THE GROUND STATE STRUCTURE OF ELECTRON’S ENSEMBLE ON ONE-DIMENSION DISORDERED LATTICE

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Abstract

The ground state of interacting particles on a disordered one-dimensional host-lattice is studied by a direct numerical method. It is shown that if the concentration of particles is small, then even a weak disorder of the host-lattice breaks the long-range order of Generalized Wigner Crystal, replacing it by the sequence of blocks (domains) of particles with random lengths. The mean domains length as a function of the host-lattice disorder parameter is also found. It is shown that the domain structure can be detected by a weak random field, whose form is similar to that of the ground state but has fluctuating domain walls positions. This is because the generalized magnetization corresponding to the field has a sufficiently sharp peak as a function of the amplitude of fluctuations for small amplitudes.

1 Introduction

Low-dimensional and layered conductors possess a number of interesting and unusual properties and have been of considerable interest in the last decades. In particular, it is possible to separate electron subsystem and that of dopant ions in a number of these conductors. As a result, the potential, produced by the dopants in the conducting electron layers is almost constant and conducting characteristics are essentially determined by the inter-electron (or inter-holes) repulsion.

Another interesting subclass of these conductors consists of lattice electrons systems, where the charge carriers tunneling between host-lattice sites is suppressed by their mutual Coulomb repulsion. As a result, the charge carriers are
These are the MOSFETs (metal-oxide-semiconductor field-effect transistors) and a variety of other semiconducting heterostructures. The quasi-one-dimensional organic conductors and artificial systems like arrays of quantum dots, networks and chains of metallic nano-grains with tunnel junctions (provided by various organic molecules) also belong to this class.

The ground state (GS) and the low-temperature properties of these systems have been extensively studied. The first theoretical result is due to Hubbard, who considered the GS of one-dimensional (1D) repulsing particles on a periodic host-lattice in the limit of strong interaction, where the dynamic effects are negligible and particles are localized with high accuracy on the lost-lattices sites. It was shown in that the corresponding GS has, in general, an incommensurable structure determined only by the particle density

$$c_e = N_e/L,$$

where $N_e \gg 1$ and $L \gg 1$ are the total numbers of particles and host lattice sites, but does not depend on pair potential $V$, provided that $V$ is non-negative, convex and decays at infinity faster then $|x|^{-1}$.

Hubbard also suggested an explicit form of the GS in this case. The form was justified and clarified in and it is known now as the Generalized Wigner crystals (GWL). According to the GWL theory, the position $x_k$ of $k$-th particle is given by the simple formula:

$$x_k = a_0\left[k/c_e + \phi\right], k = 1, ..., N_e,$$

where $\left[...\right]$ denotes the integral part, $\phi$ is an arbitrary constant (initial) phase and $a_0$ is the distance between the host lattice sites. It follows from the formula that the only two inter-particle distances

$$x_{k+1} - x_k = \left[1/c_e\right], \left[1/c_e + 1\right]$$

can appear in the GS, depending on $\phi$ and $c_e$. Thus, the inter-particle distances do not coincide in general with the minima of potential energy of the system. This leads, in particular, to rather unusual zero-temperature dependence of $c_e$ on the chemical potential $\mu$, which proved to be fractal (devil staircase).

The low-temperature thermodynamics of 1D GWL was considered in. In it was shown that 2D systems are characterized by an effective reduction of the dimension that allows one to find their GS, which proved to be a natural 2D generalization of 1D Hubbard description (see (2)).

Note, however, that the majority of 1D self-localized conductors are disordered. For example, in semiconductors on the base of MOSFET the disorder is due random impurities, in nanostructures the disorder is due to the fluctuations of tunneling junctions, and in the 1D charge transfer salts the disorder results from imperfections of their chemical structure. That is why the influence of host-lattice disorder on the GS properties is of great interest, especially taking into account that in the 1D case even a weak disorder of the host-lattice
can affects essentially the GS structure and low temperature thermodynamic properties. It suffices to recall the Larkin-Imry-Ma result [10, 11], according to which an arbitrary weak random field destroys the long-range order in 1D and 2D systems.

As was mentioned above, the systems under consideration have been extensively studied both theoretically and experimentally. However, the majority of theoretical results are obtained in the frameworks of rather simple models, providing often only qualitative estimates.

In this situation is it natural to use numerical methods of analysis of thermodynamic properties of 1D systems, since in the 1D case rather large systems (up to $N_e \sim 10^4 - 10^5$ particles) can be studied by the transfer-matrix method. However, the use of the method to find the the low temperature asymptotic regime is rather limited by the exponential growth (or decay) of the entries of transfer matrix. This implies the considerable decrease of calculation accuracy or even an overflow in numerical co-processor registers.

In this paper we propose a new numeric method for the study of GS of the system in question, i.e., classical 1D repulsing particle on a disordered host-lattice in the limit of low particle density (1). This condition is the case for many 1D lattice systems, including quasi-one-dimensional organic conductors, chains of nano-objects, etc.

2 Model

We will describe the one-dimensional system of repulsing particles [3,12,13] on disordered host-lattice by the extended Hubbard model determined by the Hamiltonian [14]

$$\hat{H} = -t \sum_{<\alpha,\beta>,\sigma} \hat{c}^+_{R_\alpha,\sigma} \hat{c}_{R_\beta,\sigma} + U \sum_{\alpha} \hat{n}_{R_\alpha,\uparrow} \hat{n}_{R_\alpha,\downarrow} + \frac{1}{2} \sum_{\alpha \neq \beta} V(|R_\alpha - R_\beta|) \hat{n}_{R_\alpha} \hat{n}_{R_\beta}. \quad (3)$$

where $<\alpha,\beta>$ means summation over the nearest neighbors, $\{R_\alpha\}$ are the sites of host-lattice ($\alpha = 1, 2, \ldots, L$), $\hat{c}^+_{R_\alpha,\sigma}$ and $\hat{c}_{R_\alpha,\sigma}$ are the creation and annihilation operators on the site $R_\alpha$ with spin $\sigma$ ($\sigma = \uparrow, \downarrow$), $U$ is the interaction energy of two particles on the same site of the host-lattice, $\hat{n}_{R_\alpha,\sigma} = \hat{c}^+_{R_\alpha,\sigma} \hat{c}_{R_\alpha,\sigma}$ is the number operator at the site $R_\alpha$.

We will consider systems for which the potential has the power-low decay at infinity, i.e.,

$$V(|x|) \sim |x|^{-\gamma}, \quad \gamma > 0, \quad |x| >> a_0. \quad (4)$$

where $a_0$ is the length fixing the order of magnitude the distance between the adjacent host-lattice sites, i.e., is the period of translation invariant lattice, the mean distance between the sites of a disordered lattice, etc. (cf. (2)).

The thermodynamic stability requires that $\gamma > 1$ [7]. Thus, we write

$$\gamma = 1 + \delta, \quad \delta > 0. \quad (5)$$
and assume that $V$ of (4) is positive (repulsive) and convex. The last condition is important and its violation may change significantly the results (see e.g. [15]).

Note that the systems for which $-1 < \delta \leq 0$ has also been studied recently (see e.g. [16, 17, 18]). One can call these systems the “strong” long ranged. In this case one has to either take into account certain truncation 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 [16, 17]. On the other hand, the systems where with $\delta > 0$) can be called the “weak” long ranged. They admit the traditional statistical mechanics description, possessing, however, certain special properties if $\delta$ is small (say, $0 < \delta \leq 2$).

We will consider in this paper the limit of low particle density $c_e$ of (1)

$$c_e = N_e / L << 1.$$  (6)

Besides, we will neglect both the dynamic effects ($t = 0$) and the effects of Fermi statistics ($U \to \infty$) [3]. The last limit leads to so called spinless fermions model. As a result, the only potential energy of particle repulsion has to be taken into account and the Hamiltonian (3) can be replaced by

$$H = \frac{1}{2} \sum_{\alpha \neq \beta} V(|R_\alpha - R_\beta|) n_{R_\alpha} n_{R_\beta},$$  (7)

where $\{ n_{R_\alpha} \}$ are the classical occupation numbers: $n_{R_\alpha} = 0, 1$.

It is convenient to pass from the occupation numbers $\{ n_{R_\alpha} \}$ of the host-lattice sites $\{ R_\alpha \}$ to the coordinates $\{ x_k \}$ of particles ($k = 1, \ldots, N_e$), i.e., the coordinates of points of the host-lattice where the occupation numbers equal 1. We obtain instead of (7)

$$H = \sum_{j<k} V(|x_j - x_k|).$$  (8)

It was shown in [19] that in the low-temperature limit the major contribution into partition function of (7) is due to the particle configurations which are close to equidistant ones, i.e., to the ground state configuration of the Wigner crystal with the same $c_e$. In other words, if $l_0 = a_0 / c_e$ is the period of the Wigner crystal, hence the coordinate $r_k$ of its $k$-th site is $r_k = kl_0$, and if $x_k$ is the coordinate of $k$-th site of Generalized Wigner Crystal, then the typical shifts between $r_k$ and $x_k$ are

$$s = < |x_k - r_k| > \sim a_0 \ll l_0,$$  (9)

where the symbol $< \ldots >$ denotes the averaging with respect to the host-lattice disorder which we assume as usually to be translation invariant in the mean [20].

We denote the shifts

$$s_k = x_k - r_k$$  (10)

and expand the Hamiltonian (7) with respect to the small parameter $\overline{s}/l_0 \simeq a_0/l_0 << 1$:
\[ H \approx H_{WC}(c_e) + \frac{1}{2} \sum_{j,k} b_{j-k}(s_j - s_k)^2. \]  

(11)

Here \( H_{WC} \) is a constant (the ground state energy of Wigner crystal with a given density) and

\[ b_{j-k} = b(|r_j - r_k|) = b(|j - k| l_0) = \frac{1}{2} \frac{\partial^2 V(x)}{\partial x^2} \bigg|_{x = |j - k| l_0}. \]

Omitting \( H_{WC} \) and using the nearest neighbor approximation, we obtain from (11)

\[ H = b_1 \sum_{\alpha=1}^{N_e-1} (s_\alpha - s_{\alpha+1})^2. \]  

(12)

Note that in the above nearest neighbor approximation we take into account the interaction between the nearest particles but not the nearest host-lattice sites. Since the typical distance between particles is \( l_0 = a_0/c_e \), hence \( l_0 >> a_0 \) (see (9)) in the low concentration limit (6), the approximation seems fairly reasonable.

It is convenient to measure the energy in units of \( b_1 a_0^2 \). Then (12) became

\[ H = \sum_{k=1}^{N_e-1} (s_k - s_{k+1})^2, \]  

(13)

where now \( H \) and the dynamic variables \( \{s_k\} \) are dimensionless. It was shown in [19] that if the temperature is low enough, then it suffices to consider the case where \( k \)-th particle occupies only one of two host-lattice sites adjacent to the \( k \)-th site \( r_k \) of the corresponding Wigner crystal (see Fig. 1).
We will call these sites clusters, each cluster consists of two sites of the host lattice and contains only one particle which can occupy one of these two host-lattice sites. In this case the shifts (10) can be written as:

\[ s_k = \sigma_k \lambda_k^\sigma, \quad \lambda_k^\sigma \geq 0, \tag{14} \]

where \( \{\sigma_k = \pm 1\} \) are the standard Ising spins and \( \{\lambda_k^\sigma\} \) are the random distances of the cluster sites from the site \( r_k \) of the Wigner crystal of the same density. We will assume that the distances \( \{\lambda_k^\sigma\} \) are independent and identically distributed for all \( k = 1, 2, \ldots, N_e \), hence the left hand and the right hand distances \( \lambda_k^+ \) and \( \lambda_k^- \) are typically different.

It follows from (14) that the shifts (10) can be viewed as Ising-type spins with random lengths \( \lambda_k^\sigma \), \( k = 1, \ldots, N_e \). To make more explicit the dependence of Hamiltonian (13) on the dynamic variables \( \{\sigma_k\} \) and the frozen disorder described by the random spin lengths \( \{\lambda_k^\sigma\} \), we write

\[ \lambda_k^\sigma = \alpha_k \sigma_k + \beta_k, \quad \alpha_k = (\lambda_k^+ - \lambda_k^-)/2, \quad \beta_k = (\lambda_k^+ + \lambda_k^-)/2 \geq 0, \tag{15} \]

i.e., \( \{\alpha_k\} \) and \( \{\beta_k\} \) do not depend on \( \{\sigma_k\} \) and are independent for different \( k \). By using this parametrization, we can rewrite (13) as

\[ H(\{\sigma_k\}) = C - 2 \sum_k \beta_k \beta_{k+1} \sigma_k \sigma_{k+1} - \sum_k h_k \sigma_k \tag{16} \]

where \( C \) does not depend on \( \{\sigma_k\} \) and can be omitted, \( \{\beta_k\} \) are given by (14) and

\[ h_k = 2\beta_k (\alpha_{k+1} + \alpha_{k-1} - 2\alpha_k). \tag{17} \]

Thus, the Hamiltonian (13) is thermodynamically equivalent to that (10) of the one-dimensional Ising model with random interaction and random short correlated external field (recall that \( \{\alpha_k\} \) and \( \{\beta_k\} \) are independent for different \( k \)). Since \( \{\lambda_k^\sigma\} \) are non-negative, independent and identically distributed for all \( k = 1, 2, \ldots, N_e \) and \( \sigma = \pm 1 \), it follows from (15) that \( \{\beta_k\} \) are non-negative, independent and identically distributed and \( \{h_k\} \) are symmetrically distributed, in particular

\[ < h_k > = 0. \tag{18} \]

We obtain the periodic host-lattice setting putting \( \lambda_k^\sigma = 1 \) for all \( k \). In this case (10) corresponds to the one-dimensional ferromagnetic Ising model with the nearest-neighbor interaction.

In general, each realizations of \( 2N_e \) random lengths \( \{\lambda_k^\sigma\} \), hence random variables \( \{\beta_k\} \) and \( \{h_k\} \) provides a realization of disorder, thus fixing the Hamiltonian to be used to find the partition function

\[ Z(L, N_e) = \sum_{\{\sigma_k = \pm\}} e^{H/T} \tag{19} \]

of our disordered system or its ground state \( \{\sigma_k^{GS}\} \):

\[ E_{GS} = \min_{\{\sigma_k = \pm\}} H(\{\sigma_k\}) = H(\{\sigma_k^{GS}\}). \tag{20} \]
3 The Ground State.

The low temperature thermodynamic properties of the model (13) have been studied in [19] using the transfer-matrix formalism. In particular, a weak local external field

\[ h = \{ \varepsilon h_k \}, \quad h_k = \delta_{k,k_0} \]  

was introduced into the Hamiltonian (13) 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

\[ H = \sum_{k=1}^{N} (s_k - s_{k+1})^2 - \varepsilon s_{k_0}. \]

Using the transfer-matrix techniques, one can calculate the free energy \( F(T, h) \) of the system and the corresponding magnetization per spin

\[ M_{loc}(T,k_0) = -\frac{1}{N_e} \left. \frac{\partial F(T,h)}{\partial \varepsilon} \right|_{\varepsilon=0} \approx \frac{F(T,0) - F(T,h)}{N_e \varepsilon}. \]  

(22)

It is reasonably to believe that if \( M_{loc}(T,k_0) > 0 \) in the low temperature limit, then the \( k_0 \)-th spin of the ground state is parallel to the field, while if \( M_{loc}(T,k_0) < 0 \), then the \( k_0 \)-th spin is antiparallel to the field. Thus, calculating \( M_{loc}(T,k_0) \) for \( k_0 = 1, 2, \ldots, N_e \) 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 (22) is of the order \( 1/N_e \ll 1 \) 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:

\[ \varepsilon \ll T, \varepsilon_{sf}, \]  

(23)

where \( \varepsilon_{sf} \) is typical “spin flip” energy. However, in view of possible local energy degeneration \( \varepsilon_{sf} \) 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.

In this paper we study the ground state by a new method, which is free from the above disadvantage. The main idea of the method is as follows. Let us divide the system into \( n \) parts (subchains) \( C_m, \quad m = 1, \ldots, n \) with the endpoints \( p_0, p_2, \ldots, p_n \), where \( p_0 = 1, p_n = N_e \) and

\[ p_0 < p_1 < p_2 < \ldots < p_{n-1} < p_n. \]

The lengths of the \( m \)-th subchain is \( l_m = p_{m+1} - p_m + 1, \quad m = 0, 1, \ldots, n-1 \). Thus, the \( m \)-th subchain contains \( l_m \) spins

\[ \sigma_{p_m}, \sigma_{p_m+1}, \ldots, \sigma_{p_m+1}, \sigma_{p_m+1}. \]
and the spin $\sigma_{p_{m}}$ ($m = 1, 2, ..., n-1$) belongs to the two neighboring subchains, i.e., $\sigma_{p_{m}}$ is the last “spin” of $m$-th subchain and the first spin of $(m+1)$-th subchain.

It is convenient to index the spins in each subchain as

$$\sigma_{p_{m}+j-1} = \sigma_{m,j},$$

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

$$\sigma_{m,1}, \sigma_{m,2}, \ldots, \sigma_{m,l_{m}-1}, \sigma_{m,l_{m}}.$$

Now we carry out the direct enumeration of the states (the direct search for the configurations with minimum energy) in each of $n$ subchains.

According to (13), the energy of $m$-th subchain is:

$$H_{m} = H_{m}(\sigma_{m,1}, \sigma_{m,2}, \ldots, \sigma_{m,l_{m}}) = -2 \sum_{j=1}^{l_{m}-1} \beta_{m,j} \beta_{m,j+1} \sigma_{m,j} \sigma_{m,j+1} - \sum_{j=1}^{l_{m}-1} h_{m,j} \sigma_{m,j}$$

Let $H_{m}^{\text{min}}$ be the minimum of $H_{m}$ over the spin configurations of the subchain and let

$$\sigma_{m,1}^{\text{min}}, \sigma_{m,2}^{\text{min}}, \ldots, \sigma_{m,l_{m}-1}^{\text{min}}, \sigma_{m,l_{m}}^{\text{min}}.$$  \hspace{1cm} (24)

be a corresponding spin configuration: $H_{m}^{\text{min}} = H_{m}(\sigma_{m,1}^{\text{min}}, \ldots, \sigma_{m,l_{m}}^{\text{min}})$.

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

$$\sigma_{m,l_{m}} = \sigma_{m+1,1}, \quad m = 1, 2, \ldots, n-1,$$  \hspace{1cm} (25)

then the union of all the subchain minimizing configurations (24) is a ground state configuration $\sigma_{GS} = \{\sigma_{k}^{GS}\}$ of the whole Hamiltonian (16):

$$\sigma_{GS} = (\sigma_{1}^{GS}, \sigma_{2}^{GS}, \ldots, \sigma_{n-1}^{GS}) = (\sigma_{0,1}^{\text{min}}, \sigma_{0,2}^{\text{min}}, \ldots, \sigma_{0,l_{0}}^{\text{min}}, \sigma_{1,1}^{\text{min}}, \ldots, \sigma_{n-1,l_{n-1}}^{\text{min}}),$$

and the corresponding total minimum energy (20) is

$$E_{GS} = \sum_{m=0}^{n-1} H_{m}^{\text{min}}.$$  \hspace{1cm} (26)

A similar idea has been recently used to study ground states of certain rather complex (in particular frustrated) translation invariant spin models [21, 22].

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 (25). If the conditions are not satisfied, repeat
the procedure.

Note, however, that the procedure does not guarantee that the ground state
is unique.

The choice of an optimal number \( n \) 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 \( t_0 \sim n2^{N_e/n} \). It is thus reasonable to choose \( n \) so that \( t_0 \) is several seconds,
i.e., \( n \sim N_c/10 - N_c/20 \), where \( N_c = 10^4 - 10^5 \) and even more. Increase in \( n \)
leads to decrease in enumeration time, but at the same time, to increase in the
number of attempts (number of generations of division points \( \{p_m\} \)).

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 (25)
is modified. For example, if we take into account the near- and next-neighbors
interaction, then the matching conditions (25) are

\[
\begin{align*}
\sigma_{m,l}^{\min} & = \sigma_{m+1,l}^{\min} \\
\sigma_{m,l}^{\min} & = \sigma_{m+1,l+1}^{\min}
\end{align*}
\]

By using the method, we studied the ground state of the Hamiltonian (10). It
is convenient to quantify the amount of disorder by writing the random spin
length (14) as

\[
\lambda_{k}^\sigma = 1 - \xi_k^\sigma, \quad \xi_k^\sigma = 2A\eta_k^\sigma,
\]

where \( \{\eta_k^\sigma\} \) are independent random variables uniformly distributed over the
interval \([0,1]\) (\( \langle \eta_k^\sigma \rangle = 1/2 \)) and \( A \) is the “disorder” strength, \( 0 \leq A \leq 1/2 \).
The limiting case \( A = 0 \) corresponds to the ordered system (the translation
invariant Ising model) and \( A = 1/2 \) corresponds to complete disorder, where
the spin lengths \( \{\lambda_{k}^\sigma\} \) are uniformly distributed over the interval \([0,1]\).

The examples of the ground state spin configurations for \( N_e = 10^4 \) are
presented in Fig. [2].

We see that the ground state consists of “domains” [19] of blocks of spins of
the same sign, the domains concentration increasing rapidly with the increase
of disorder parameter \( A \).

It follows from (15) and (16) that interaction in our Ising model is ferro-
magnetic although random. Thus, the ground state of (16) without the second
term is ferromagnetic (collinear), i.e., with all the spins either “up” or “down”. 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 [10, 11, 23] implies that the ferromagnetic
ground state is unlikely for any \( 0 \leq A \leq 1/2 \). Thus, it is not completely un-
expected 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” non-collinear type. On the other hand, our numerical method allows us to detect an explicit form of a ground state, having the domain structure.

Figure 2: The orientation of spins in the ground state of the system for $N_e = 10^4$ and two values of the disorder parameter $A$ of (27). 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 $A$.

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 (13) (or of (16)) are

$$\delta \varepsilon \sim A^2,$$

while 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. Thus, the domain is stable if its length $l_{\text{dom}}$ satisfies the inequality

$$\delta \varepsilon \sqrt{l_{\text{dom}}} \lesssim \varepsilon_{\text{dom}}.$$

We obtain then [19, 24]:

$$l_{\text{dom}} \sim A^{-4},$$

hence

$$c_{\text{dom}} = l_{\text{dom}}^{-1} \sim A^4.$$  \hspace{1cm} (28)

In particular, it follows from (28) and (29) 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 (solid boxes).

The approximation by the function

$$c_{\text{dom}} = (A/A_0)^d$$

is given by the solid line. The best fitting is for $A_0 = 0.88885$ and $d = 4.06031$ (quite close to those, obtained in [19] and (29)). Thus, we have a sufficiently good agreement between the numerical data and the fitting curve for $A \leq 1/2$. 

10
4 Probing field.

In this section we confirm our results of previous section on the form of the ground states of model (16) by probing its ground state by an external field of special form. Denote $H_I$ the r.h.s. of (16) without $C$. Given a collection $b = \{b_k\}$, consider the perturbed Hamiltonian

$$H_I - \varepsilon \sum_{k=1}^{N} b_k \sigma_k$$

and the corresponding generalized magnetization

$$M(T, b) = -\frac{1}{N_e} \frac{\partial F(T, b, \varepsilon)}{\partial \varepsilon} \bigg|_{\varepsilon = 0} = \frac{1}{N_e} \sum_{k=1}^{N_e} b_k < \sigma_k >_G,$$

where $F(T, b, \varepsilon)$ is the free energy of (30) and $< ... >_G$ denotes the corresponding Gibbs mean. By using the terminology of spin glass theory (see e.g. [25]), we can view (31) as the overlap between external field $\{b_k\}$ and the local magnetization $\{< \sigma_k >_G\}$.

It follows from the r.h.s. of (31) that the inequality

$$|M(T, b)| \leq \left( \frac{1}{N_e} \sum_{k=1}^{N_e} b_k^2 \frac{1}{N_e} \sum_{k=1}^{N_e} < \sigma_k >^2_G \right)^{1/2}$$

holds for a generic $\{b_k\}$ and that it becomes the equality only for an external field proportional to $\{< \sigma_k >_G\}$:

$$\overline{b}_k = a < \sigma_k >_G, \ k = 1, ..., N_e,$$

where $a$ is a constant, i.e.,

$$M(T, \overline{b}) = a \sum_{k=1}^{N_e} < \sigma_k >^2_G.$$

The constant $a$ can be chosen to be 1 if we normalize $\{b_k\}$ by the condition

$$\sum_{k=1}^{N_e} b_k^2 = 1.$$

Since we are interested in the ground state $\{\sigma_k^{GS} = \pm 1\}$ of the Hamiltonian (16), which we identify with the domain walls configuration of the previous section, we put $T = 0$ in the above formulas and arrive to the following algorithm to detect $\{\sigma_k^{GS}\}$. Pick a class of external fields containing $\{\sigma_k^{GS}\}$ and satisfying (34) and vary $\{b_k\}$ over the class. The configuration $\{\sigma_k^{GS}\}$ will be obtained as a maximizer of the generalized magnetization (31):

$$M(0, \{\sigma_k^{GS}\}) = \frac{1}{N_e} \sum_{k=1}^{N_e} (\sigma_k^{GS})^2 = 1.$$
In general, this will only prove that the corresponding maximizer is a local minimum of the Hamiltonian \(^{13}\) of the model, it is reasonable to believe but the larger is the class the closer is the minimizer to the genuine ground state.

Figure 3: The domain concentration \(c_{dom}\) as the function of disorder parameter \(A\). Solid boxes are the results of our numeric calculation, solid line is the fitting by function \(c_{dom} = (A/A_0)^d\).

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

\[
b_k = \sigma_k^{GS} + f_k, \quad (36)
\]

where

\[
f_k = \begin{cases} -2\sigma_k^{GS} & k \in (d_m, d_m + \Delta_m) \quad m = 1, 2, \ldots, n, \\ 0, & \text{otherwise}; \end{cases} \quad (37)
\]

\[
\Delta_m = (-1)^{\eta_m}[B\rho_m], \quad (38)
\]

\(B \geq 0\) is a non-negative constant, \([\ldots]\) 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 \(\{\sigma_k^{GS}\}\). The direction of the shift of the \(m\)-th domain wall is determined by \(\eta_m\) and the amplitude of the shift is determined by \(B\). In particular, the probe field \(^{36}\) coincides with \(\{\sigma_k^{GS}\}\) if \(B = 0\).
To find the free energy $F(T, b, \varepsilon)$ corresponding to (16), we use the transfer-matrix method. We set for $s_k^\pm = \pm \lambda_k^\pm$, $k = 1, 2, \ldots, N_e$

$$
\hat{P}_k(T, b) = \begin{pmatrix}
\exp \left( -\frac{(s_k^+ - s_{k+1}^-)^2 - \varepsilon b s_k^+}{2} \right) & \exp \left( -\frac{(s_k^+ - s_{k+1}^-)^2}{2} - \varepsilon b s_k^- \right) \\
\exp \left( -\frac{(s_k^- - s_{k+1}^+)^2}{2} \right) & \exp \left( -\frac{(s_k^- - s_{k+1}^+)^2 - \varepsilon b s_k^-}{2} \right)
\end{pmatrix}, \quad (39)
$$

assume the periodic boundary conditions ($\sigma_{N_e+1} = \sigma_1$) and write

$$
F(T, b, \varepsilon) = -T \log \left( \text{Tr} \left[ \prod_{k=1}^{N_e} \hat{P}_k(T, b) \right] \right), \quad (40)
$$

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

Using (39) - (40), one can calculate numerically the generalized magnetization (31) for the class (36) – (38) of probing fields as the function of amplitude $B$ of fluctuations of the domains walls:

$$
M(T, b) \approx \frac{F(T, b, 0) - F(T, b, \varepsilon)}{N_e \varepsilon}. \quad (41)
$$

Fig. 4 (curve 1) presents the generalized magnetization (31) as a function of $B$ for field (36) and $T \to 0$.

Figure 4: Curve 1. The generalized magnetization $M(0, b)$ as the function of $B$ for the fields (36) – (38). Curve 2. The analogous curve for the probe fields with $s_k^{GS} = \sigma_k^{GS} \lambda_k^\pm$ instead of $\sigma_k^{GS}$ in the r.h.s. of (39).

We see that the magnetization is maximal for $B = 0$, where the fluctuations (37) are absent, hence the probe field (36) 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 the if we replace the maximizing field \( \sigma^{\text{GS}}_k \) in (36) by \( s^{\text{GS}}_k = \alpha_k \sigma^{\text{GS}}_k \) (see (14)) and compute again numerically the corresponding generalized magnetization, we obtain a curve (see curve 2 of Fig. 4), which is quite similar to that of curve 1 of Fig. 4 except the magnitude of maximum, which is now \( 1 - A \).

The magnitude can be explained as follows. In view of (14) and (15) the maximum is

\[
\frac{1}{N_e} \sum_{k=1}^{N_e} s^{\text{GS}}_k \sigma^{\text{GS}}_k = \frac{1}{N_e} \sum_{k=1}^{N_e} \sigma_k \sigma^{\text{GS}}_k + \frac{1}{N_e} \sum_{k=1}^{N_e} \beta_k.
\]

The second term on the right is \( < \beta_k > = 1 - A \), if \( N_e \) is large enough, thus the first term has to vanish for \( N_e >> 1 \) 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.

5 Results and Discussion.

The ground state of interacting particles on a disordered one-dimensional host-lattice is studied using a new numerical method. It is shown that if the concentration of particles is small enough, then even a weak disorder in host-lattice site positions leads to the formation of the “domains” of particles and to the breaking the long-range order pertinent to the Generalized Wigner crystal in the absence of disorder. The nature of the domains can be explained by using the Hubbard formula (2) for particle positions in the Generalized Wigner crystal. Indeed, in the case of the translation invariant host-lattice the phase \( \phi \) in the formula is an arbitrary constant, just fixing the origin of the host-lattice. In the disordered case each domains has its own phase, i.e., \( \phi \) is a step function with random steps and the mean domain length \( l_{\text{dom}} \) is just the mean length of steps.

It is also shown that the formula \( l_{\text{dom}} \sim A^{-4} \) (28) is valid in a sufficiently wide range of disorder parameter \( A \): \( 0 \leq A \leq 0.5 \) (see Fig. 4).

The above results are then confirmed by studying the weak perturbations of the Hamiltonian (16) of the model by random external fields, 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 (41) 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.
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