \dots, L, \quad (3.1)$$

where  $\{\chi_u\}_{u=1}^L$  are independent and identically distributed random variables with the common probability density  $w$ , and assume that

$$\langle \chi \rangle = 0. \quad (3.2)$$

Note that here and below we assume without loss of generality that the period  $a_0$  of the “unperturbed” chain [see, e.g., (1.1), (2.2), (2.4), etc.] is one:

$$a_0 = 1. \quad (3.3)$$

Thus, according to (3.1), (3.2), a realization of our disordered chain is, in fact, a realization of the collection of random variables  $\{\chi_u\}_{u=1}^L$ , and the corresponding Hamiltonian (the energy) of the system is [cf. (1.7)]

$$\frac{1}{2} \sum_{s \neq t} V(r_s - r_t) n_{r_s} n_{r_t}, \quad (3.4)$$

where now the host chain coordinates  $r_s$  and  $r_t$  are random assuming values (3.1), (3.2).

Applying an argument similar to that used in beginning of Sec. 2.2 to introduce the nearest-neighbor approximation in the translation invariant case [see (2.7)], we obtain the analogous approximation in the disordered case replacing the total interaction energy (3.4) by [cf. (2.7)]

$$H_{NN} = \sum_{j=1}^{N-1} V(x_{j+1} - x_j), \quad (3.5)$$

$$1 < x_1 < \dots < x_j < \dots < x_N < N, \quad (3.6)$$

where now every electron coordinate  $x_j, j = 1, \dots, N$  runs over the set of the host-chain sites (3.1)–(3.3). Note again that the nearest-neighbor approximation means that we take into account the interaction between *the nearest electrons but not the nearest host-chain sites*. The effect of other terms of (1.8) will be considered in Sec. 4.

Recall also that in the translation invariant case ( $\chi_u = 0, u = 1, \dots, l$ ) this approximation was already sufficient in order to carry out a rather detailed analysis of the ground state and the low-temperature properties of the system. This is notably because we were able to write the partition function  $Z(L, N)$  of (2.8) as

$$Z(L, N) = (\mathbf{1}, T^N \mathbf{1}), \quad (3.7)$$

where  $T$  is the (triangular) transfer matrix with entries

$$T(u, v) = e^{-V(u-v)/T} \theta(u-v), \quad u, v = 1, \dots, L. \quad (3.8)$$

Here  $\theta$  is the Heaviside function and  $\mathbf{1}$  is the  $L$ -dimensional vector whose components equal 1. This  $L \times L$  matrix can be diagonalized by the discrete Laplace transformation [see (2.11), (2.12)], thereby providing the technical background for further analysis.

Passing to the disordered case, we obtain again (3.7), however now the corresponding transfer matrix is random since its entries are [cf. (3.8)]

$$T(u, v) = e^{-V(r_u - r_v)/T} \theta(r_u - r_v), \quad u, v = 1, \dots, L, \quad (3.9)$$

where  $r_u$  and  $r_v$  run over the set of random sites (3.1)–(3.3) of the disordered host chain. This  $L \times L$  matrix is a particular case of the so-called Euclidean random matrices arising in condensed matter theory and adjacent fields, see, e.g., review works [25–27]. The matrices are not simple to deal with and have not been studied in detail. Thus, we will study the problem numerically, by a certain direct method.

Before proceeding in this direction, let us discuss briefly a related general topic of the theory of disordered systems. It is evident that the characteristics of disordered systems of finite size depends nontrivially on the realizations of disorder, i.e., fluctuate from sample to sample. However, the specific extensive characteristics, i.e., those per unit volume or per particle (free energy, entropy, specific heat, magnetization, conductivity, etc.), become deterministic in the macroscopic limit. This is known as the *self-averaging property*, which is assumed, sometimes implicitly, in practically all works on disordered systems [26].

The property is a consequence of the spatial homogeneity of the probability distribution (spatial homogeneity in mean) and of the decay of spatial correlations between random parameters entering the Hamiltonian of the system (interaction, external field, particle coordinates, etc.) and determining the disorder.

The mechanism by which the self-averaging property occurs under these conditions is follows (see, e.g., [26, 28]). Every extensive observable  $O_D$  becomes additive if the  $d$ -dimensional domain  $D$  (the  $d$ -dimensional cube for simplicity) of volume  $|D|$  occupied by the system is macroscopically large. This means that by partitioning  $D$  into a collection of smaller but still macroscopically large congruent subdomains  $\{D_j\}_j$  separated by the “mesoscopic corridors” of width  $R \ll |D|^{1/d}$ , we can write the specific observable  $O_D/|D|$  up to the surface terms as the arithmetic mean of its values in the subdomains:

$$O_D/|D| = \sum_j (|D|/|D_j|) O_{D_j}/|D_j| + O(|D|^{-1/d}). \quad (3.10)$$

Note that a similar partitioning is carried out in statistical mechanics of translation invariant systems while proving the existence of the macroscopic (thermodynamic) limit [29, 30].

The statistical properties of the term in (3.10) are the same in view of the spatial homogeneity in mean and if  $R$  is sufficiently large ( $R \gg a_0$ ), then the terms in (3.10) are statistically independent in view of the decay of correlations. Hence, every  $O_{D_j}$  assumes all its possible values independently of the others and if the number  $|D|/|D_j|$  of subdomains is large enough, then the sum (3.10) contains practically all possible realizations of some  $O_{D_j}$  (precisely which one is unimportant since all of them are identically distributed due to the spatial homogeneity in mean). In other words, the summation over  $j$  in (3.10) is equivalent to the summation over all possible realizations of any  $O_{D_j}$ , i.e., its averaging with respect to the corresponding probability distribution. Thus, for macroscopic domains the specific variable  $O_D/|D|$  coincides with its mean  $\langle O_D/|D| \rangle$  value, i.e., is a nonrandom quantity. The quantity coincides with the mean value of any  $O_{D_j}/|D_j|$  if  $D_j$ 's are large enough up to fluctuating error terms of order  $|D|^{-a}$ ,  $a = \min\{1/2, 1/d\}$ .

Recall that in our case, disorder is determined by the collection  $\{\chi_u\}_{u=1}^L$  of the independent and identically distributed random variables in (3.1), (3.2). Thus, the averaging operation  $\langle \dots \rangle$  is the integration of the quantity in question calculated for a given realization of the collection with the density

$$W(\{\chi_1 \dots \chi_L\}) = \prod_{u=1}^L w(\chi_u), \quad (3.11)$$

where  $w$  is the common probability density of the collection  $\{\chi_u\}_{u=1}^L$ .

The above scheme has to be somewhat modified in the case of slow decaying but oscillating interactions and corresponding correlations [31] or for the mean-fields (i.e., for the infinite range) type models [32], both quite popular in the spin glass theory [33], but the essence of the scheme is quite similar in all cases and is analogous to that of the proof of the law of large numbers in probability theory.

It can be shown that the free energy of the classical disordered system, determined by the random host chain with coordinates (3.1), (3.2) and by energy (1.8), where  $V$  satisfies (1.1), (1.2), is self-averaging, see, e.g., [28, 31, 32] for related results, in particular, for the validity of the self-averaging property under rather general conditions of spatial ergodicity of random variables  $\{\chi_s\}_{s=1}^L$  instead the condition to be independent and identically distributed.

On the other hand, self-averaging quantities are not only important characteristics of disordered systems. The systems can also possess a number of important non-self-averaging characteristics, e.g., the spectrum of elementary excitations, the structure of the corresponding states, in particular, the ground state, certain thermodynamic characteristics, such as the hierarchy of relaxation times, related non-ergodic phenomena, and even the order parameter in certain mean field models of spin glasses [26, 32, 33].

All the above makes the studies of disordered systems both noninteracting (like localization and percolation phenomena) and interacting (like many body localization, thermalization and phase transitions) quite difficult and requires new ideas and techniques, or, at least, appropriate modifications of those worked out in translation invariant theories. This, among others, motivate an extensive use of numerical methods in the field (see, e.g., [34] concerning the “classical” simulation methods such as Monte Carlo and molecular dynamics methods).

We will consider the ground state and the low-temperature excitations of electrons on the disordered host chain confining ourselves the simplest case of the density  $c_e = 1/q$  of (1.6) and (2.26). We assume also that  $c_e$  is sufficiently small, which is typical for narrow-band semiconductors, quasi-one-dimensional organic conductors, and nanochains. In this case, the electron positions  $\{x_j\}_{j=1}^N$  deviate slightly from those  $\{j\bar{l} + \phi\}_{j=1}^N$  of Hubbard’s generalized Wigner crystal with the same electron density  $c_e$ , where [see (2.2) and (2.4)]

$$\bar{l} = 1/c_e = q \gg 1. \tag{3.12}$$

In other words, in the case of small concentrations and low temperatures, the leading contribution to the thermodynamic functions is due to the electron configurations in which  $j$ th electron occupies one of the sites of a small (relative to  $\bar{l}$ ) neighborhood of  $j\bar{l}$ . We will call these neighborhoods clusters (see, for example, [35–37]), denote them  $C_j$  and assume (for simplicity) that all clusters consists of the same nonrandom number  $v \sim 1$  of the host-chain sites. Thus, the total number  $vN$  of sites belonging to the clusters is small with respect to the total number  $L$  of sites of the host chain, since  $Nv/L = c_e^{-1}v \ll 1$ .

Let us write the coordinates of the host-chain sites belonging to the  $j$ th cluster as [see (2.4), (3.1)–(3.3), and (3.12)]

$$C_j = \{r_j^m\}_{m=1}^v, \quad r_j^m = r_{jq+m-1-[v/2]}, \tag{3.13}$$

where  $r_u$  is defined in (3.1).

Note that in general one has to assume that  $C_j$  contains  $m_j^-$  particles to the left of  $j$ ,  $m_j^+$  particles to the right of  $j$  and that these numbers are independent and identically distributed random variables, hence  $v_j = m_j^+ + m_j^- + 1$  are also independent and identically distributed to provide the translation invariance in mean and the decay of correlations properties.

The same property of the translation invariance in mean implies that the physical information on the system is independent of the shift of the host chain by any  $\tau$  [cf. (2.4)]. It is convenient then to write the possible electron coordinates in the  $j$ th cluster in the form

$$r_j^m = jq + s_j^m + \tau, \tag{3.14}$$

where

$$\tau = \frac{1}{N} \sum_{j=1}^N \left( \frac{1}{v} \sum_{m=1}^v r_j^m - jq \right) \tag{3.15}$$

is the “mean center of inertia” of cluster and

$$s_j^m = m - 1 - [v/2] - \tau + \chi_{jq+m-1-[v/2]}. \tag{3.16}$$

We will call  $s_j^m$ ’s the shifts. It follows from (3.1), (3.2), and (3.14) that the shifts are independent and identically distributed random variables, since  $\{\chi_u\}_{u=1}^L$  of (3.1)–(3.3) possess this property, thereby providing the translation invariance in mean and the decay of correlation of the model.

According to (3.2) and (3.16), the typical value of the shifts is

$$\bar{s} = \langle s_j^m \rangle \simeq v \ll q \tag{3.17}$$

and since the arithmetic mean in (3.15) coincides with the probabilistic mean of the summand in the limit of infinite  $N$ , we have

$$\tau = \begin{cases} -1/2, & v \text{ is even} \\ 0, & v \text{ is odd} \end{cases} + O(N^{-1/2}). \tag{3.18}$$

An example of a 1D disordered host chain with clusters, corresponding to  $v = 2$ , is presented in Fig. 3.1(a), where every cluster contains two host-chain sites, adjacent from the left and right to the sites of Hubbard’s generalized Wigner crystal positions. The examples of electron configurations are presented in Fig. 3.1(b).

In this case we have

$$\begin{aligned} s_j^1 &= jq - 1 + \chi_{jq-1} - jq + 1/2 = -1/2 + \chi_{jq-1}, \\ s_j^2 &= jq + \chi_{jq} - jq + 1/2 = 1/2 + \chi_{jq}. \end{aligned} \tag{3.19}$$

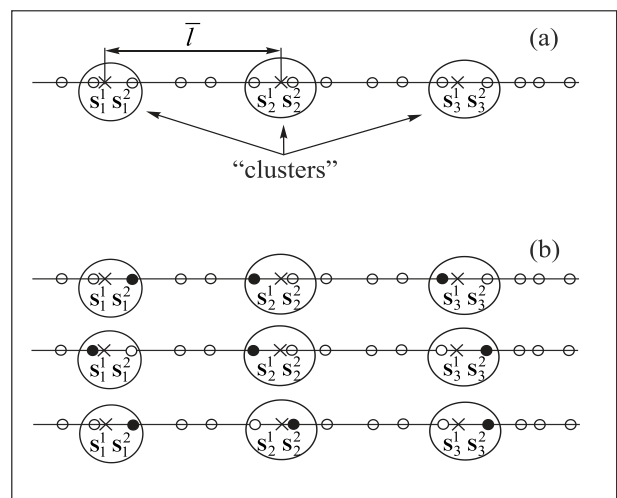


Fig. 3.1. (a) The example of a 1D disordered host-lattice chain ( $\times$  = the ideal Wigner lattice positions  $jq$ ,  $\circ$  = host-lattice sites). (b) Several possible electron configurations on this chain.

By the way, we have for translation invariant case  $\chi_u = 0$ ,  $u = 1, \dots, L$ :

$$\begin{aligned} \nu = 2: & s^1 = -1/2, s^2 = +1/2, \\ \nu = 3: & s^1 = -1, s^2 = 0, s^3 = +1, \\ \nu = 4: & s^1 = -3/2, s^2 = -1/2, s^3 = 1/2, s^4 = 3/2, \end{aligned} \quad (3.20)$$

i.e., definition (3.16) of shifts implies that, in the absence of disorder, their values coincide with those of quantum spins of  $1/2$ ,  $1$ , and  $3/2$ .

The above argument determines the *cluster approximation*. Let us find an effective Hamiltonian corresponding to the approximation. For this, we rewrite the Hamiltonian (3.5), (3.6) in terms of shifts (3.16) and expand the result up to the second order with respect to the shifts, i.e., up to the second order in the small parameter  $\bar{s}/\bar{l} \simeq \nu/q \ll 1$  [see (3.17)]. We obtain

$$\begin{aligned} H_{NN} = & (N-1)V(\bar{l}) + V'(\bar{l})(s_N^{mN} - s_1^{m1}) + \\ & + \frac{1}{2}V''(\bar{l}) \sum_{j=1}^{N-1} (s_{j+1}^{m_{j+1}} - s_j^{m_j})^2 + \dots, \end{aligned} \quad (3.21)$$

where the first term is the ground-state energy  $\mathcal{E}_{WC}$  of the generalized Wigner crystal with a given density  $c_e$  and the second term is of the order 1. Omitting these two terms and taking into account the convexity of  $V$ , we obtain the effective Hamiltonian

$$J \sum_{j=1}^{N-1} (s_{j+1}^{m_{j+1}} - s_j^{m_j})^2, \quad J = \frac{1}{2}V''(\bar{l}) > 0 \quad (3.22)$$

that describes the low-energy part of the Hamiltonians (3.4), (3.5), and (3.6) spectra. Since the typical distance between electrons is  $\bar{l} \gg 1$  in the low-concentration limit [see (3.12)], the cluster approximation seems fairly reasonable.

It is convenient to measure the energy in units of  $J$ . Then (3.22) became

$$H_C = \sum_{j=1}^{N-1} (s_{j+1}^{m_{j+1}} - s_j^{m_j})^2, \quad (3.23)$$

where now the Hamiltonian and the shifts are dimensionless.

To determine completely model (3.23), we have to specify the common probability distribution of the collection

$$\Sigma_{N\nu} = \{s_j^{m_j}\}_{j=m=1}^{N,\nu} \quad (3.24)$$

of shifts. According to (3.2) and (3.16), the shifts are independent and identically distributed in  $j$  and independent in  $m_j$ . Hence, the joint probability distribution of the collection (3.24) of the shifts is [cf. (3.11)]

$$W(\Sigma_{N\nu}) = \prod_{j=1}^N \prod_{m=1}^{\nu} w\left(s_j^{m_j} - m + 1 + [\nu/2] + \tau\right), \quad (3.25)$$

where  $w$  is the common probability density of random variables  $\{\chi_u\}_{u=1}^L$  in (3.1)–(3.3) assumed to be independent and identically distributed.

The partition function of the cluster model determined by Hamiltonian (3.23) is

$$Z(N, T, \Sigma_{N\nu}) = \sum_{\Sigma_{N\nu}} \exp\left\{-\frac{H_C}{T}\right\}. \quad (3.26)$$

According to the discussion of the self-averaging property in Sec. 3.1, the free energy per site

$$\begin{aligned} f(N, T, \Sigma_{N\nu}) &= N^{-1}F(N, T, \Sigma_{N\nu}), \\ F(N, T, \Sigma_{N\nu}) &= -T \ln Z(N, T, \Sigma_{N\nu}) \end{aligned} \quad (3.27)$$

of the cluster model (3.23) calculated for a fixed realization of shifts of (3.24) possesses the self-averaging property, thus coincides with its mean

$$\langle f(N, T, \Sigma_{N\nu}) \rangle = \int f(N, T, \Sigma_{N\nu}) W(\Sigma_{N\nu}) d\Sigma_{N\nu} \quad (3.28)$$

with respect to the joint probability density (3.25) of the shifts up to a fluctuating error term proportional to  $N^{-1/2}$ .

For the computer calculations, we used the rectangular density

$$w(x) = \frac{1}{A} \begin{cases} 1, & |x| < A/2 < 1/2, \\ 0, & 1/2 > |x| > A. \end{cases} \quad (3.29)$$

The parameter  $A$  is the measure of disorder in the system. The complete disorder corresponds to  $A \rightarrow 1$ . On the other hand, if  $A \ll 1$  the random shifts (3.16) are slightly dispersed around the right-hand side of (3.16) with  $\chi_u = 0$  and the limiting case  $A = 0$  corresponds to the equidistant ground-state configurations with period  $q$  (see Sec. 2). In the absence of disorder, the shifts are  $\pm 1/2$  [see (3.20)] and the ground state is obtained if all shifts are equal. Hence, the second and the third terms of the right-hand side of (3.21) are zero, and we obtain the energy of the generalized Wigner crystal.

In what follows, we confine ourselves to the case  $\nu = 2$ . We redefine the shifts [see (3.19) and Fig. 3.1] as follows:

$$s_j^1 \rightarrow s_j^-, s_j^2 \rightarrow s_j^+ \quad (3.30)$$

and write

$$s_j^{\sigma_j} = \sigma_j \lambda_j^{\sigma_j}, \quad \sigma_j = \pm, \lambda_j^{\sigma} \geq 0, \quad (3.31)$$

where  $\{\lambda_j^{\sigma}\}_{j=1, \sigma=\pm}^N$  are independent random variables according to (3.1). We conclude that in this case the shifts (3.16) can be viewed as Ising-type spins with random lengths  $\lambda_j^{\sigma_j}$ ,  $j = 1, \dots, N$ , cf. (3.20). To make more explicit the dependence of Hamiltonian (3.23) on the  $\{\sigma_j\}_{j=1}^N$  and the frozen disorder described by the random spin lengths  $\{\lambda_j^{\sigma_j}\}_{j=1}^N$ , we write

$$\lambda_j^{\sigma_j} = \alpha_j \sigma_j + \beta_j, \quad \alpha_j = (\lambda_j^+ - \lambda_j^-) / 2, \quad (3.32)$$

$$\beta_j = (\lambda_j^+ + \lambda_j^-) / 2 \geq 0,$$

where  $\{\alpha_j\}_{j=1}^N$  and  $\{\beta_j\}_{j=1}^N$  do not depend on  $\{\sigma_j\}_{j=1}^N$  and are statistically independent for different  $j$ . By using this parametrization and omitting the constant term, we can write (3.23) as

$$H_I(\{\sigma_j\}) = -\sum_{j=1}^{N-1} I_j \sigma_j \sigma_{j+1} - \sum_{j=1}^N h_j \sigma_j, \quad (3.33)$$

where

$$I_j = 2\beta_j \beta_{j+1},$$

$$h_j = 2\beta_j (\alpha_{j+1} + \alpha_{j-1} - 2\alpha_j), \quad (3.34)$$

and  $\{\alpha_j\}_{j=1}^N, \{\beta_j\}_{j=1}^N$  are given by (3.32).

Thus, the Hamiltonian (3.23) is thermodynamically equivalent to that (3.33), (3.34) of the one-dimensional disordered Ising model with random ferromagnetic interaction and random short correlated external field (recall that  $\alpha_j$  and  $\beta_j$  are independent for different  $j$ ).

Note that our effective Ising model is ferromagnetic just because of the convexity property (1.3) of the potential, see (3.23).

Since  $\{\lambda_j^{\sigma_j}\}_{j=1, \sigma_j=\pm}$  are nonnegative, independent and identically distributed in  $j$  and  $\sigma_j = \pm 1, j = 1, 2, \dots, N$ , it follows from (3.32) that  $\{\beta_j\}_{j=1}^N$  are nonnegative, independent and identically distributed and  $\{h_j\}_{j=1}^N$  are symmetrically distributed (stochastically oscillating), in particular,

$$\langle h_j \rangle = 0. \quad (3.35)$$

We obtain the periodic host-lattice setting if  $\lambda_j^{\sigma_j} = 1/2$  for all  $j$ . In this case, (3.33), (3.34) corresponds to the one-dimensional ferromagnetic Ising model with the nearest-neighbor interaction.

In the disordered case and  $\nu = 2$  we have in view (3.19), (3.29)–(3.31)

$$\sigma_j^{\sigma_j} = \frac{1}{2} \sigma_j (1 - A \xi_j^{\sigma_j}), \quad (3.36)$$

where  $\{\xi_j^{\sigma_j}\}_{j=1, \sigma_j=\pm}^N$  are independent random variables that are uniformly distributed over the interval  $[-1, 1]$ .

### 3.2. The low-temperature thermodynamics

Denote

$$\Lambda_N = \{\lambda_j^{\sigma_j}\}_{j=1, \sigma_j=\pm}^N \quad (3.37)$$

the realization of random spin lengths of (3.31), hence, random variables of (3.32). The partition function of our model (3.33) is [cf. (3.26)]

$$Z(N, T, \Lambda_N) = \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \dots \sum_{\sigma_N=\pm 1} \exp\left(-\frac{H_I(\{\sigma_j\})}{T}\right). \quad (3.38)$$

The free energy per site  $f(N, T, \Lambda_N)$  corresponding to (3.38) is defined by formulas analogous to those in (3.27). It can be shown (see, e.g., [28]) that  $F(N, T, \Lambda_N) = Nf(N, T, \Lambda_N)$  satisfies (3.10), hence, possesses the self-averaging property according to the discussion in Sec. 3.1 coinciding with its mean

$$f(N, T) = \langle f(N, T, \Lambda_N) \rangle = -\frac{T}{N} \langle \log Z(N, T, \Lambda_N) \rangle \quad (3.39)$$

up to an error term of the order  $O(N^{-1/2})$ .

We will find the mean free energy per site in the cluster model by using another than (3.9) version of the transfer matrix method. Namely, in view of (3.33) we can present (3.38) as a product of  $2 \times 2$  random transfer matrices

$$\hat{P}(j) = \{P_j(\sigma', \sigma'')\}_{\sigma', \sigma''=\pm},$$

$$P_j(\sigma', \sigma'') = \exp\left(-\frac{\epsilon_j(\sigma', \sigma'')}{T}\right), \quad (3.40)$$

where, according to (3.33), (3.34),

$$\epsilon_j(\sigma', \sigma'') = I_j \sigma' \sigma'' - \frac{1}{2} (h_j \sigma' + h_{j+1} \sigma''). \quad (3.41)$$

Imposing the cyclic boundary condition

$$\sigma_j = \sigma_{j+N}, \quad j = 1, \dots, N, \quad (3.42)$$

we obtain for (3.38)

$$Z(N, T, \Lambda_N) = \text{Tr} \left( \prod_{j=1}^N \hat{P}(j) \right), \quad (3.43)$$

where the symbol  $\text{Tr}$  denotes the trace of a  $2 \times 2$  matrix. The representation (3.43) allows us to carry out fast numerical calculation of the free energy.

Note that in general the multiplication of two  $2 \times 2$  matrices requires  $\sim 2^3$  steps of calculation (one have to calculate  $2^2$  matrix elements, where each element is a sum of 2 terms). Thus, the total calculation time is  $\sim 2^3 N$ . In the case of the direct calculation of the right hand side of (3.38) this time is  $\sim 2^N$ .

Besides, it is shown in the next section that an appropriate numerical method makes it possible to find the ground-state configuration of our model of the one-dimensional Wigner glass on disordered host lattice.

Figure 3.2 shows the entropy

$$s(T) = -\frac{1}{N} \frac{\partial}{\partial T} f(N, T) \quad (3.44)$$

as a function of temperature calculated by using (3.43) for  $\nu = 2$  and several values of the disorder parameter  $0 \leq A < 1$  [see (3.36)]. The mean free energy  $f(N, T)$  is found numerically by using (3.39) and (3.43) and by identifying the operation  $\langle \dots \rangle$  in (3.39) with the arithmetic mean of  $\log Z(N, T, \Lambda_N)$  over a sufficiently large number of realization of  $\Lambda_N$ .

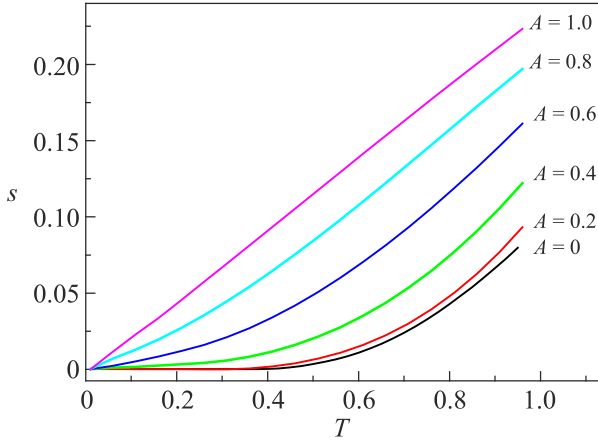


Fig. 3.2. The plots of  $s(T)$  for different values of disorder parameter  $A$ .

Note that  $s(T \rightarrow 0) = 0$  as it has to be for any model (even classical) with a discrete phase space. Moreover, for any  $A > 0$  of (3.36) the entropy is linear for low temperatures (in particular,  $s'(T = 0) \neq 0$ , see Fig. 3.3).

This is an indication of the gapless nature of the excitation spectrum of our model and raises a natural question on the nature and properties of corresponding elementary excitations. To answer the question one needs to know more about the ground state of the model.

### 3.3. The ground state

In general, every realization of the collection (3.37) of  $2N$  random “spin lengths”, hence the random variables  $\{\alpha_j\}_{j=1}^N$  and  $\{\beta_j\}_{j=1}^N$  of (3.31), (3.32) and (3.34), provides a realization of disorder, thus fixing the Hamiltonian to be used to find the ground state of our disordered system:

$$\sigma^{GS} = \{\sigma_k^{GS}\}_{k=1}^N \quad (3.45)$$

defined by

$$E_{GS} = \min_{\{\sigma_k = \pm\}} H_I(\{\sigma_k\}_{k=1}^N) = H_I(\sigma^{GS}). \quad (3.46)$$

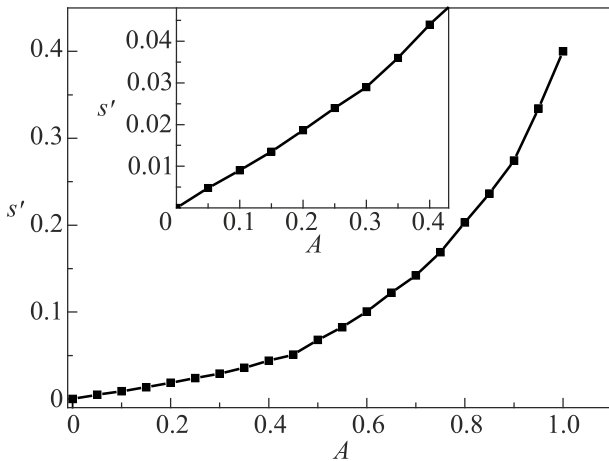


Fig. 3.3. The dependence  $s'(T \rightarrow 0)$  on  $A$ .

#### 3.3.1. Matching subchains

The low-temperature thermodynamic properties of the model (3.23) have been studied in [46] using the transfer-matrix formalism. In particular, a weak local external field

$$h = \{\varepsilon \tilde{h}_k\}_{k=1}^N, \quad \tilde{h}_k = \delta_{k,k_0} \quad (3.47)$$

was introduced into the Hamiltonian (3.23) as a tool of analysis of the ground state. Here  $\varepsilon$  is a small constant and  $\delta_{k,k_0}$  is Kronecker symbol. In other words, the field affects only the  $k_0$ th spin and the corresponding Hamiltonian is

$$H = H_I - \varepsilon \sigma_{k_0},$$

where  $H_I$  is defined in (3.33). Using the transfer-matrix techniques, one can calculate the free energy of the system and the corresponding magnetization per spin

$$M_{\text{loc}}(T, k_0) = -\frac{1}{N} \left. \frac{\partial F}{\partial \varepsilon} \right|_{\varepsilon=0} \approx (F|_{\varepsilon=0} - F) / N\varepsilon. \quad (3.48)$$

It is reasonable to believe that if  $M_{\text{loc}}(T, k_0) > 0$  in the low-temperature limit, then the  $k_0$ th spin of the ground state is parallel to the field, while if  $M_{\text{loc}}(T, k_0) < 0$ , then the  $k_0$ th spin is antiparallel to the field. Thus, calculating  $M_{\text{loc}}(T, k_0)$  for  $k_0 = 1, 2, \dots, N$  one can obtain the orientations of all the spins of ground state.

However, the method seems to have certain disadvantages. First, since  $h$  affects only *one* spin, the local magnetization (3.48) is of the order  $1/N \ll 1$  for sufficiently large systems. Hence, the method can only be applied to the cases, where the length of the system is not too large, thus the boundary conditions may seriously effect the ground state. Second, the amplitude  $\varepsilon$  of the local field should be small:

$$\varepsilon \ll T, e_{sf}, \quad (3.49)$$

where  $e_{sf}$  is typical “spin flip” energy. However, in view of possible local energy degeneration  $e_{sf}$  can be zero for certain spins, thus the sign of  $M(T, k_0)$  is rather sensitive to the value of  $\varepsilon$  and the applicability of the method to rather large systems is again questionable.

Thus, we will study the ground state by a another method, main idea is as follows. Let us divide the system into  $\mathcal{P}$  parts (subchains) with overlaps: the end-points of every subchain coincide with the corresponding end-points of the adjacent subchains. Denote

$$1 = p_0 < p_1 < p_2 < \dots < p_{j-1} < p_{\mathcal{P}} = N \quad (3.50)$$

the end-points of subchains and

$$l_k = p_{k+1} - p_k + 1, \quad k = 0, 1, \dots, \mathcal{P} - 1 \quad (3.51)$$

the lengths of the subchains. Thus, the  $k$ th subchain contains  $l_k$  spins

$$\sigma_{p_k}, \sigma_{p_k+1}, \dots, \sigma_{p_{k+1}-1}, \sigma_{p_{k+1}}. \quad (3.52)$$

It should be noted again, that the spin  $\sigma_{p_k}$  ( $k = 1, 2, \dots, \mathcal{P} - 1$ ) belongs to the *two* neighboring subchains, i.e.,  $\sigma_{p_k}$  is the last spin of  $k$ th subchain and the first spin of  $(k + 1)$ th subchain.

It is convenient to index the spins in each subchain as

$$\sigma_{p_k+j-1} = \sigma_{k,j}, \quad (3.53)$$

i.e., the first index indicates that spin belongs to the  $k$ th subchain and the second one is the number of the spin in the subchain. In this notation the  $k$ th subchain consists of the spins

$$\sigma_k = (\sigma_{k,1}, \sigma_{k,2}, \dots, \sigma_{k,l_k-1}, \sigma_{k,l_k}). \quad (3.54)$$

Now we carry out the direct enumeration of the states (the direct search for the configurations with minimum energy) in each of  $\mathcal{P}$  subchains.

According to (3.33), the energy of  $k$ th subchain is

$$H_k(\sigma_k) = \sum_{j=1}^{l_k-1} I_{k,j} \sigma_{k,j} \sigma_{k,j+1} - \sum_{j=1}^{l_k-1} h_{k,j} \sigma_{k,j}. \quad (3.55)$$

Let  $H_m^{\min}$  is the minimum of  $H_m$  over the spin configurations of the  $k$ th subchain (including its end spins) and let

$$\sigma_k^{\min} = (\sigma_{k,1}^{\min}, \sigma_{k,2}^{\min}, \dots, \sigma_{k,l_k-1}^{\min}, \sigma_{k,l_k}^{\min}) \quad (3.56)$$

be a corresponding spin configuration, i.e.,  $H_m^{\min} = H_m(\sigma_k)$ .

Now we claim that if the last spin of each subchain is equal to the first spin of the next subchain, i.e., if

$$\sigma_{k,l_k}^{\min} = \sigma_{k+1,1}^{\min}, \quad k = 0, 1, \dots, \mathcal{P} - 2, \quad (3.57)$$

then the union of all the subchain minimizing configurations (3.56) is a ground-state configuration  $\sigma^{GS}$  of the whole Hamiltonian (3.33):

$$\begin{aligned} \sigma^{GS} &= \{\sigma_k^{GS}\}_{k=1}^N = \\ &= (\sigma_{0,1}^{\min}, \sigma_{0,2}^{\min}, \dots, \sigma_{0,l_0}^{\min}, \sigma_{1,1}^{\min}, \sigma_{1,2}^{\min}, \dots, \sigma_{1,l_1}^{\min}, \dots, \sigma_{\mathcal{P}-1,1}^{\min}, \dots, \sigma_{\mathcal{P}-1,2}^{\min}, \dots, \sigma_{\mathcal{P}-1,l_{\mathcal{P}-1}}^{\min}), \end{aligned} \quad (3.58)$$

and the corresponding total minimum energy (3.46) is

$$E_{GS} = \sum_{k=0}^{\mathcal{P}-1} H_k^{\min}. \quad (3.59)$$

A similar idea has been recently used to study the ground states of certain rather complex (in particular, frustrated) translation invariant spin models [47].

A more detailed description of the above procedure of minimization of spin Hamiltonians is given at the end of this section.

Note that the procedure does not guarantee that the obtained ground state is unique. However, this does not contradict to the fact that the energy assumes the absolute minimum on this configuration. In fact, the nonuniqueness of

minimizing configuration (ground state) is rather common for macroscopic systems. For instance, there are two ground states (of the same energy) in the ferromagnetic Ising model at zero temperature and zero external field (all the spins are either up or down), and a continuum of ground states for the classical ferromagnetic Heisenberg model at zero temperature and zero external field. Moreover, in the frustrated spin systems, especially those of the spin glass type like our model (3.33), (3.34), there is the macroscopic number of ground states (of the same energy).

We believe, however, that the ground state found by our procedure is typical, i.e., the overwhelming majority of ground states of our model have the same structure differing only by the lengths of domains and their positions. In fact, our procedure can be modified to find all the ground states.

The above suggests a direct numerical algorithm to search ground states: split the system into subchains, minimize the energy of every subchain and check the matching conditions (3.57). If the conditions are not satisfied, repeat the procedure. The choice of an optimal number  $\mathcal{P}$  of subchains depends on the computer efficiency. Since in this scheme we perform the direct enumeration of the states (direct energy minimization) for each subchain, the typical calculation time is  $t_0 \sim n2^{N/n}$ . An increase in  $\mathcal{P}$  leads to a decrease in enumeration time but also to an increase in the number of attempts (the number of generations of division points  $\{p_k\}$ ).

It should be noted that the proposed method is rather universal and can be applied for a wide class of 1D disordered systems. An important advantage of the methods is that the direct minimization of energy is carried out independently in each subchain, thus the corresponding operations can be easily adapted to the parallel calculations. Besides, the method can be modified to deal with systems with larger number of interaction neighbors. In this case the conditions (3.57) is modified. For example, if we take into account the near- and next-neighbors interaction, then the matching conditions are [cf. (3.57)]

$$\begin{cases} \sigma_{k,l_k-1}^{\min} = \sigma_{k+1,1}^{\min} \\ \sigma_{k,l_k}^{\min} = \sigma_{k+1,2}^{\min} \end{cases}$$

Using the proposed method, we have studied the ground state of the Hamiltonian (3.33) numerically and the examples of the ground-state spin configurations for  $N = 10^4$  are presented in Fig. 3.4. As seen, the ground state consists of “domains” [46] of blocks of spins of the same sign, the domains concentration increasing rapidly with the increase of disorder parameter  $A$ .

It follows from (3.32) and (3.33) that interaction in our Ising model is ferromagnetic although random. Thus, the ground state of (3.33) without the second term is ferromagnetic (collinear), i.e., with all the spins either “up” or “down”.



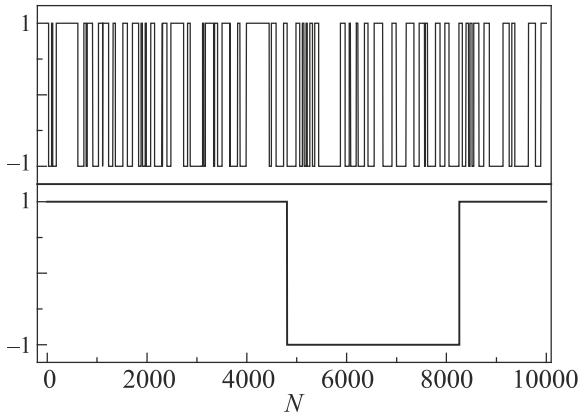


Fig. 3.4. The orientation of spins in the ground state of the systems for  $N = 10^4$  and two values of the disorder parameter  $A$  of (3.36). The top corresponds to  $A = 0.4$ , the bottom to  $A = 0.2$ . The ground states have the domain structures and the domain concentration increases with  $A$ .

Since, however, in our case the second term (random field) is of the same order of magnitude as the first one (interaction), an argument similar to that of the well known Larkin–Imry–Ma criterion [41, 42, 48] implies that the ferromagnetic ground state is unlikely for any  $0 < A \leq 1$ . Thus, it is not completely unexpected that the ground state is not collinear. However, the Larkin–Imry–Ma argument does not suggest a detailed form of the genuine ground state, except that it has to be of a “spin glass” noncollinear type. On the other hand, our numerical method allows us to detect an explicit form of a ground state, having the domain structure.

We can also estimate the concentration  $c_{\text{dom}}$  of the domain walls if  $A$  is small enough. Indeed, the typical fluctuations of the pair interaction of (3.23) [or of (3.33)] are  $\delta\varepsilon \sim A^2$ , while the energy of creation of a domain wall is  $\varepsilon_{\text{dom}} \sim (\lambda_k^+ + \lambda_k^-)^2 \sim 1$ , if  $A$  is not too close to 1. Let  $l_{\text{dom}}$  be the typical domain length, i.e.,

$$l_{\text{dom}} = N / N_+, \quad (3.60)$$

where  $N_+$  is the number of sites for which the spins are up. Then the domain is stable if  $l_{\text{dom}}$  satisfies the inequality  $\delta\varepsilon\sqrt{l_{\text{dom}}} \lesssim \varepsilon_{\text{dom}}$ . We obtain then [46, 49]:

$$l_{\text{dom}} \sim A^{-4}, \quad (3.61)$$

hence

$$c_{\text{dom}} = l_{\text{dom}}^{-1} \sim A^4. \quad (3.62)$$

In particular, it follows from (3.61) and (3.62) that the ground state consists of a single “ferromagnetic” domain for  $A = 0$ . We have calculated by the same method the domain concentration  $c_{\text{dom}}$  for a series of disorder parameter value  $A$ . The results are presented in Fig. 3.5.

Note that a similar problem with random variables  $\xi_j^{\sigma'}$  uniformly distributed over the interval  $[0,1]$  is considered in [46, 50].

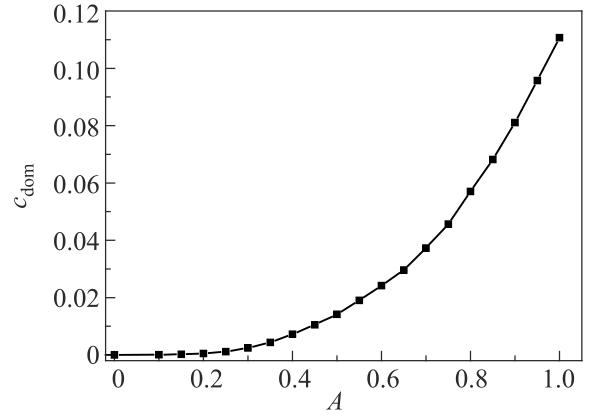


Fig. 3.5. The domain concentration  $c_{\text{dom}}$  as the function of disorder parameter  $A$ .

We present now a more detailed description of our procedure [see (3.50)–(3.59)] of minimization of Hamiltonian (3.33), (3.34). Let us consider the Hamiltonian

$$H = \sum_{k=1}^{N-1} u_k(\sigma_k, \sigma_{k+1}) \quad (3.63)$$

giving the energy of a configuration  $\sigma = \{\sigma_k\}_{k=1}^N$  of a spin chain of length  $N$  with pair interaction  $u_k$ . The Hamiltonian (3.33), (3.34) is a particular case of (3.63).

We will discuss the simplest nontrivial case  $\mathcal{P} = 2$  of our procedure, where the chain is divided into two subchains [the general case (3.50)–(3.54) of an arbitrary number  $j$  of subchains is analogous, but just a bit more tedious]. Then  $1 = p_0 < p_1 < p_2 = N$  are the endpoints (3.50) of the subchains,  $(\sigma_{0,1}, \dots, \sigma_{0,l_0})$  and  $(\sigma_{1,1}, \dots, \sigma_{1,l_1})$  are their spin configurations (3.54),  $l_k = p_{k+1} - p_k + 1$ ,  $k = 0, 1$  are their lengths (3.51), and

$$\begin{aligned} H_0 &= \sum_{j=1}^{l_0-1} u_j(\sigma_{0,j}, \sigma_{0,j+1}), \\ H_1 &= \sum_{j=1}^{l_1-1} u_{l_0+j-1}(\sigma_{1,j}, \sigma_{1,j+1}) \end{aligned} \quad (3.64)$$

are their energies (Hamiltonians) [cf. (3.55)].

Let  $\sigma_k^{\min}$ ,  $k = 0, 1$  be the minimizing configurations (3.56) of the subchains, i.e.,  $\min_{\sigma_k} H_m(\sigma_k) = H_m(\sigma_k^{\min})$ ,  $k = 0, 1$ . Assume that the matching condition (3.57) holds, i.e., that  $\sigma_{0,l_0}^{\min} = \sigma_{1,1}^{\min}$ . Then

$$H(\sigma') = H_0(\sigma_0^{\min}) + H_1(\sigma_1^{\min}), \quad (3.65)$$

where  $\sigma'$  is the union of these subchain minimizing configurations  $\sigma_0^{\min}$  and  $\sigma_1^{\min}$ . We claim that  $\sigma'$  is a minimization configuration for the whole chain, i.e., a ground state of the chain Hamiltonian. Indeed, assume that there exists another spin configuration  $\sigma''$  of the whole chain, which gives a lower energy than  $\sigma'$ :

$$H(\sigma'') < H(\sigma'). \quad (3.66)$$

Using the same division points  $(p_0, p_1, p_2)$  for  $\sigma''$  and denoting  $\sigma''_0$  and  $\sigma''_1$  corresponding “subconfigurations” of  $\sigma''$ , which satisfy the matching condition (by definition), we can write  $H(\sigma'') = H_0(\sigma''_0) + H_1(\sigma''_1)$ . This, (3.65) and (3.66) yield

$$H_0(\sigma''_0) + H_1(\sigma''_1) < H_0(\sigma''_0^{\min}) + H_1(\sigma''_1^{\min}),$$

or

$$(H_0(\sigma''_0) - H_0(\sigma''_0^{\min})) + (H_1(\sigma''_1) - H_1(\sigma''_1^{\min})) < 0.$$

The last inequality implies that at least one of the terms on its left is negative, i.e., that we have at least one of the inequalities

$$H_0(\sigma''_0) < H_0(\sigma''_0^{\min}), \quad H_1(\sigma''_1) < H_1(\sigma''_1^{\min}).$$

However, neither of these inequalities is possible, since  $H_m(\sigma''_k^{\min})$ ,  $k = 0, 1$  are the absolute minima of for subchain energies (3.64).

We came to a contradiction, which proves our claim, according to which if the matching conditions (3.57) hold for the minimum energy configurations of all the subchains, then the union of these configurations is a minimization configuration (a ground state) of the whole chain and the corresponding minimum energy is the sum of the minimum energies of the subchains [see (3.59)].

### 3.3.2. The “probing field” approach

In this section we confirm our results of the previous subsection on the form of ground states of model (3.33) via probing the ground state by an external field of special form, determined by a collection  $b = \{b_k\}_{k=1}^N$ :

$$H = H_I - \varepsilon \sum_{k=1}^N b_k \sigma_k, \quad (3.67)$$

and the corresponding generalized magnetization

$$M(T, b) = - \frac{1}{N} \frac{\partial F}{\partial \varepsilon} \Big|_{\varepsilon=0} = \frac{1}{N} \sum_{k=1}^N b_k \langle \sigma_k \rangle_G, \quad (3.68)$$

where  $F$  is now the free energy of (3.67) and  $\langle \dots \rangle_G$  denotes the corresponding Gibbs mean. By using the terminology of spin glass theory (see, e.g., [33]), we can view (3.68) as the overlap between external field  $b = \{b_k\}_{k=1}^N$  and the field of local magnetization  $\{\langle \sigma_k \rangle_G\}_{k=1}^N$ , where

$$\langle \sigma_k \rangle_G \quad (3.69)$$

is the mean local magnetization at site  $k$  of our effective spin system, i.e., the Gibbs average of the spin at a given site  $k$  corresponding to the Hamiltonian (3.33), (3.34).

It follows from the r.h.s. of (3.68) that the inequality

$$|M(T, b)| \leq \left( \frac{1}{N} \sum_{k=1}^N b_k^2 \frac{1}{N} \sum_{k=1}^N \langle \sigma_k \rangle_G^2 \right)^{1/2}$$

holds for a generic  $\{b_k\}$  and that it becomes the equality only for an external field proportional to  $\{\langle \sigma_k \rangle_G\}_{k=1}^N$ :

$$\bar{b}_k = a \langle \sigma_k \rangle_G, \quad k = 1, \dots, N, \quad (3.70)$$

where  $a$  is a constant, i.e., [see (3.68) and (3.70)]

$$M(T, \bar{b}) = a \sum_{k=1}^N \langle \sigma_k \rangle_G^2. \quad (3.71)$$

The constant  $a$  can be chosen to be 1 if we normalize  $\{\bar{b}_k\}_{k=1}^N$  by the condition

$$\sum_{k=1}^N \bar{b}_k^2 = 1. \quad (3.72)$$

Since we are interested in the ground state  $\sigma^{GS}$  of the Hamiltonian (3.33), which we identify with the domain walls configuration of the previous subsection, we put  $T = 0$  in the above formulas and arrive to the following algorithm to detect  $\sigma^{GS}$ . Pick a class of external fields containing the assumed ground state  $\sigma^{GS}$  and satisfying (3.72) and vary  $b$  over the class. The configuration  $\sigma^{GS}$  will be obtained as a maximizer of the generalized magnetization (3.68):

$$M(0, \sigma^{GS}) = \frac{1}{N} \sum_{k=1}^N (\sigma_k^{GS})^2 = 1. \quad (3.73)$$

Let now  $d_1, d_2, \dots$  be the coordinates of domain walls of the spin configuration found in the previous section ( $\langle d_m - d_{m-1} \rangle = l_{\text{dom}}$ ). Consider the following class of random external (probing) fields:

$$b_k = \sigma_k^{GS} + f_k, \quad (3.74)$$

where

$$f_k = \begin{cases} -2\sigma_k^{GS}, & k \in (d_m, d_m + \Delta_m), \quad m = 1, 2, \dots, j, \\ 0, & \text{otherwise} \end{cases}, \quad (3.75)$$

$$\Delta_k = (-1)^{\eta_k} [B\rho_k], \quad (3.76)$$

$B \geq 0$  is a nonnegative constant, [...] denotes the integer part,  $\{\eta_m\}$  are the independent distributed random variables, assuming (0, 1) with probability 1/2 and  $\{\rho_m\}$  are independent random variables with exponential distribution  $P(x) = B^{-1} \exp(-x/B)$ . Thus, the random variables  $\{f_k\}$  provide generic fluctuations of the positions of domain walls of the ground-state configuration  $\{\sigma_k^{GS}\}$  of the  $k$ th subchain. The direction of the shift of the  $k$ th domain wall is determined by  $\eta_k$  and the amplitude of the shift is determined by  $B$ . In particular, the probe field (3.74) coincides with  $\{\sigma_k^{GS}\}$  if  $B = 0$ .

To find the free energy  $F$  corresponding to (3.33), we use the modification of the transfer-matrix method corresponding to (3.67) where the role of the transfer matrices play [cf. (3.40)]

$$\hat{P}(j, b) = \begin{pmatrix} \exp\left(-\frac{\epsilon_k(\sigma^+, \sigma^+) - \epsilon b_k \sigma_k^+}{T}\right) & \exp\left(-\frac{\epsilon_k(\sigma^+, \sigma^-)}{T}\right) \\ \exp\left(-\frac{\epsilon_k(\sigma^-, \sigma^+)}{T}\right) & \exp\left(-\frac{\epsilon_k(\sigma^-, \sigma^-) - \epsilon b_k \sigma_k^-}{T}\right) \end{pmatrix}, \quad (3.77)$$

where  $\epsilon_k(\sigma^+, \sigma^+)$  is defined in (3.41). Assume the periodic boundary conditions ( $\sigma_{j+1} = \sigma_1$ ) and write the corresponding free energy

$$F(N, T, b) = -T \log \left( \text{Tr} \left[ \prod_{k=1}^N \hat{P}_k(T, b) \right] \right), \quad (3.78)$$

where  $\text{Tr}$  denotes the trace of a  $2 \times 2$  matrix.

Using (3.77), (3.78), one can calculate numerically the generalized magnetization (3.68) for the class (3.74)–(3.76) of probing fields as the function of amplitude  $B$  of fluctuations of the domains walls:

$$M(T, b) \approx (F|_{\epsilon=0} - F) / N\epsilon. \quad (3.79)$$

Figure 3.6 (curve 1) presents the generalized magnetization (3.68) as a function  $B$  for field (3.74) and  $T \rightarrow 0$ .

We see that the magnetization is maximal for  $B = 0$ , where the fluctuations (3.75) are absent, hence the probe field (3.74) coincides with  $\{\sigma_k^{GS}\}$ . However, for  $B > 0$  the generalized magnetization decays rather fast with the growth of  $B$ , i.e., it is a rather sensitive characteristic of the proximity of the external field to the maximizing one.

It is also worth noting that if we replace the maximizing field  $\{\sigma_k^{GS}\}_{k=1}^N$  in (3.74) by  $\{s_k^{GS} = \sigma_k^{GS} \lambda_k^{\sigma_k^{GS}}\}_{k=1}^N$  [see (3.31)] and compute again numerically the corresponding generalized magnetization, we obtain a plot [see curve 2 of Fig. 3.6], which is quite similar to plot 1 of Fig. 3.6, except the value of maximum, which is now  $M = 1 - A/2$ .

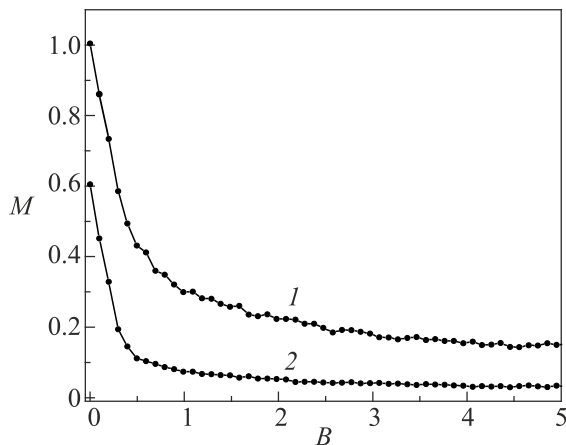


Fig. 3.6. The generalized magnetization  $M(0, b)$  as the function of  $B$  for the fields (3.74)–(3.76) (curve 1). The analogous curve for the probe fields with  $s_k^{GS} = \sigma_k^{GS} \lambda_k^{\sigma_k^{GS}}$  instead of  $\sigma_k^{GS}$  in the r.h.s. of (3.74) (curve 2).

The value can be explained as follows. In view of (3.31) and (3.32) the maximum  $M$  of (3.68) is

$$\frac{1}{N} \sum_{k=1}^N s_k^{GS} \sigma_k^{GS} = \frac{1}{N} \sum_{k=1}^N \alpha_k \sigma_k^{GS} + \frac{1}{N} \sum_{k=1}^N \beta_k.$$

The second term on the right is  $\langle \beta_k \rangle = 1 - A/2$ , if  $N$  is large enough. As for the first term, it vanishes in this case according our numerical results.

This can be viewed as a manifestation of a certain robustness of our numerical algorithm to detect the ground state provided that the probe field takes into account the sign structure of the ground state.

Thus, we showed that if the concentration of electron is small enough, then even a weak disorder in host-lattice site positions leads to the formation of the “domains” of electron and to the breaking the long-range order pertinent to the generalized Wigner crystal in the absence of disorder.

Note also that, according to Sec. 3.1, one has to distinguish two classes of characteristics of disordered systems: the self-averaging and non-self-averaging ones. The former are usually proportional to the volume (or the number of particles) of the system and, being divided by the volume, become nonrandom in the macroscopic limit. In our case, this is the free energy (3.27) and (3.78), the ground state energy (3.46), the domain wall concentration (3.62), and the generalized magnetization (3.68). For these characteristics it suffices to find their disorder average, since their values for practically all realizations of disorder coincide with the average if the size of system is large enough. Accordingly, we have calculated the statistical averages of the above quantities for various strength of disorder and size of the system and found that their fluctuations vanish rather fast with the growth of  $N$ .

The second class of characteristics of disordered systems, e.g., the ground state (3.45) and local magnetization (3.69), consists of characteristics, which depend essentially on the realizations of disorder and their fluctuations are not small for macroscopic systems, if, of course, the disorder is not too small. For these characteristic, one has to find their whole probability distribution.

### 3.3.3. Random domains distribution

Here we describe an analytical method for the analysis of the ground-state properties of the cluster model in the limit of weak disorder in the positions of host-lattice sites. We will base our analysis on the Hamiltonian (3.23).

Following (3.31), (3.32) and (3.36), we write  $s_k$  as

$$s_k^{\sigma_k} = \frac{1}{2} \left[ (2 + A\xi_k^+ + A\xi_k^-) \sigma_k + A(\xi_k^+ - \xi_k^-) \right],$$

where  $\sigma_k$  is are standard Ising spins and  $A$  is the disorder parameter. Recall, that the case of  $A = 0$  corresponds to the absence of disorder and the ground state of the system with the Hamiltonian (3.23) is a single domain, composed either of  $s_k^+$  or  $s_k^-$  (the ground state is doubly degenerate). At  $A \neq 0$  the degeneracy is lifted, thus, the energies of domains that consist of spins directed up and down, become different. The energies of domains with the length  $l$  are equal to

$$\varepsilon(l)^+ = \sum_{k=1}^l (s_k^+ - s_{k+1}^+)^2 \quad (3.80)$$

and

$$\varepsilon(l)^- = \sum_{k=1}^l (s_k^- - s_{k+1}^-)^2 \quad (3.81)$$

depending on the direction of the spin. Their difference

$$\delta\varepsilon(l) = \varepsilon(l)^+ - \varepsilon(l)^- \quad (3.82)$$

is a random (fluctuating) variable. Suppose that the domain consisting of upward spins is energetically favorable. Since  $\delta\varepsilon$  is random and its mean is zero, its energy grows with  $l$  roughly as the length  $l^{1/2}$  and sooner or later this domain will inevitably become unfavorable. It should be noted that the formation of a domain composed of spins in the opposite direction is associated with losses of energy due to the formation of a domain wall. This energy is also random

$$\varepsilon_{dw} = (s_l^\pm - s_{l+1}^\mp)^2. \quad (3.83)$$

If  $\varepsilon^+ > \varepsilon^- + \varepsilon_{dw}$ , then a domain wall of the down spins appears. Next, at some length of the domain the inequality  $\varepsilon^- > \varepsilon^+ + \varepsilon_{dw}$ , becomes valid and a domain wall of the up spin appears. Hence, the condition for the formation of a domain wall is

$$|\delta\varepsilon(l)| \geq \varepsilon_{dw}. \quad (3.84)$$

When  $A \ll 1$  it becomes possible to estimate the average length  $\bar{l}$  of the domain. The fluctuation of the pair interaction energy is equal to [see (3.36)]:

$$\delta_0 \approx (s_k^+ - s_{k+1}^+)^2 \approx (s_k^- - s_{k+1}^-)^2 \approx A^2.$$

Consequently,

$$\delta\varepsilon(l_{\text{dom}}) \sim \delta_0 \sqrt{l_{\text{dom}}} = A^2 \sqrt{l_{\text{dom}}}. \quad (3.85)$$

According to (3.83),

$$\varepsilon_{dw} = \left( 2 - A(\xi^+ + \xi^-) \right)^2, \quad (3.86)$$

then the average energy of domain wall formation is

$$\langle \varepsilon_{dw} \rangle = 4 - 8A \langle \xi \rangle + 2A^2 (\langle \xi^2 \rangle + \langle \xi \rangle^2) \approx 4. \quad (3.87)$$

Substituting (3.87) and (3.85) into (3.84), we get

$$A^2 \sqrt{l_{\text{dom}}} \sim 4, \quad l_{\text{dom}} \sim A^{-4}.$$

The concentration of domain walls  $c_{\text{dom}} \sim 1/l_{\text{dom}}$  can be written as [46, 50]

$$c_{\text{dom}} = (A/A_0)^4. \quad (3.88)$$

The ground state with an arbitrary parameter  $A$  is studied numerically in previous subsections. It was shown there that for an arbitrary weak disorder ( $A \neq 0$ ) the long-range order of the system vanishes. This result is in complete agreement with the stability criterion formulated in [41, 42].

Formula (3.88) give the explicit form of the dependence  $c_{\text{dom}}(A)$  in the limit of weak disorder  $A \ll 1$  thereby continuing the direction of study initiated in [41, 42]. We will develop further this direction and obtain the domain wall distribution.

According to (3.80)–(3.82),

$$\delta\varepsilon(l) = A^2 \sum_{k=1}^l s_k, \quad (3.89)$$

where

$$s_k = (\xi_k^+ - \xi_{k+1}^+)^2 - (\xi_k^- - \xi_{k+1}^-)^2. \quad (3.90)$$

Since the typical values of  $l$  in (3.89) are large and the terms of the sum are statistically independent, we can use the central limit theorem of probability theory, according to which the probability distribution of  $\delta\varepsilon(l)$  tends to a normal distribution with mathematical expectation  $M$  and variance  $D$ . Because of symmetry  $s_k$ ,  $M = 0$  (each term includes  $\xi_k^\pm$  and  $\xi_{k+1}^\pm$ ) and because of the independence of terms

$$D[\delta\varepsilon(l)] = A^4 \{ lD[s_k] + 2(l-1)K[s_k, s_{k+1}] \}, \quad (3.91)$$

with the correlator

$$K[x, y] = \langle xy \rangle - \langle x \rangle \langle y \rangle,$$

and the symbol  $\langle \dots \rangle$  denoting the average over the distribution of  $\xi$ 's. Then

$$\begin{aligned} D[s_k] &= \left\langle \left[ (\xi_k^+ - \xi_{k+1}^+)^2 - (\xi_k^- - \xi_{k+1}^-)^2 \right]^2 \right\rangle = \\ &= \left\langle (\xi_k^+ - \xi_{k+1}^+)^4 \right\rangle + \left\langle (\xi_k^- - \xi_{k+1}^-)^4 \right\rangle - \\ &- 2 \left\langle \left[ (\xi_k^+ - \xi_{k+1}^+) (\xi_k^- - \xi_{k+1}^-) \right]^2 \right\rangle = 2(d_1 - d_2), \end{aligned}$$

where

$$\begin{aligned} d_1 &= \left\langle (\xi_k^+ - \xi_{k+1}^+)^4 \right\rangle = \left\langle (\xi_k^- - \xi_{k+1}^-)^4 \right\rangle = \\ &= 2 \langle \xi^4 \rangle - 8 \langle \xi \rangle \langle \xi^3 \rangle + 6 \langle \xi^2 \rangle^2, \end{aligned}$$

$$d_2 = \left\langle \left[ (\xi_k^+ - \xi_{k+1}^+)(\xi_k^- - \xi_{k+1}^-) \right]^2 \right\rangle = 4D^2[\xi].$$

Due to the statistical independence and equivalence of the distributions of  $\xi_k^+$  and  $\xi_k^-$  we have

$$\begin{aligned} & \langle (\xi_k^+ - \xi_{k+1}^+)^2 - (\xi_k^- - \xi_{k+1}^-)^2 \rangle = \\ & = \langle (\xi_{k+1}^+ - \xi_{k+2}^+)^2 - (\xi_{k+1}^- - \xi_{k+2}^-)^2 \rangle = 0. \end{aligned}$$

Consequently,

$$\begin{aligned} K[s_k, s_{k+1}] &= \left\langle \left[ (\xi_k^+ - \xi_{k+1}^+)^2 - (\xi_k^- - \xi_{k+1}^-)^2 \right] \times \right. \\ & \left. \times \left[ (\xi_{k+1}^+ - \xi_{k+2}^+)^2 - (\xi_{k+1}^- - \xi_{k+2}^-)^2 \right] \right\rangle = 2(k_1 - k_2), \end{aligned}$$

where

$$\begin{aligned} k_1 &= \left\langle \left[ (\xi_k^+ - \xi_{k+1}^+)(\xi_{k+1}^+ - \xi_{k+2}^+) \right]^2 \right\rangle = \\ &= \left\langle \left[ (\xi_k^- - \xi_{k+1}^-)(\xi_{k+1}^- - \xi_{k+2}^-) \right]^2 \right\rangle = \\ &= 3\langle \xi^2 \rangle^2 + \langle \xi^4 \rangle - 4\langle \xi^3 \rangle \langle \xi \rangle, \\ k_2 &= \left\langle \left[ (\xi_k^+ - \xi_{k+1}^+)(\xi_{k+1}^- - \xi_{k+2}^-) \right]^2 \right\rangle = \\ &= \left\langle \left[ (\xi_k^- - \xi_{k+1}^-)(\xi_{k+1}^+ - \xi_{k+2}^+) \right]^2 \right\rangle = 4D^2[\xi]. \end{aligned}$$

We consider the case of the random variables  $\xi$  uniformly distributed over the interval  $[-1, 1]$ . Then we have

$$\langle \xi^n \rangle = \frac{1}{2} \int_{-1}^1 \xi^n d\xi = \frac{1 - (-1)^{n+1}}{2(n+1)}. \quad (3.92)$$

Consequently

$$\begin{aligned} d_1 &= \frac{16}{15}, \quad d_2 = \frac{4}{9}, \quad D[s_k] = 2\left(\frac{16}{15} - \frac{4}{9}\right) = \frac{56}{45}, \\ k_1 &= \frac{8}{15}, \quad k_2 = \frac{4}{9}, \quad K[s_k, s_{k+1}] = 2\left(\frac{8}{15} - \frac{4}{9}\right) = \frac{8}{45}. \end{aligned}$$

Introduce

$$D_0 = \lim_{l \rightarrow \infty} \frac{D[\delta\varepsilon(l)]}{l},$$

then (3.91) implies

$$D_0 = A^4 \{D[s_k] + 2K[s_k, s_{k+1}]\} = \frac{8A^4}{5}, \quad (3.93)$$

and we obtain for the probability density of  $\delta\varepsilon(l)$

$$f(\delta\varepsilon(l)) = \frac{1}{\sqrt{2\pi D_0 l}} \exp\left(-\frac{(\delta\varepsilon(l))^2}{2D_0 l}\right). \quad (3.94)$$

To calculate the mean length of the domains it is necessary to calculate the joint probability distribution of the domain lengths  $l$  and domain wall energies  $\varepsilon_{dw}$ . We will find this

distribution for  $A \ll 1$ . We note that the terms in (3.89) are bounded from above:  $|s_k| \leq 1$  while the energy to form a domain wall is bounded from below. Indeed, in accordance with (3.86),

$$\varepsilon_{dw}^{\min} = 4(1-A)^2. \quad (3.95)$$

The condition (3.84) of forming a domain wall implies the lower bound on the number of terms in (3.89)

$$\varepsilon_{dw}^{\min} \leq \varepsilon_{dw} \leq |\delta\varepsilon| \leq A^2 \sum_{k=1}^l |s_k| \leq A^2 l.$$

Consequently, we have

$$l \geq l_0 \sim \varepsilon_{dw}^{\min} / A^2 = 4(1-A)^2 / A^2.$$

Thus, if  $l < l_0$  the probability of forming domain walls is equal to zero. In other words, there is a minimal length  $l_0$  of the domain. In the regime  $A \ll 1$  the value  $l_0 \gg 1$ , hence, the distribution of  $\delta\varepsilon(l)$  can be considered normal.

We will now find the distribution of the domain lengths given a fixed energy of the domain wall formation  $\varepsilon_{dw}$  (so-called conditional distribution). At  $l \geq l_0 \gg 1$ , the length of domains can be considered as a continuously variable. According to (3.84), the probability of forming a domain with the length  $l$  is equal to

$$P(|\delta\varepsilon(l)| \geq \varepsilon_{dw}) = 1 - \Phi_0(|\delta\varepsilon(l)| < \varepsilon_{dw}),$$

where  $\Phi_0(|\delta\varepsilon(l)| < \varepsilon_{dw})$  is the distribution of the absolute value of a normally distributed random variable (so-called semi-normal distribution). The transition from a normal to a semi-normal distribution in our case is possible, since  $M = \langle \delta\varepsilon(l) \rangle = 0$  according to (3.94). Thus, we can write

$$\begin{aligned} \Phi_0(|\delta\varepsilon(l)| < \varepsilon_{dw}) &= \sqrt{\frac{2}{\pi D_0 l}} \int_0^{\varepsilon_{dw}} \exp\left(-\frac{\varepsilon^2}{2D_0 l}\right) d\varepsilon = \\ &= \left[ \varepsilon^2 = \frac{l\varepsilon_{dw}^2}{x} \right] = \frac{\varepsilon_{dw}}{\sqrt{2\pi D_0}} \int_l^\infty \exp\left(-\frac{\varepsilon_{dw}^2}{2D_0 x}\right) \frac{1}{x^{3/2}} dx = 1 - G(\varepsilon_{dw}, l), \end{aligned}$$

where

$$G(\varepsilon_{dw}, l) = \frac{\varepsilon_{dw}}{\sqrt{2\pi D_0}} \int_0^l \exp\left(-\frac{\varepsilon_{dw}^2}{2D_0 x}\right) \frac{1}{x^{3/2}} dx$$

is the Levy distribution, which represents a steady distribution with a so-called ‘‘heavy tail’’. Recall that in this case  $\varepsilon_{dw}$  is the distribution parameter. Therefore,

$$P(|\delta\varepsilon(l)| \geq \varepsilon_{dw}) = G(\varepsilon_{dw}, l) = \int_0^l g(\varepsilon_{dw}, x) dx,$$

where

$$g(\varepsilon_{dw}, x) = \frac{\varepsilon_{dw}}{\sqrt{2\pi D_0}} \exp\left(-\frac{\varepsilon_{dw}^2}{2D_0 x}\right) \frac{1}{x^{3/2}}. \quad (3.96)$$

In order to find the distribution of the domain lengths  $w(l)$ , it is necessary to average (3.96) over the distribution of the energy of domain walls  $\rho_{dw}$

$$w(l) = \int_0^\infty g(\varepsilon, l) \rho_{dw}(\varepsilon) d\varepsilon.$$

According to (3.86), in the limit  $A \ll 1$  the function  $\rho_{dw}(\varepsilon)$  is a distribution of the sum of two independent and uniformly distributed random numbers, i.e., the triangular Simpson distribution

$$\rho_{dw}(\varepsilon) = \frac{4}{(\varepsilon_{dw}^{\max} - \varepsilon_{dw}^{\min})^2} \begin{cases} 0, & \varepsilon \notin (\varepsilon_{dw}^{\min}, \varepsilon_{dw}^{\max}) \\ (\varepsilon - \varepsilon_{dw}^{\min}), & \varepsilon \in [\varepsilon_{dw}^{\min}, \varepsilon_{dw}^{\text{mid}}] \\ (\varepsilon_{dw}^{\max} - \varepsilon), & \varepsilon \in [\varepsilon_{dw}^{\text{mid}}, \varepsilon_{dw}^{\max}]. \end{cases} \quad (3.97)$$

Here  $\varepsilon_{dw}^{\max} = 4$  [see (3.83)],  $\varepsilon_{dw}^{\min} = \varepsilon_{dw}^{\max} (1 - A)^2$  [see (3.95)], and  $\varepsilon_{dw}^{\text{mid}} = (\varepsilon_{dw}^{\max} + \varepsilon_{dw}^{\min}) / 2 = \varepsilon_{dw}^{\max} (1 - A + A^2 / 2)$ . By integrating we get

$$w(l) = -2D_0 \frac{\text{Erf}\left(\frac{\varepsilon_{dw}^{\min}}{\sqrt{2D_0}l}\right) + \text{Erf}\left(\frac{\varepsilon_{dw}^{\max}}{\sqrt{2D_0}l}\right) - 2\text{Erf}\left(\frac{\varepsilon_{dw}^{\text{mid}}}{\sqrt{2D_0}l}\right)}{(\varepsilon_{dw}^{\max} - \varepsilon_{dw}^{\min})^2} \approx -\frac{D_0}{2} \text{Erf}'\left(\frac{x}{\sqrt{2D_0}l}\right) \Big|_{x=\varepsilon_{dw}^{\text{mid}}}.$$

Here  $\text{Erf}(x)$  is the error function. As a result,

$$w(l) \approx \frac{\varepsilon_{dw}^{\text{mid}}}{\sqrt{2\pi D_0}} \exp\left(-\frac{(\varepsilon_{dw}^{\text{mid}})^2}{2D_0 l}\right) \frac{1}{l^{3/2}}. \quad (3.98)$$

As indicated above, the given expression is formally valid only at  $l > l_0$ , but if we integrate with respect to (3.98), the main contribution will come from the region  $l \gg 1$  (which is typical for distributions with a “heavy tail”), i.e., the lower limit of integration is arbitrary to a large extent. Moreover, the numerical modeling we performed showed that the distribution of (3.98) is a good approximation of the probability that domain walls will form in the whole range of  $l$  (see Fig. 3.7). Therefore, the lower limit of integration over (3.98) can be set equal to zero. The average over the distribution is infinite, while the harmonic mean is

$$l_{\text{dom}} = \left\langle \frac{1}{l} \right\rangle^{-1} = \left( \int_0^\infty \frac{w(l)}{l} dl \right)^{-1} = \frac{(\varepsilon_{dw}^{\text{mid}})^2}{3D_0}.$$

Using (3.61) and (3.62), we can write

$$c_{\text{dom}} \approx \frac{6D_0}{(\varepsilon_{dw}^{\text{mid}})^2} \approx \frac{3A^4}{10}. \quad (3.99)$$

The obtained expression can be compared with the results of numerical calculations (see Sec. 3.3.1.) The plot of  $c_{\text{dom}}$  as function of  $A$  is presented in Fig. 3.8. Solid curve

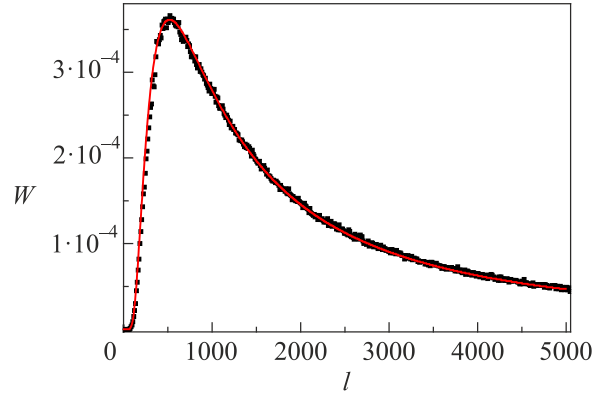


Fig. 3.7. (Color online) The domain distribution with respect to the lengths  $l$ . Points show the results of numerical simulation at  $A = 0.25$ . The solid line is the distribution (3.98).

corresponds to (3.99) and solid boxes are the results of numerical simulation (see Fig. 3.5). Good agreement between the numerical simulation and the obtained analytical formula holds until  $A \lesssim 1/2$ .

Thus, it is shown in this section that in the framework of an effective magnetic (cluster) model an arbitrarily weak disorder destroys the long-range order: the system is broken down into ferromagnetic domains having a random length. The obtained formula relates the typical size of these domains with the disorder parameter  $A$ , which characterizes the spread of host-lattice sites. In the terms of the initial (electron) model this means that the ground state is a sequence of the generalized Wigner crystal fragments adjacent one to another via the segments occupied by the domain walls (in terms of the magnetic model). Each of these fragments is described by (2.4) for a certain fixed value of the phase  $\phi$ . For  $\nu = 2$ , it means that the ground-state structure in each fragment is realized by random shifts of the electrons *in the same direction*, for example, all  $s_j = s^+$  [see (3.36)]. In an adjacent segment, therefore, all  $s_j = s^-$ , etc. In positions where the domain walls are formed,  $\phi$  changes sharply its value. In other words,

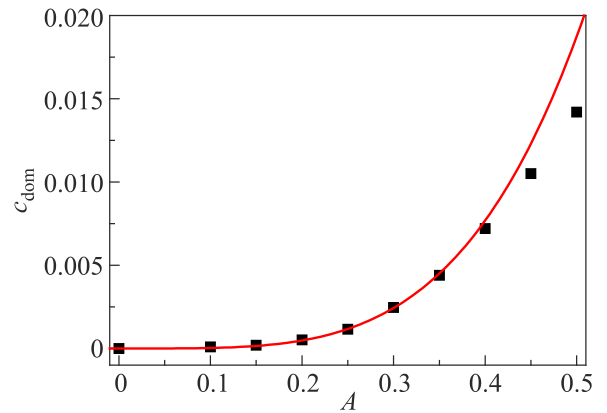


Fig. 3.8. The dependence  $c_{\text{dom}}$  on  $A$ . Boxes indicate the results of numerical simulation (see Fig. 3.5). Solid curve corresponds to  $c_{\text{dom}} = 3A^4 / 10$  [see (3.99)].

the ground state of a 1D electron ensemble on a weakly disordered host-lattice is described by formula (2.4), in which phase  $\phi$  is a random step function. Consequently, a typical length of the domain  $l_{\text{dom}}$  is the average distance over which there is a “phase failure”  $\phi$ . This result is also confirmed by studying the weak perturbations of the Hamiltonian (3.33) of the model by random external fields (see Sec. 3.3.2), which “probes” the domain structure of the ground state via random variations (fluctuations) of the domain walls. It is shown that the generalized magnetization per particle (3.79), corresponding to the field, is maximal if the amplitude of fluctuations is small and decays sufficiently fast with the growth of the amplitude, i.e., that the magnetization is rather sensitive to the proximity of the form of the field to that of the ground state.

Note, that we obtain the translation invariant version of the proposed above disordered cluster model just by setting  $\chi_u = 0$ ,  $u = 1, \dots, L$  or  $A = 0$ , in the above formulas, thereby arriving to the model treated in Sec. 2. In the case of  $v = 2$  we have  $\lambda_j^+ + \lambda_j^- = 1$ ,  $j = 1, 2, \dots, N$  [see (3.32)]. Then  $\beta_j = (\lambda_j^+ + \lambda_j^-)/2 = 1/2$  and  $I_j$  in (3.34) is equal to  $1/2$ . If  $c_e = 1/q$  [see (2.1)], then  $\alpha_j = \text{const}$  and  $h_j$  in (3.34) is zero. The Hamiltonian (3.33) is then 1D Ising model with “ferromagnetic” nearest neighbor exchange  $I = 1/2$  and zero external magnetic field  $h_j$ ,  $j = 1, \dots, L$ .

On the other hand, if  $c_e = p/q$ , with  $p \neq 1$ , then the external field is a periodic function with period  $\tilde{T} = [1/\delta m]$  [see (2.32)], attaining its extrema ( $h = \pm 1$ ) at the endpoints of  $\tilde{T}$  interval. At the positions where  $h_j = -1$  the exchange energy of  $j$ th spin with 2 neighbors is equal to the energy of flipped  $j$ th spin in the field  $h_j$ . This leads to an additional degeneracy of the ground state: the ferromagnetically ordered spin chain has the same energy as the ferromagnetically ordered spin chain in which every  $\tilde{T}$ th spin is flipped. These flipped spins in term of electron model are nothing else that defectons, described in Sec. 2.4. Next near neighbor interactions remove this degeneracy forming superstructure of these flipped spins (defectons).

#### 4. Beyond the nearest-neighbor approximation in the cluster model

It is of interest to study the influence of the range of potential of the interelectron repulsion on the thermodynamic properties of the system under study.

Starting from the one-dimensional version

$$H = \sum_{1 \leq j < k \leq N} V(x_k - x_j)$$

of the general classical Hamiltonian (1.8) and repeating the procedure leading from (3.5) to (3.22), we obtain

$$H = \sum_{i=1}^{N-1} H_i, \quad (4.1)$$

where

$$H_i = J_i \sum_{j=1}^{N-i} \left( s_{j+i}^{m_{j+i}} - s_j^{m_j} \right)^2$$

and

$$J_i = \frac{1}{2} \frac{\partial^2 V(x)}{\partial x^2} \Big|_{x=i\bar{r}}.$$

The Hamiltonian  $H_1$  corresponds to the interaction between nearest neighbors [see (3.22)],  $H_2$  corresponds to next nearest-neighbor interaction, etc.

To illustrate the situation we confine ourselves to the interactions between  $\mathcal{M}$  neighboring electrons, using instead of Hamiltonian (4.1), we study

$$H_{\mathcal{M}} = \sum_{i=1}^{\mathcal{M}} H_i. \quad (4.2)$$

To calculate the partition function of the system with Hamiltonian (4.2), it is again convenient to use the transfer matrix formalism [see (3.40), (3.43), (3.77), (3.78)]. We consider now the case of  $\mathcal{M} = 2$ . Since in this case we have the interaction of nearest and next to nearest neighbors, the corresponding transfer matrices  $\hat{P}(j)$  are of the size  $v^2 \times v^2$  (recall, that  $v$  is the number of states of the variables  $s_j$ ):

$$\{\hat{P}(j)\}_{a,b} = A_{\omega' \rho'}^1(2j) A_{\omega'' \rho''}^1(2j+1) A_{\rho' \rho''}^2(2j+1) A_{\omega'' \omega'}^2(2j+2), \quad (4.3)$$

where

$$\{A^k(j)\}_{\omega \rho} = \exp \left( -\frac{\varepsilon_j^k(\omega, \rho)}{T} \right). \quad (4.4)$$

The indexes  $\omega', \omega'', \rho', \rho'' = 1, \dots, v$ .

$$a = \omega' + v(\rho' - 1), \quad b = \omega'' + v(\rho'' - 1); \quad a, b = 1, \dots, v^2.$$

Analogous formulas can be obtained for any  $\mathcal{M}$ .

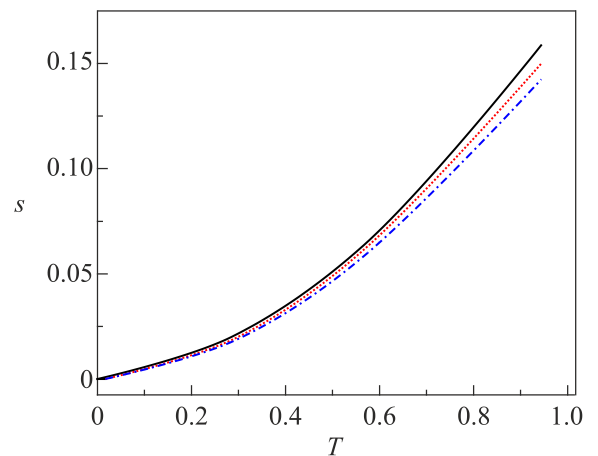


Fig. 4.1. The dependences of specific entropy  $s(T)$  for  $c_e = 1/2$ ,  $A = 0.6$  and  $V(r) = 1/r$ . Solid curve (black) corresponds to  $\mathcal{M} = 1$ , dashed curve to  $\mathcal{M} = 2$ , dashed-dotted curve (blue) to  $\mathcal{M} = 3$ .

Assuming for simplicity of subsequent formulas that  $N = 2n$  and imposing the cyclic boundary conditions [see (3.42)], we obtain the analog of (3.43):

$$Z(N, T) = \text{Tr} \left( \prod_{j=1}^N \hat{P}(j) \right).$$

Using the above formula, the plots of specific entropy  $s(T)$  (3.44) are calculated for  $c_e = 1/2$ , different  $\mathcal{M}$  and pair potential  $V(r) = 1/r$ . The results are presented in Fig. 4.1. It shows that the entropy slightly decreases as  $\mathcal{M}$  increases. It is caused by the fact that the condition of the frustration creation becomes stronger and, hence, the concentration of these frustrations decreases.

1. F. Bouchet, S. Gupta, and D. Mukamel, *Physica A* **389**, 4389 (2010).
2. A. Campa, T. Dauxois, and S. Ruffo, *Phys. Rep.* **480**, 57 (2009).
3. T. Dauxois, S. Ruffo, and L. Cugliandolo (eds.), *Long-Range Interacting Systems, Lecture Notes of the Les Houches Summer School 2008*, Oxford University Press, Oxford (2009).
4. J. Jedrzejewski and J. Miekisz, *Europhys. Lett.* **50**, 307 (2000). arXiv:cond-mat/9903163v1.
5. A.A. Slutskin and L. Yu. Gorelik, *Fiz. Nizk. Temp.* **19**, 1199 (1993) [*Low Temp. Phys.* **19**, 852 (1993)].
6. J. Hubbard, *Phys. Rev. B* **17**, 494 (1978).
7. L. A. Pastur, V. V. Slavin, and A. V. Yanovsky, *Fiz. Nizk. Temp.* **46**, 857 (2020) [*Low Temp. Phys.* **46**, 724 (2020)].
8. E. Y. Andrei, *2D Electron Systems on Helium and Other Substrates*, Kluwer Academic Publishers, New York (1997).
9. H. Nejoh and M. Aono, *Appl. Phys. Lett.* **64**, 2803 (1995).
10. M. S. Bello, E. I. Levin, B. I. Shklovskii, and A. L. Efros, *Sov. Phys. JETP* **53**, 822 (1981).
11. A. A. Slutskin, M. Pepper and H. A. Kovtun, *Europhys. Lett.* **62**(5), 705 (2003).
12. I. F. Ljuskutov, A. G. Naumovets, and V. L. Pokrovsky, *Two-Dimensional Crystals*, Naukova Dumka, Kiev (1988).
13. J. Hubbard, *Generalized Wigner Lattices and Band Motion Effects*, in: *Quasi One-Dimensional Conductors II, Lecture Notes in Physics 96*, S. Barisic, A. Bjelis, J. R. Cooper, and B. Leontic (eds.), Springer Verlag, Berlin, Heidelberg, New York (1979).
14. V. L. Pokrovsky and G. V. Uimin, *J. Phys. C* **11**, 3535 (1978).
15. S. Aubry, *J. Phys. C: Solid State Phys.* **16**, 2497 (1983).
16. P. Bak and R. Bruinsma, *Phys. Rev. Lett.* **49**, 249 (1982).
17. S. E. Burkov and Ya. G. Sinai, *Russ. Math. Surv.* **38**, 235 (1983).
18. D. Mattis, *The Many Body Problem*, World Scientific, Singapore (1993).
19. T. L. Hill, *Statistical Mechanics*, Dover, New York (1987).
20. V. V. Slavin and A. A. Slutskin, *Phys. Rev. B* **54**, 8095 (1996).
21. V. V. Slavin, *Fiz. Nizk. Temp.* **29**, 900 (2003) [*Low Temp. Phys.* **29**, 674 (2003)].
22. V. V. Slavin, *Phys. Status Solidi (b)* **242**, 2033 (2005).
23. B. Valenzuela, S. Fratini, and D. Baeriswyl, *Phys. Rev. B* **68**, 045112 (2003).
24. D. Baeriswyl, in: *Nonlinearity in Condensed Matter*, by A. R. Bishop, D. K. Campbell, P. K. Kumar, and S. E. Trullinger (eds.), *Springer Series in Solid State Sciences* **69**, 183 (1987).
25. A. Goetschy and S. E. Skipetrov, *Phys. Rev. E* **84**, 011150 (2011).
26. I. M. Lifshitz, S. A. Gredeskul, and L. A. Pastur, *Introduction in the Theory of Disordered Systems*, New York, Wiley (1988).
27. G. Parisi, in: *Application of Random Matrices in Physics*, E. Brézin, V. Kazakov, D. Serban, P. Wiegmann, and A. Zabrodin (eds.), Springer, Heidelberg (2006).
28. L. A. Pastur and A. L. Figotin, *Teor. Math. Phys.* **35**, 193 (1978).
29. D. Ruelle, *Statistical Mechanics*, W. A. Benjamin (ed.), New York (1969).
30. G. E. Uhlenbeck and G. W. Ford, *Lectures in Statistical Mechanics*, American Mathematical Society, Providence, R.I. (1963).
31. K. M. Khanin and Ya. G. Sinai, *J. Statist. Phys.* **20**, 573 (1979).
32. L. A. Pastur and M. V. Shcherbina, *J. Statist. Phys.* **62**, 1 (1991).
33. M. Mezard, G. Parisi, and M. A. Virasoro, *Spin Glass Theory and Beyond*, World Scientific Publishing Co., Inc., Teaneck, NJ (1987).
34. K. Binder and W. Kob, *Glassy Materials and Disordered Solids*, World Scientific Publishing, Singapore (2005).
35. V. V. Slavin and A. A. Slutskin, *Physica B* **364**, 321 (2005).
36. V. V. Slavin, *Solid State Commun.* **131**, 355 (2004).
37. V. V. Slavin, *Int. J. Mod. Phys. C* **15**, 955 (2004).
38. V. V. Slavin, *Phys. Status Solidi (b)* **241**, 2928 (2004).
39. N. Mott, *Metal-Insulator Transitions*, Taylor and Francis, London (1974).
40. A. A. Slutskin, V. V. Slavin, and H. A. Kovtun, *Phys. Rev. B* **61**, 14184 (2000).
41. A. I. Larkin, *Sov. Phys. JETP* **31**, 784 (1970).
42. Y. Imry and S. K. Ma, *Phys. Rev. Lett.* **35**, 1399 (1975).
43. S. Fratini, B. Valenzuela, and D. Baeriswyl, *J. Phys. IV France* **12**, 69 (2002); arXiv:0209518v1.
44. S. Fratini, B. Valenzuela, and D. Baeriswyl, *Phys. Rev. B* **68**, 045112 (2003); arXiv:0302020v2.
45. E. H. Lieb and F. Y. Wu, *Physica A* **321**, 1 (2003).
46. V. V. Slavin, *Phys. Status Solidi (b)* **241**, 2928 (2004).
47. Y. I. Dublenych, *Phys. Rev. Lett.* **109**, 167202 (2012).
48. J. Cardy, *Scaling and Renormalization in Statistical Physics*, Cambridge University Press (1996).
49. A. A. Slutskin and H. A. Kovtun, *Fiz. Nizk. Temp.* **31**, 784 (2005) [*Low Temp. Phys.* **31**, 594 (2005)].
50. L. A. Pastur, V. V. Slavin, and A. A. Krivchikov, *Int. J. Mod. Phys. C* **25**(8), 1450028 (2014).



Одновимірні вузькозонні провідники  
(Огляд)

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Розглянуто одновимірні ґраткові моделі та відповідні їм результати, що описують низькотемпературні властивості квазіодновимірних ґраткових систем з далекодіючою взаємодією. Широко відомим прикладом таких систем є вузькозонні низьковимірні провідники з далекодіючим потенціалом електрон-електронного відштовхування. В розглянутих моделях частинки розташовані на одновимірній ґратці-матриці (ланцюжку), трансляційно-інваріантній або неупорядкованій, та взаємодіють через далекодіючий потенціал відштовхування. В першій частині приведено результати щодо трансляційно-інваріантної ґратки-матриці, а саме: низькотемпературна термодинаміка, несумірний основний стан та пов'язана з ним

структура «чортових» сходів, різні характеристики як функції відповідних параметрів, самокалізація частинок, нова гілка елементарних збуджень тощо. Далі розглянуто неупорядкований випадок, коли вузли ґратки-матриці випадково флюктують навколо вузлів періодичного ланцюжка. Низькотемпературну термодинаміку та структуру основного стану таких систем досліджено в рамках певної моделі, яку називають кластерною та яка є досить розумним наближенням при низьких температурах і малих концентраціях частинок. За допомогою аналітичних та чисельних методів проаналізовано термодинаміку та основний стан моделі. Останній виявляється послідовністю випадкових доменів, розподіл яких досліджено детально.

Ключові слова: одновимірні системи, неупорядковані системи, структура основного стану.