Interaction of charged particles on surfaces

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The dependence of the energy of interaction between charged particles forming a two-dimensional lattice on the type of lattice is investigated. It is shown that all but triangular lattices are unstable with respect to the shear mode. The characteristic energy changes connected with such motions are quite small ($\sim 10^{-2}$ of the energy of interaction between the nearest neighbors) even at lattice deformations $\sim 100\%$.

PACS numbers: 63.10. + a, 68.40. + e

Two-dimensional systems of charged particles can, as is well known, form ordered structures at sufficiently low temperatures, namely a two-dimensional Wigner crystal.^{1, 2} For the case of a system of electrons on the surface of liquid helium, an original method of investigating its properties was proposed³ and the corresponding phase transition was observed with its aid in experiment.⁴

Charged particles or dipoles that interact with one another can exist also on surfaces of solids⁵, and although the possibility of formation of a Wigner crystal is greatly hindered in this case by the presence of the stronger quantum-chemical interaction, in individual situations one can nevertheless expect structures close to those of the Wigner type. For example, one can speak of the presence of a partly filled zone of surface states (intrinsic or induced by adsorbed atoms) on the surfaces of solids, films, and other surface structures; other cases are also possible.

One might expect the characteristic energy (per particle) of formation of a crystal to be of the order of ηU , where U is the energy of the interaction between the nearest neighbors, and the numerical coefficient η depends on the type of the lattice and on the concrete type of interaction. Numerical calculations and experiments^{4, 6-9} have shown, however, that the temperature of the phase transition on the surface of liquid helium is lower by two orders of magnitude than the indicated value. In the present paper we wish to note that this is a general phenomenon and the quantity ηU is responsible only for the establishment of short-range order, while the energy connected with the difference between the different lattices, which properly speaking is responsible for their formation, is much lower.

That part of the energy (per particle) which is of interest to us can be obtained by expanding the potential in a Fourier series in the coordinates

$$\frac{\varepsilon}{e^{2}}S^{\nu_{n}}\Phi = 2\pi^{\nu_{n}}\int_{0}^{\infty}\frac{d\rho}{\rho^{\nu_{n}}}\left\{-1 + \frac{1}{4\pi\rho}\sum_{n,m=-\infty}^{\infty} \exp\left[-\frac{(an^{2}/b + bm^{2}/a + 2mn\cos\varphi)}{4\rho\sin\varphi}\right]\right\},$$
(1)

where e is the absolute value of the electron charge, $\overline{\epsilon} = (\epsilon_1 + \epsilon_2)/2$ is the average dielectric constant of the two media on both sides of the surface, S is the area of the unit cell of the lattice, a, b, and φ are the lengths of the vectors of the unit cell and the angle between them, Φ is the potential, and the prime on the summation sign means that the term with n = m = 0 has been left out.

The unit cell of the lattice is defined by two independent parameters, a useful choice of which is $(b/a)\sin\varphi$ $=\xi_1$ and $(b/a)\cos\varphi = \xi_2$. Investigation of the dependence of the energy on ξ_1 leads to a well known result: the lowest energy is possessed by lattices with $a \sim b$, and we shall not discuss it here. More interesting is the dependence on ξ_2 at fixed a and ξ_1 . Variation of this parameter corresponds to the gliding of one-dimensional particle chains relative to one another with the distance between the chains kept constant; this can be easily verified by noting that ξ_1 is the ratio of the distance between neighboring chains to the distance between the particles in the chain. In such motions the changes of the potential at an individual site are connected only with the changes of the oscillating parts of the potentials of the chains. Since this part of the chain potential decreases exponentially with increasing distance from the chain, the changes of the particle energy in such lattice motions should contain an additional factor $\exp(kz)$, where $k = 2\pi/a$ is the modulus of the reciprocal-lattice vector of the chain and $z = b \sin \varphi$ is the distance between the chains. This factor is small enough $(\sim 10^{-2} \text{ at})$ $\xi_1 \sim 1$), so that allowance for the influence of the chains other than the nearest ones should not change the estimate.

To prove this statement, we write down that part of the potential which is of interest to us:

$$\frac{\varepsilon}{e^2}\Phi = \frac{8}{a}\sum_{m_n=1}^{\infty} K_0(2\pi nm\xi_1)\cos(2\pi nm\xi_2), \qquad (2)$$

where K_0 is a Macdonald function.¹⁰ This expression can be represented in a simpler form, using the asymptotic representation for K_0 (Ref. 10):

$$K_{\circ}(z) = \left(\frac{\pi}{2z}\right)^{\frac{1}{2}} e^{-z} \left[1 - \frac{1}{8z}\theta\right], \quad 0 \leq \theta \leq 1,$$
(3)

$$\frac{\varepsilon}{e^2} \Phi = \frac{8}{a} \left(\frac{\pi}{2z}\right)^{\frac{1}{2}} \sum_{n,m=1}^{\infty} e^{-znm} \frac{\cos(unm)}{(nm)^{\frac{1}{2}}} \xi_{n,m}, \quad u = 2\pi\xi_2, \quad z = 2\pi\xi_1, \quad (4)$$

where $\xi_{n,m}$ are determined by using θ from (3).

The simplest estimates of $\tilde{\Phi}'_{u}$ with the aid of the formulas for the geometric progression show that

$$\Phi_u' = -A \sin u, \quad A > 0$$

at $\xi_1 \sim 1$, i.e., the sign of the derivative of $\tilde{\Phi}$ with respect to the considered parameter is determined by the nearest chains and the lowest harmonic. This phenomenon is connected with the fact that the contributions made to the potential by the higher spatial harmonics

are exponentially small [see Eqs. (3) and (4)].

We have thus shown that at $\xi_1 \sim 1$ and at fixed *a* the potential Φ decreases monotonically from a maximum to a minimum when ξ_2 is varied from zero to $\frac{1}{2}$, and by the same token [see Eq. (2)] we have completely described the dependence of Φ on ξ_2 .

At fixed b we obtain similarly $(a/b)\cos\varphi = \frac{1}{2}$ at the minimum. This leads to the known result^{2, 6-9} that the lowest energy is possessed by a regular triangular lattice.

We emphasize once more that the dependence of the energy on ξ_2 is monotonic and is of the order of smallness $\exp(-2\pi\xi_1) \sim 10^{-2}$ not only at small displacements of the particles, but also in the case of ~100% lattice deformations. This character of the dependence of the energy on ξ_2 offers evidence of instability of all but triangular lattices to the corresponding long-wave shear modes, while the fact that the dependence remains monotonic at deformations ~100% is evidence that transitions of one type of lattice to another encounter barriers that might lead to a possible coexistence of different lattices.

It follows also from the foregoing, obviously, that the Wigner-crystal production temperature cannot greatly exceed the amplitude of the considered energy oscillations, and should consequently be less than $\eta e^2/\overline{\epsilon}a$. This can be verified also directly by using the known

formula for the mean squared amplitude of the displacements of crystal particles (Ref. 11, \$137) as applied to the shear mode. Such an estimate is given, e.g., in Ref. 12.

In conclusion the author thanks I. E. Dzyaloshinskii, Sh. M. Kogan, V. B. Shikin, and B. I. Shklovskii for helpful discussions.

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Translated by J. G. Adashko