

Yu. E. Lozovik. *Ion and electron clusters.* Clusters consisting of electrons or ions, trapped in external fields, are studied. The following are examples of the physical realizations of such clusters: 1) ions, electrons, or other particles in radio-frequency or Penning traps; 2) electrons in potential wells, created by impurities or contact phenomena at a boundary in semiconductors; inclusions of one semiconductor in another; 3) electrons trapped above a dielectric particle or drop by image forces. As the temperature is lowered a hierarchy of structural changes, associated, as it turned out, with sequential freezing of degrees of freedom and manifested in the change in the character of the spectra, and of the type of motions of the particles, etc., is realized in these systems.¹ The properties of these systems were analyzed 1) in the low-temperature case (with the help of a variant of the theory of self-consistent vibrational approximation, taking into account systematically all effects of the same order of magnitude in the displacements of the particles from a lattice site)^{2,3}; 2) with the help of modeling by means of molecular dynamics and Monte Carlo methods; and, in the quantum case, 3) with the help of a variational calculation.

In the case of an external oscillator potential (harmonic trap) such systems are analogous to the Thompson atom. Coulomb charges form in the ground state of the system shell structures with quasicrystalline angular order within a shell. Filling of successive shells starts with definite numbers of particles N (see Table I). An analog of the periodic system of the "elements" was constructed, and the energies of the clusters and their symmetry and structure (for the three- and two-dimensional cases) were found. Both the global and the local minima of the system, differing significantly in structure (their energies differ only in the fourth decimal place), were determined. The size of the clusters slowly increases as N increases.

As the temperature T increases the potential energy of a cluster increases almost linearly in both the global and local minima (partial equilibrium). As T increases there arises a

hierarchy of changes in the structure of the clusters. In three-dimensional clusters for $T_1 \sim 10^{-3} - 10^{-4}$ (in dimensionless units) the crystalline structure within one shell melts, and then at $T_2 \sim 10^{-1}$ radial spreading of the shells occurs. In two-dimensional clusters rotation of the shells relative to one another starts at $T'_1 \sim 10^{-3} - 10^{-4}$; hopping of particles between shells occurs at $T'_2 \approx 10^{-2}$; and, radial spreading of the shells occurs at $T'_3 \sim 10^{-1}$. These structural changes are manifested both in the character of the dependence of the mean-square displacements $\langle u^2 \rangle$ from the equilibrium position on the time t (for example, the function $\langle u^2 \rangle = f(t)$ undergoes oscillations and infrequent discontinuities for $T > T'_2$) and in the form of the spectrum of the oscillations. Prior to the first structural change ($T < T_1$) the spectrum of the velocity autocorrelation function is discrete and after the first structural change it is continuous. As the number of particles increases, the occupation number of the shells at the center of a cluster approaches the coordination numbers of a Wigner crystal, and as T increases the standard melting occurs in the system (in two-dimensions, in two stages⁴).

Qualitatively close temperature-dependent global and local structures appear for charges on a sphere, in a circle, or in a cylinder (a beam of cooled particles in an accelerator,

TABLE I. Table of the occupation numbers of shells of two-dimensional Coulomb clusters.

N	1-5	6-8	9-10	11-13	14-15	16
N_1, N_2, N_3	$N = N$	$\begin{matrix} 1, \\ N-4 \end{matrix}$	$\begin{matrix} 2, \\ N-2 \end{matrix}$	$\begin{matrix} 3, \\ N-3 \end{matrix}$	$\begin{matrix} 5, \\ N-5 \end{matrix}$	1, 5, 10
N	17-18	19-21	...	56-58
N_1, N_2, N_3	1, 6, $N-7$	1, 7, $N-8$...	$\begin{matrix} 1, 6, 12, 18, \\ N-37 \end{matrix}$

etc.). In the first case, if the characteristic interaction energies of the charges are of the order of the binding energy on a sphere, the system becomes unstable. At very low temperatures T , when quantum properties become important, the ground state of the clusters is calculated variationally—with the help of the trial function $\psi = \exp(-V/2T^*)$, where V is the total potential energy and T^* is the trial parameter. Averaging over such a ψ is equivalent to thermodynamic averaging for a classical system with temperature T^* . After scaling transformations of the coordinates and the energy the behavior of the system in a harmonic trap depends only on one quantum parameter $\lambda = \frac{\hbar^2}{2m} e^{-8/3} \alpha^{1/3}$ (e is the charge and α is the parameter of the trap). Minimization gives the dependence $T^* = f(\lambda)$, so that the hierarchy of transitions in a classical system with changing T^* corresponds to a hierarchy of transitions in the quantum parameter λ (for example, to a change in α , which is equivalent to a change in the density).

The predicted phenomena can be observed for laser-cooled charges,⁵ for electrons above a helium drop or cryocrystallite,⁶ and for electrons in a semiconductor cluster.

Similar effects should also occur for clusters of a different nature, for example, clusters of dipoles, vortices, etc., as well as for particles forming short-range order in amorphous materials. In connection with the latter system, in particular, it would be interesting to study the reorientations of shells and other changes, which can simulate premelting, contribute to low-temperature properties, etc.

The hierarchy of transitions in two-dimensional electronic clusters in a magnetic field could be manifested (see Ref. 7) in the fractional quantum Hall effect.

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