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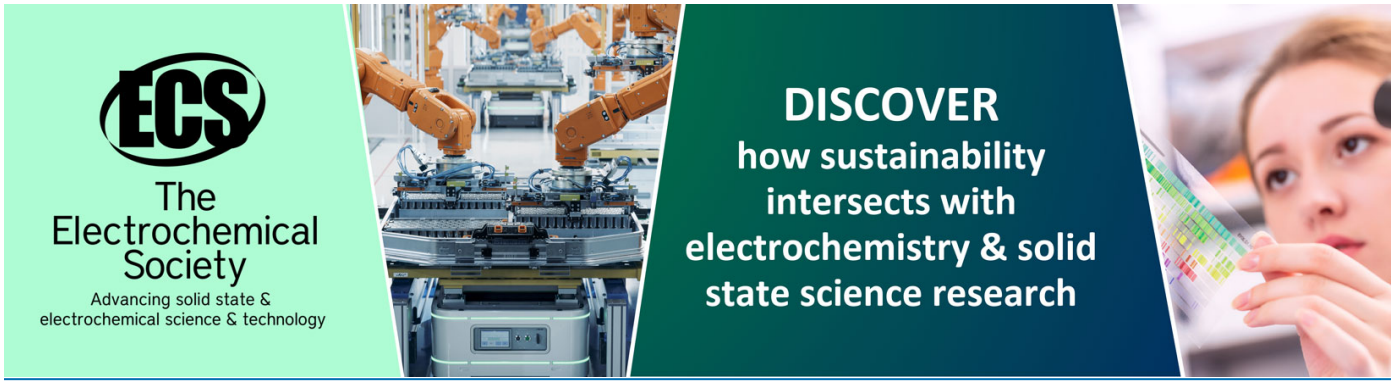

Theory of electron states in two-dimensional Wigner clusters

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Abstract. The results of modeling a finite system of interacting two-dimensional electrons placed at zero temperature into an external parabolic potential well are presented. The structure of the 2D Wigner cluster is found. The distribution functions of interelectron distances and the coordination numbers of internal and external electrons are obtained. The "string-zigzag" transition is analyzed. The low-temperature specific heat of the system is determined. An electronic Wigner crystal on a sphere is also considered.

1. Introduction

The Wigner crystal [1, 2], is a system of repulsing charged particles with compensating uniformly distributed opposite charges. If the repulsion is strong enough, the charged particles will form a crystal. The Wigner crystal was initially proposed as a hypothetical model of a metal, where positive ions are smeared and electrons are localized into a crystal lattice. This model is orthogonal to the usual adiabatic model, in which electrons are smeared out due to Fermi statistics and heavy ions are static. It was used by Wigner in order to interpolate the thermodynamic properties of a metal between weakly interacting and strongly interacting electrons for an intermediate case.

Unfortunately, 3D systems are usually electrically neutral. With a large interaction force in such systems, unlike charges are bound into atoms instead of ordering similar charges into the crystal lattice.

A.V. Chaplik [3] (see, also [4]) pointed out that, in a two-dimensional system, positive and negative charges can be separated - some are on the gate electrode, while others are in the two-dimensional system itself. Then the requirement to smear opposite charges is eliminated and the Wigner crystal becomes accessible. The realization of a two-dimensional Wigner crystal is the cherished dream in physics of solid low-dimensional systems. Unfortunately, this is hindered by the relatively low electron interaction constant, despite the fact that the electron crystallization is expected at its value of about 100.

Main efforts were pooled in the theoretical study of infinite Wigner crystals (see, e.g., [5] and references therein). The problem of the Wigner crystal is related to the problem of the string-zigzag transition [6] in an infinite system of electrons placed in a one-dimensional parabolic confining potential. Such a system can be interpreted as a transition in the formation of two

Wigner crystal layers from one layer. Note, that recently, however, the signature in exciton spectrum of the 2D Wigner crystal was observed [7].

In fact, the Wigner crystal was observed in the electron system on the liquid helium surface [8], where very low electron densities are attainable, and the Coulomb interaction is practically not screened due to the dielectric constant of the medium. Another representative of systems with the Wigner crystal is, e.g., a dusty plasma crystal, a system implemented in microgravity (see, e.g. [9, 10] and references therein). In such a system, massive charged dust particles are not smeared out due to the Fermi energy and can form a crystal.

The Wigner clusters with a limited but large number of particles have their own nontrivial properties. The systems with few electrons were studied both experimentally [11] and theoretically [12]-[13]. Electrons in an isotropic potential well form a near-isotropic distribution with polycrystalline core with a shell structure (see [14]-[18], and references therein).

In contrast to the previous papers, here we study the formation of a two-dimensional cluster from a system of a large number (50-200) of electrons placed in a two-dimensional symmetric and asymmetric confining potential. Our approach is based on computer simulations accompanied by theoretical estimates.

2. Computer simulations

We consider a two-dimensional system of N classical electrons placed in a field with potential $U = k(x^2 + \beta y^2)/2$. An imaginary installation for the 2D confinement of electrons is shown in figure 1. Electrons repel each other with the Coulomb potential $e^2/|\mathbf{r}_i - \mathbf{r}_j|$, $\mathbf{r} = (x, y)$. The temperature is assumed to be zero.

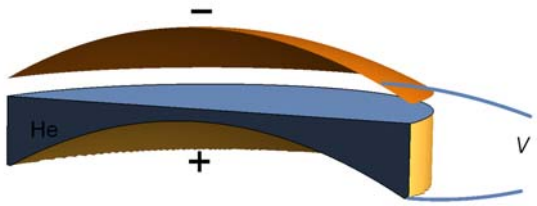

Figure 1. Electrons on the liquid He surface are surrounded by upper and bottom parabolic metallic gates, producing a parabolic well in the center of the He container. Electrons are collected in the center of the well.

Under these conditions, electrons will minimize the total potential energy. This means that they will be located near the minimum of the external potential at the maximum possible relative distance. The inner part of such a cluster should obviously be a periodic lattice. The system energy was minimized at $N = 50, 100, 200$. The results of computer calculations of the arrangement of electrons for different β are shown in figure 2. If $\beta = 1$, then, on the average, the electrons system should occupy a circular region (figures 2(e) and 2(f)). On the contrary, if $\beta \to \infty$, the electrons will be pressed to the abscissa axis.

3. 1D cluster and string-zigzag transition

The different cluster shapes replace each other via the increase in the number of electron rows. The first electrons protruding beyond the $y = 0$ line arise at $\beta \sim 18.7$. This is the beginning of the string-zigzag transition in the final system. The transition occurs due to the loss of stability of the central electrons in the cluster, and then of the surrounding electrons, by sequentially decreasing β. The region of the electrons unstable on the $y = 0$ line gradually grows. Then electrons with $y \neq 0$ lose their stability, and the third row appears. The circular area is formed gradually.

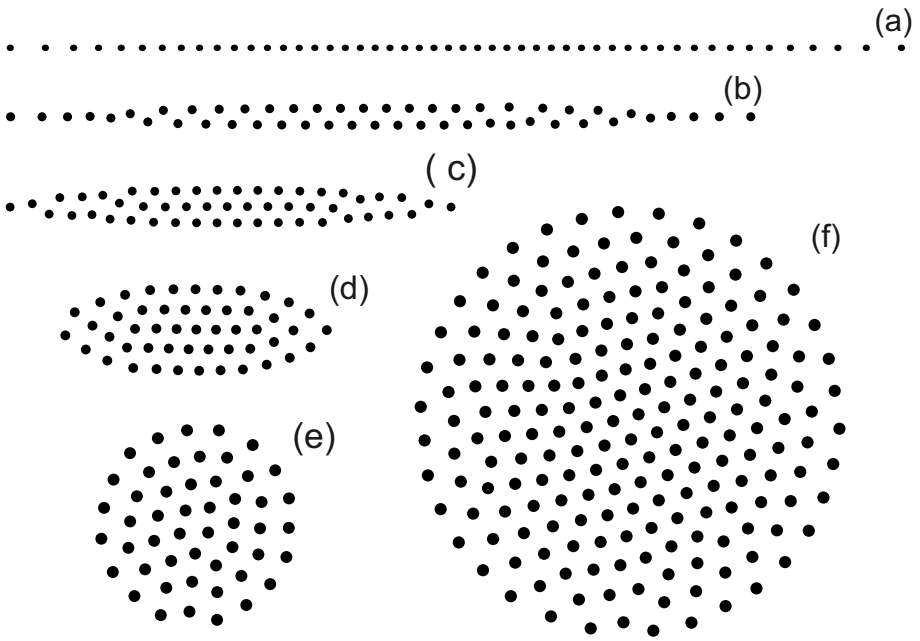

Figure 2. Cluster structure at (a) $N = 50$, $\beta = 20$, (b) $N = 50$, $\beta = 10$, (c) $N = 50$, $\beta = 5$, (d) $N = 50$, $\beta = 2$, (e) $N = 50$, $\beta = 1$, (f) $N = 200$, $\beta = 1$.

Let us examine why the restructuring process takes place gradually. The electron density on the $y = 0$ line decreases towards the x axis the edges. The potential from neighboring electrons is $\sum_j 1/\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} \approx \sum_j 1/|x_i - x_j| - (y_i - y_j)^2/2|x_i - x_j|^3$. The lateral potential decreases in density to the edges quadratically. When this part of the potential becomes greater than the potential of the well, the central minimum of the electron energy turns into a maximum: the equilibrium at the center becomes unstable.

For this reason, with a relatively small β, electrons in the line center lose their stability, and, at the edges they retain their rest.

The structures of clusters of N electrons, depending on the asymmetry of the potential well, are shown in the figures. When the crystal degenerates into one-dimensional, its density decreases towards the edges due to a decrease in pressure. When decreasing to 18.7, the one-dimensional crystal loses its stability, turning into a zigzag one, and then increases the number of layers.

4. One-dimensional cluster. Analysis

Let us analyze the nature of the electron distribution within a one-dimensional cluster. According to figure 2, the cluster has a finite size, and the electron density is higher in the center of the cluster. The equilibrium position of electrons satisfies the system

$$\sum_{j \neq i} \frac{\mathrm{sign}(x_i - x_j)}{(x_i - x_j)^2} - k x_i = 0. \tag{1}$$

We consider the electron distribution in a continuous model with use of mean density $c(x)$. First, let the density be constant. In this case all electrons to the right from the given one will press on it with the force

$$c^2 \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} c^2.$$

If electrons are placed in the well with potential $kx^2/2$, density c begins to depend on the coordinate x. The force applied to an element of electron gas $c(x)dx$ should be equated to the force from the well $kxc(x)dx$. Hence, we have:

$$\frac{\pi^2}{6}\frac{dc^2(x)}{dx} = -c(x)kx, \qquad c(x) = c(0) - \frac{3kx^2}{2\pi^2}. \tag{2}$$

The distribution boundaries $\pm L$ are determined by the condition $c(L) = 0$. The total number of electrons in a cluster is $N = 2\pi(\frac{2c(0)}{3})^{3/2}/\sqrt{k}$. As a function of x_i, density $c(x_i) = 1/(x_{i+1} - x_i)$ from the computer calculation and the function $c(x)$, in accordance with (2), are shown together in figure 3. This shows their good agreement.

The large density in the central part of the elongated cluster converts it to a zigzag while the edges stay intact.

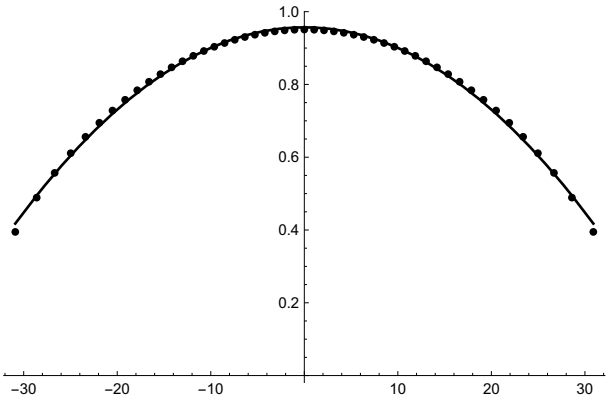

Figure 3. Electron density *versus* distance (dotted) for the 1D cluster in figure 2(a), in comparison with the analytical result (line).

5. 2D cluster

When $\beta = 1$, the crystal occupies, on the average, a circular area. Inside the central part of the circular region, electrons are located equidistantly, minimizing the mutual repulsion energy. On a small scale, electrons form a triangular crystal lattice. Typically, each electron has a hexagonal coordination. However, the inner part is periodic, but polycrystalline. The lattice contains defects, such as crystalite boundaries and pentagonal-coordinated point defects.

The periodicity violation results from the competition of the isotropic surface pressure from the well and the requirement for the minimum of the mutual electron-electron interaction energy repulsion. The lattice periodicity requires the point symmetry group C_6, and the surface energy minimization requires the symmetry group O_2, the competition between which is allowed by breaking the crystal into blocks-crystallites. In other words, polycrystallinity is a result of the minimization of the cluster surface energy and the spatial periodicity of the lattice.

In this case, the intercrystaline boundary length must be of the order of outer perimeter of the cluster, so that the orders of the energies of the outer and intercrystaline boundaries could coincide. Therefore, the number of clusters should be of the order of unity.

The same competition melts the outer cluster part. Approximately two edge layers near the circle border have a highly damaged structure. This surface layer "melting" is due to the need to combine the minimum surface energy of the crystal and the spatial periodicity of the lattice. The competition of these two factors leads to melting.

6. Wigner cluster on a spherical surface

This system has an advantage from the point of view of the transition to an infinite crystal, since all points in it are initially equivalent and, therefore, there are no edge effects. The spherical cluster resembles fullerenes. However, their ordering is different.

Figure 4 shows the result of the energy minimization of the energy of 60 Coulomb particles in the assumption that the sphere itself does not affect the Coulomb interaction. The lattice consists of hexagonal and pentagonal faces and corresponds to icosahedral symmetry, like the C_{60} fullerene. However, not atoms but the most of internodes form the densest triangular lattice in this cluster, unlike graphene (and most C60 cells). The reason for this difference originates from the fact that carbon atoms attract each other, forming the densest packing on the sphere, while electrons repeal each other, so, their internodes tend to attract each other.

If we consider the spherical Wigner cluster as a part of an infinite lattice, then attention is drawn to the presence of local symmetry of the axes sixth (compatible with the translational symmetry of the two-dimensional lattice) and fifth orders (incompatible with it). This structure hints at the possibility of quasi-crystallinity in an infinite planar lattice.

A large spherical Wigner cluster can be considered as a part of an infinite lattice. However, the spherical Wigner cluster has a local symmetry axes of the sixth order compatible with the translational symmetry of the two-dimensional lattice) and fifth orders (incompatible with it). This structure hints at the possibility of quasi-crystallinity in an infinite planar lattice.

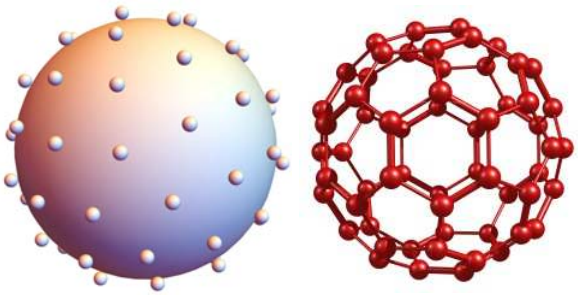

Figure 4. Wigner cluster of 60 electrons on a sphere (left) in comparison with fullerene C_{60} (right).

7. Low temperature specific heat

To determine the specific heat of the Wigner cluster, a spectrum of its vibration frequencies is required. Consider the system of classical Newton equations for crystal electrons

$$m\frac{d^2r_{n,i}}{dt^2} = \frac{d^2U}{dr_{n,i}dr_{m,j}}r_{m,j}, \tag{3}$$

where the indices m, n refer to the electron number, and i, j - to the coordinate. The squares of the frequencies ω_k are the eigenvalues of the force matrix

$$\frac{1}{m}\frac{\partial^2 U}{\partial r_{n,i}\partial r_{m,j}}.$$

The specific heat at a constant number of electrons in a cluster is given by the formula

$$C = \frac{\partial E}{\partial T} = \frac{\partial}{\partial T}\sum_k \omega_k f\left(\frac{\omega_k}{k_B T}\right), \tag{4}$$

where k_B is the Boltzmann constant, $f(x) = 1/(e^x - 1)$ is the Bose function. When the temperature decreases, the leading contribution arises from the terms with minimum frequencies. Note that, near the Wigner cluster stability threshold, one or a group of frequencies vanish. In this case, these terms become the main ones, contributing to the specific heat. Exactly at the threshold, $C = k_B\nu$, where ν is the number of frequencies that simultaneously vanish.

The multiplicity of degeneracy ν is dictated by the symmetry of the problem. Let us introduce the collective coordinate of the electrons across the u line. The initial symmetry of the system dictates the parity of the energy expansion in u: $E = au^2 + bu^4$. The frequency vanishing at some value of the parameters $s = s_0$ gives $a = \alpha(s - s_0)$. Then, the equilibrium value of u is $u_0 = \pm\sqrt{\alpha(s - s_0)/b}$. A valid solution exists for $\alpha(s - s_0)/b > 0$. In this case two equilibrium states arise and $\nu = 2$. Otherwise, the minimum is reached at $u_0 = 0$ and there is only one equilibrium state of the chain and $\nu = 1$. The critical vibration frequency vanishes like $\sqrt{|s - s_0|}$.

Another degeneracy arises from the global system symmetry. In particular, if $\beta = 1$, the system possesses the rotational $O(2)$ symmetry. If $b \neq 1$ the system has C2v group symmetry. The zigzag system has a symmetry depending on the electron numbers. For example, the clusters (b) and (c) in figure 2 have symmetry under reflection in the vertical axis. It should be emphasized that our consideration neglects electron spins. This degeneracy reflects in the low-temperature specific heat.

8. Conclusions

We have studied the 2D Wigner clusters confined in parabolic 2D wells. It was found that, under a change of the well eccentricity from strong to small, these clusters are the reconstructions from the 1D chain to a round cluster with a 2D polycrystal interior. Its exterior is melted down due to the concurrence between the crystal ordering and the surface tension. The interelectron valence angles demonstrate the narrow distribution around the value $\pi/3$ corresponding to the coordinate number 6.

The "string-zigzag" transition was also found. It was established that this transition first touches the chain center, subsequently propagating to the edges when the eccentricity drops. These findings are supported by the analytical estimations.

Acknowledgement

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