

Pinning of a two-dimensional Wigner crystal by charged impurities

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The magnitude of pinning of the classical Wigner crystal as a function of the distance between the crystal and a charged impurity is calculated numerically. The pinning magnitude is shown to be very asymmetric with respect to the sign of the impurity charge. Donors are found to pin effectively only in a narrow layer at a finite distance from the crystal, whereas acceptors pin strongly in a relatively wide region adjacent to the crystal plane. It is shown that pinning of the crystal by a close acceptor cannot be described by the conventional model of periodic coupling because at small distances the acceptor is built into the lattice.

I. INTRODUCTION

A two-dimensional (2D) Wigner crystal formed in a low-density electron system due to Coulomb repulsion between electrons was discovered first on a helium surface, where electrons have a huge effective mass so that their kinetic motion is suppressed.¹ The interest in this object was revived recently when the existence of a correlated dissipative phase in 2D heterostructures subject to a strong magnetic field at filling factors close to $\nu = \frac{1}{5}$ was observed.²⁻⁴ In this phase, the nonlinear resistance R_{xx} was shown^{3,4} to have a threshold in an external electric field, similar to depinning of the collective motion of a quasi-one-dimensional charge-density wave in Peierls conductors⁵ and of electrons on a helium film adsorbed on a dielectric surface.⁶ A two-dimensional Wigner solid was also revealed at large filling factors $\nu > 1$ in Si metal-oxide-semiconductor field-effect transistor samples with extremely high mobility.^{7,8}

Pinning by an arbitrarily small random potential is a crucial property of an electron solid. This phenomenon destroys the linear conductance at zero temperature and results in a threshold behavior of the I - V dependence. The pinning is also responsible for the loss of low-frequency oscillations in the electron crystal⁹ that was intensively studied in recent experiments on absorption of sound and rf waves in the regime of fractional quantum Hall effect.^{4,10}

The existing theories of collective pinning are based mostly on the model of white-noise random potential that implies the existence of numerous shallow potential wells. However, in real semiconductor structures the most likely candidates for a pinning center are charged impurities (donors and acceptors) for which this approach may be inadequate. These centers are, generally, of two types: the distant ones introduced intentionally into the material (dopants) and the residual impurities which are small in number but can be situated close to the electron plane. The first type creates a long-range random potential which can, if it is strong enough, break the electron system into separate regions.^{11,12} However, the magnitude of this potential can be significantly suppressed by screen-

ing effects of a close metallic gate and of the 2D electron system itself. The last mechanism of screening is especially effective when the spatial scale of the potential which is equal to the distance between 2D electrons and remote dopants (spacer width) is much larger than the interelectron distance. In this work we consider the case when the screening effects are strong, and the electron density is almost uniform. We show that, in this situation, the remote dopants are extremely ineffective for pinning: the magnitude of the pinning potential is exponentially smaller than that of the one-electron random potential. Hence we concentrate on pinning of the classical Wigner crystal by residual impurities situated in the spacer.

Our goal is to find out at which distance a donor and an acceptor are most effective for pinning. This issue is not trivial because of a crucial role of the crystal deformation in the vicinity of the impurity. In Sec. II, we study a charged impurity at a distance $d \gg a$ from the electron plane, where a is the Wigner lattice constant. The height of the pinning barrier V_p is shown to be proportional to the small exponential $\exp(-4\pi d/\sqrt{3}a)$. This results from the fact that potential of such an impurity in the electron plane is smooth and has a large spatial scale.

The opposite case of a very close impurity is considered in Sec. III. The ground state of the crystal with a close donor differs from that with a distant donor. At large d , the donor is situated opposite to the site of lattice which is elastically deformed around it. At small distances, the donor binds an electron, and the resulting dipole favors an interstitial position and weakly interacts with the rest of electrons. As a result of such strongly nonlinear screening, the pinning energy V_p is small and vanishes when d tends to zero. An analogous transformation happens with an acceptor: it favors an interstitial at large d , while at small d it is built into the electron lattice. In contrast to the donor, pinning by acceptor at $d \rightarrow 0$ is strong.

In order to find where the transition between the two ground states occurs for both types of impurities and to study the pinning barrier V_p in the whole range of d , we

carried out a numerical simulation described in Sec. IV. We find that the transition points are $d=0.45a$ for the donor and $d=0.63a$ for the acceptor, respectively. A noticeable pinning by donor exists only in the narrow region above the transition, $d=(0.5-0.6)a$. The acceptor pins strongly everywhere in the small- d phase, $d<0.63a$, and the pinning energy V_p is one order of magnitude larger than that for the donor. Thus the interaction of the electron solid with charged impurities turns out to be highly asymmetric with respect to the charge. This is caused by the strongly nonlinear nature of the screening and is in contrast to an identical role played by impurities of opposite signs in the mobility of the electron gas. In addition, the pinning energy V_p (for either kind of impurities) and the cross section of scattering in the gas depend differently on the impurity distance d , so that different groups of impurities may dominate pinning of the crystal and the electron mobility in the gas.

The main observable characteristics of the pinning by many randomly situated impurities are the correlation length ξ_c and the threshold electric field E_{th} . The former represents the scale at which the long-range order in the crystal disappears; it can be found in experiments on sound absorption from the characteristic pinning frequency.¹⁰ The quantity E_{th} manifests itself in the I - V measurements as a critical field at which depinning occurs, and the crystal begins to slide. Specific expressions for both parameters depend on the pinning regime. In the strong pinning case, the crystal is relatively soft and adjusts its phase to each impurity position, ξ_c being of the order of interimpurity distance $n_i^{-1/2}$. In the weak pinning regime, the crystal is relatively rigid, and $\xi_c \gg n_i^{-1/2}$. As shown in Sec. V for a homogeneous distribution of impurities in the spacer, acceptors always create a strong pinning, whereas donors, depending on their concentration, provide a strong or intermediate one. Estimates for ξ_c and E_{th} are given for both types of impurities assuming the strong pinning limit.

II. A DISTANT CHARGED CENTER

Consider the triangular lattice of the classical Wigner crystal placed in a plane with the 2D coordinate \mathbf{r} . Suppose the lattice interacts with a positively charged impurity (donor) which creates for each electron in the plane the Coulomb potential

$$U(\mathbf{r}) = -\frac{e^2}{\kappa(r^2 + d^2)^{1/2}}, \quad (1)$$

where κ is the dielectric constant and d is the distance between the impurity and plane. In this section we dwell on the case when $d \gg a$, where a is the lattice constant.

If the donor is shifted on distance \mathbf{s} along the plane, its energy $V(\mathbf{s})$ will change periodically in \mathbf{s} with the lattice period. First, we shall calculate the dependence $V(\mathbf{s})$ in the approach of an absolutely rigid crystal. In this case $V(\mathbf{s})$ is given by the sum over all the lattice sites

$$V(\mathbf{s}) = \sum_{m,n} U(\mathbf{r}_{mn} - \mathbf{s}), \quad (2)$$

$$\mathbf{r}_{mn} = m \mathbf{a}_1 + n \mathbf{a}_2, \quad (3)$$

where the vectors

$$\mathbf{a}_1 = a \mathbf{e}_x, \quad \mathbf{a}_2 = \frac{a}{2} \mathbf{e}_x + \frac{\sqrt{3}a}{2} \mathbf{e}_y \quad (4)$$

are the basis of the triangular lattice. The sum (2) has the translational symmetry of the crystal and can be expanded in the Fourier series

$$V(\mathbf{s}) = \frac{1}{|\mathbf{a}_1 \times \mathbf{a}_2|} \sum_{\mathbf{p}} U_{\mathbf{p}} e^{i\mathbf{p} \cdot \mathbf{s}}, \quad (5)$$

where the sum is evaluated over all the vectors \mathbf{p} of the reciprocal lattice, and

$$U_{\mathbf{p}} = \int d^2r e^{i\mathbf{p} \cdot \mathbf{r}} U(\mathbf{r}) \quad (6)$$

is the Fourier transform of the donor potential. The value of $U_{\mathbf{p}}$ decreases exponentially with increasing $|\mathbf{p}|$ as given by

$$U_{\mathbf{p}} = -\frac{2\pi e^2}{\kappa p} e^{-pd}. \quad (7)$$

Hence, at $d \gg a$, the sum (5) is dominated by terms with the minimal modulus $|\mathbf{p}| = 4\pi/\sqrt{3}a$ (as one can show, the contribution from higher harmonics is less than 0.5% even at $d=a$). There are six of these terms: $\pm \mathbf{p}_1$, $\pm \mathbf{p}_2$, and $\pm(\mathbf{p}_1 - \mathbf{p}_2)$, where

$$\mathbf{p}_1 = \frac{2\pi}{a} \left[\mathbf{e}_x + \frac{1}{\sqrt{3}} \mathbf{e}_y \right], \quad \mathbf{p}_2 = \frac{4\pi}{\sqrt{3}a} \mathbf{e}_y \quad (8)$$

represent basis of the reciprocal lattice. We can also omit in Eq. (5) the term with $\mathbf{p}=0$ which does not depend on \mathbf{s} and is irrelevant for the pinning. As a result, we get

$$V(\mathbf{s}) = \frac{4}{\sqrt{3}a^2} U_{\mathbf{p}} \{ \cos(\mathbf{p}_1 \mathbf{s}) + \cos(\mathbf{p}_2 \mathbf{s}) + \cos[(\mathbf{p}_1 - \mathbf{p}_2) \mathbf{s}] \}. \quad (9)$$

The potential energy (9) is minimum at a site of electron lattice $\mathbf{s}=0$, is maximum at the triangle center $\mathbf{s}=\mathbf{s}_t=(a/2, a/2\sqrt{3})$, and has a saddle point at the middle of the triangle edge $\mathbf{s}=\mathbf{s}_e=(a/2, 0)$. At these points the cosine sum in (9) is equal to 3, $-\frac{3}{2}$, and -1 , respectively. The height V_r of the barrier separating two adjacent potential minima is given by the difference

$$V_r = V(\mathbf{s}_e) - V(0) = \frac{16}{\sqrt{3}a^2} |U_{\mathbf{p}}|. \quad (10)$$

After substitution of Eq. (7) with $|\mathbf{p}| = 4\pi/\sqrt{3}a$ into (10), for the rigid crystal, we get

$$V_r = \frac{8e^2}{\kappa a} \exp \left[-\frac{4\pi d}{\sqrt{3}a} \right]. \quad (11)$$

We see that the pinning energy V_r turns out, at $d \gtrsim a$, to be much smaller than the magnitude of original potential $e^2/\kappa d$.

The pinning barrier for the negatively charged center (acceptor) can be obtained in the same way. Changing the sign of the Fourier transform $U_{\mathbf{p}}$ in Eq. (9), we find the minimum of the pinning potential at the triangle

center $\mathbf{s}=\mathbf{s}_r$, the maximum at the lattice site $\mathbf{s}=0$, and the saddle point, as for the donor, at the edge center $\mathbf{s}=\mathbf{s}_e$. As a result, the pinning barrier for the acceptor is given by

$$V_r = V(\mathbf{s}_e) - V(\mathbf{s}_r) = \frac{e^2}{\kappa a} \exp \left[-\frac{4\pi d}{\sqrt{3}a} \right] \quad (12)$$

and is eight times less than that for the donor [Eq. (11)]. Note that this asymmetry of the pinning potential with respect to the impurity charge even at large distances d exists only for the triangular and honeycomb lattices of electrons: sites and interstitial points in either of them (which correspond to minima and maxima of the potential) form different lattices and are, in the geometrical sense, not equivalent.

We have obtained expressions (11) and (12) for the pinning energy in the approximation of the rigid crystal. In fact, the crystal area near the impurity is always deformed since electrons tend to screen the impurity potential. In order to take into account this deformation one has to replace Eq. (2) by

$$V(\mathbf{s}) = \sum_{m,n} U(\mathbf{r}_{mn} + \mathbf{u}_{mn} - \mathbf{s}), \quad (13)$$

where \mathbf{u}_{mn} is the displacement of electron at the site (m,n) . When the charge center is far enough from the plane, the local displacement of the crystal can be treated in a continuous approximation. This assumes that \mathbf{u}_{mn} is a continuous function of the distance between the site and the center projection on the plane, as given by

$$\mathbf{u}_{mn} = \mathbf{u}(|\mathbf{r}_{mn} - \mathbf{s}|). \quad (14)$$

In this approximation the sum (13) takes a form (2) with the renormalized potential

$$U^*(\mathbf{r}) = -\frac{e^2}{\kappa \{[\mathbf{r} + \mathbf{u}(\mathbf{r})]^2 + d^2\}^{1/2}}, \quad (15)$$

instead of original potential (1). As a result, we arrive at formulas (11) and (12) for the pinning energy, where the Fourier transform (7) should be evaluated for the new potential $U^*(\mathbf{r})$. The sign of the effect of deformation on the pinning can be easily predicted even without this evaluation. For the donor, electrons are attracted to the center, so that $\mathbf{u}(\mathbf{r}) = -(\mathbf{r}/r)\mathbf{u}(r)$. As a result, the effective potential (15) is wider than the incipient potential (1); magnitudes of its Fourier components with large p should be less than that given by Eq. (7). Hence the deformation of the lattice should diminish the pinning by the donor (and, correspondingly, should enhance that by the acceptor).

At large spatial scales $d \gg a$ the long-range Coulomb forces dominate the equilibrium of the deformed lattice, and the existence of the crystal structure plays a minor role. Hence the displacement $\mathbf{u}(\mathbf{r})$ can be found for $d \gg a$ in the "metal surface" approximation in which

$$\text{div} \mathbf{u} = -\frac{\sqrt{3}a^2}{2} n(r), \quad (16)$$

where $n(r)$ is the electron concentration on a conducting

surface induced by a point charge. The surface charge density $en(r)$ can be found from the normal electric field near the conducting surface, as given by

$$\frac{4\pi e^2}{\kappa} n(r) = \pm \frac{d}{dz} \left[\frac{2e^2}{\kappa(r^2 + z^2)^{1/2}} \right]_{z=d}, \quad (17)$$

where plus and minus correspond to the acceptor and donor, respectively. The function $\mathbf{u}(\mathbf{r})$ can be found from Eqs. (16) and (17):

$$\mathbf{u}(\mathbf{r}) = -\frac{\mathbf{r}}{r} u(r) = \pm \frac{\mathbf{r}}{r} \frac{\sqrt{3}a^2 d}{4\pi r} \left[\frac{1}{d} - \frac{1}{(r^2 + d^2)^{1/2}} \right]. \quad (18)$$

At $d \gg a$ and $pd \gg 1$, the Fourier transform (6) of the potential $U(\mathbf{r})$ defined by Eqs. (15) and (18) has a form

$$U_p^* = -\frac{2\pi e^2 d}{\kappa} e^{-pd} \left[\frac{1}{pd} \pm \frac{1}{8} \left[\frac{a}{d} \right]^2 \left[\frac{3pd}{2\pi} \right]^{1/2} \right], \quad (19)$$

where the second term in brackets is assumed to be much smaller than the first one. Comparison of Eqs. (7) and (19) with $p = 4\pi/\sqrt{3}a$ yields for the pinning barrier V_p

$$V_p = V_r \left[1 \pm \pi \left[\frac{a}{2\sqrt{3}d} \right]^{1/2} \right], \quad (20)$$

where plus stands for the acceptor and minus for the donor. The value V_r is given by Eqs. (12) and (11) for the donor and acceptor, respectively.

Thus the deformation of the lattice by the impurity changes only the prefactor in the V_p vs d dependence not affecting the exponential term. In the limit of large d , the deformation effects become small, and the pinning energy tends to its value V_r obtained for the rigid crystal. On the other hand, the deformation changes V_p by the order of itself already at $d \sim (3-6)a$, where V_p is still exponentially small. We can conclude that in the region of $d \lesssim a$ where a noticeable pinning can exist, the deformation effects are of a crucial importance for the pinning magnitude. Since, in this region, the screening of impurity by electrons should be essentially nonlinear, numerical calculations of the V_p vs d dependence are necessary. Before presenting results of our computation in the region of intermediate d , we consider in the next section another limit $d \ll a$ which also allows an analytical treatment (at least, for the donor). This will also permit us to make important qualitative conclusions about the form of the $V_p(d)$ dependence at the intermediate d .

III. VERY CLOSE IMPURITY

When the charged impurity is situated sufficiently close to the crystal plane, the ground state of the system "impurity-crystal" differs essentially from that with a distant impurity. As we have seen in the preceding section, the ground-state position of a distant donor is against some site of the lattice symmetrically deformed around this site. At very small distances d , the donor traps an electron forming a stable dipole perpendicular to the plane of the crystal. The rest of electrons rearrange forming a triangular lattice with the dipole situated in a

most favorable position (triangle center). In order to demonstrate that this small- d phase will be the true ground state of the system, let us consider the situation of electrons in both competing states at very small d . In the small- d phase, the electrons other than that bound by the donor form an almost perfect triangular lattice since its distortion by the short dipole donor electron is negligible. In the large- d phase, the charge of one of the electrons at the lattice site is almost entirely compensated by the donor charge, the rest of electrons forming the vacancy configuration. Since the interaction between the dipole "donor electron" and the surrounding electrons in both cases is negligible, at small d the difference in energy between the large- d and small- d phase is equal to the energy of the vacancy formation in the Wigner crystal and is, of course, positive. Thus, at some finite d , the abrupt transition of the ground state from the large- d to small- d phase takes place. As easy to see, this phase transition should be a "first-order" one because one phase cannot be obtained from another by a continuous deformation.

The pinning energy in which we are interested is associated with the interaction between the dipole and the triangular electron lattice and, hence, should be weak in the reformed phase. When the dipole is shifted in the plane by \mathbf{s} , its energy changes as

$$V(\mathbf{s}) = \frac{ed^2}{2} D(\mathbf{s}), \quad (21)$$

where

$$D(\mathbf{s}) = -\frac{\partial^2 \varphi}{\partial z^2} = \frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} \quad (22)$$

is the normal second derivative of the lattice potential φ . The pinning barrier V_p is then given by

$$V_p = \frac{ed^2}{2} [D(\mathbf{s}_e) - D(\mathbf{s}_t)], \quad (23)$$

where the middle of the triangle edge \mathbf{s}_e and the center of triangle \mathbf{s}_t are the saddle point and the ground-state position, respectively. Hence, at small d , the interaction between the dipole and the lattice is weak, and distortions of the lattice caused by this interaction are negligible. In the perfect lattice, the values of the two-dimensional Laplacian (22) $D(\mathbf{s}_t)$ and $D(\mathbf{s}_e)$ can be related to that at the lattice site $D_0 = 8.89en^{3/2}/\kappa$, where n is the concentration of electrons in the lattice, as given by

$$D_t = \frac{3^{3/2} - 1}{2} D_0, \quad (24a)$$

$$D_e = \frac{1}{3} D_0. \quad (24b)$$

[As it has been shown in Ref. 13, the lattice potentials at points \mathbf{s}_t and \mathbf{s}_e can be related to the Madelung constant $|\varphi_0|$ by means of an exact renormalization procedure. Equations (24) are obtained by the same method.] After the substitution of Eqs. (24) into Eq. (23), for the asymptotic of pinning energy at small d we get

$$V_p = 1.08 \frac{e^2 n^{3/2}}{\kappa} d^2. \quad (25)$$

Analogous change of the ground-state configuration should take place for the acceptor too. At large d , the latter is situated against an interstitial position, the lattice of electrons being elastically deformed around it. At small d , the acceptor is built into the lattice playing a role of one of the lattice sites. Corresponding gain in energy due to this reconstruction of the lattice is obviously equal, at $d=0$, to the energy of interstitial. As for the pinning energy by the acceptor in the small- d phase, it is difficult to define this parameter in a quantitative way. The potential of the acceptor-lattice interaction does not have in this case a translational symmetry, and the definition of V_p as a height of the barrier between two equivalent minima of the pinning potential which we use for the donor (and for the acceptor at large d) becomes meaningless. Below we shall characterize the pinning in this phase by the energy increase at a small displacement of the acceptor from its equilibrium position, i.e., by the effective "Hook constant" of the acceptor-lattice coupling k_p . In the energy scale, the latter can be conveniently written as the energy $V_p = k_p a^2 / 8$ which corresponds to the acceptor displacement by a half of the lattice constant. Although $V_p(d)$ is hard to find analytically even at smallest d , it is clearly finite at $d=0$ and has a parabolic maximum at this point. The typical values of V_p in the small- d phase should be obviously much larger than that in the large- d phase where V_p is given by the energy required to move an additional charge from one interstitial position to another. This energy at $d=0$, according to numerical calculations in Ref. 14, is as small as $0.003e^2/\kappa a$.

We conclude that the lattice reconstruction which takes place at small d drastically affects the shape of the $V_p(d)$ dependence for both types of impurities, although in entirely different ways. Either of the dependences should have an abrupt step at the value of d where this "phase transition" occurs. In the case of acceptor, the pinning should be stronger in the small- d phase, whereas for the donor it is weak both at small and large d . Hence, for the donor, $V_p(d)$ is expected to reach its maximum in the intermediate region of d just above the transition point. These predictions, we shall see in the next section, agree with the results of numerical calculations.

IV. NUMERICAL CALCULATIONS

In this section we study numerically pinning of the Wigner crystal by charged impurities. We simulated an infinite triangular lattice of electrons in which only the electrons inside a rectangle with sides $(m-1)a$ by $ma\sqrt{3}/2$, where m is an even integer, were allowed to move. The energy of electron-electron interaction was calculated in the following way. The potential of mobile electrons and of a part of the immobile ones (including those forming the boundary of the rectangle) was calculated exactly as the sum of corresponding Coulomb terms. The part of the positive background formed by hexagonal Wigner-Seitz cells around these electrons was also taken into account explicitly. The rest of the crystal was treated as a triangular lattice of quadrupoles.

In order to study pinning effects we placed a charged

impurity at a given distance d from the plane of the crystal. The interaction between the impurity and an electron with coordinate \mathbf{r} is given by Eq. (1). The lowest-energy configuration for a fixed impurity position was obtained by relaxing the mobile electrons in an effective viscous fluid.

As mentioned in the preceding section, the ground-state configuration of the electrons differs at small and large impurity distances d . We discuss, first, how to find the transition point d_{tr} for a donor. The energy E_1 of the large- d phase, which should be favorable at large distances, was evaluated as a function of d for the donor placed opposite to the lattice site at the center of the system. We obtained the small- d phase by adding to the system an electron at an interstitial and placing the donor opposite to it. After this, the system was allowed to relax, and its energy E_2 was calculated. It turns out that both phases are stable and coexist in a wide range of distances d . The transition point d_{tr} was determined from the equation

$$E_1(d_{tr}) = E_2(d_{tr}) - \xi, \quad (26)$$

where $\xi = -3\alpha_M/4$ is the chemical potential of the Wigner crystal, $\alpha_M = 3.921$ is the Madelung constant. (All the energies and distances in this section are given in units of $e^2 n^{1/2}/\kappa$ and $n^{-1/2}$, respectively.) The chemical potential μ in the right-hand side of Eq. (26) reflects the fact that the total number of electrons in both competing phases should be the same for the infinite system.

To take into account size effects we calculated the difference $\Delta E(d, m) = E_1(d, m) - E_2(d, m)$ at four sizes of the system ($m = 8, 10, 12, 14$) and extrapolated it to $m = \infty$ by means of

$$\Delta E(d, m) = \Delta E(d, \infty) + \beta(d)/m. \quad (27)$$

The use of this equation can be justified by noting that the main size corrections arise from the fixed boundary conditions. After the electrons move towards the donor in order to screen it, the rest of the lattice acquires a unit charge. This results in an additional Coulomb energy inversely proportional to the system size, as given by Eq. (27). The actual size dependence of ΔE agrees very well with this formula. The transition point found by the size extrapolation is $d_{tr} = 0.48$.

At a given distance d , we calculated the energy of the system shifting the donor parallel to the plane of the lattice. The pinning energy V_p was calculated as the energy difference between the ground-state position (site for the large- d phase and interstitial for the small- d one) and the saddle point which is situated in both phases at the middle of the triangle side. We note that the size effects discussed above, when the energy of the two phases was compared, turn out to be very small for the pinning energy V_p in either phase: we did not observe any change in V_p for lattice sizes $m = 10$ and 14 . This is so because V_p is determined by the *difference* in energy between two close donor positions at the center of the system. Hence the size correction is canceled out.

The resulting dependence $V_p(d)$ is shown in Fig. 1(a). The function $V_p(d)$ has an abrupt step at the transition

point $d = d_{tr} = 0.48$. At larger values of d , it decays exponentially with the distance, in accordance with prediction of Sec. II. At the smallest d , the pinning energy vanishes as $V_p \propto d^2$, as given by the asymptotic (25). However, the region of parabolic dependence (25) is very narrow ($d \lesssim 0.04$) because at larger d the displacements of neighboring electrons repelling from the stable dipole "donor electron," which were not taken into account in the derivation of Eq. (25), become important. The height of the pinning barrier turns out to be much smaller than its asymptotic value [dashed curve in Fig. 1(a)] because it is much easier to shift two neighboring electrons for the saddle-point position of the dipole than three electrons in the ground-state configuration. Therefore the deformation lowers the energy more effectively in the saddle point than it does in the ground state. As a result, the energy difference V_p between these two points begins to decrease starting from $d \simeq 0.14$ and changes its sign at $d = 0.29$

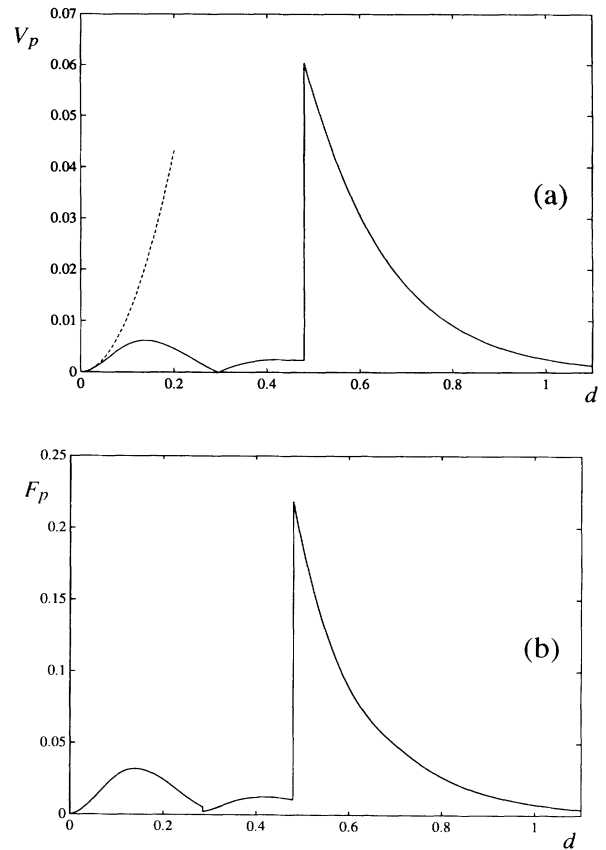


FIG. 1. (a) Pinning energy V_p as a function of the distance d between a donor and the Wigner crystal plane with 77 mobile electrons ($m = 10$). Energy and distance are given in units of $e^2 n^{1/2}/\kappa$ and $n^{-1/2}$, respectively. Dashed curve shows the asymptotic in the limit of small d [Eq. (25)]. The abrupt step at $d = 0.48$ is caused by the change of the ground-state configuration of the system donor crystal (Sec. III). (b) Maximum coupling force F_p for a donor as a function of the distance d for $m = 10$. The maximum force was found along the line connecting two neighboring lattice sites for the large- d phase ($d > 0.48$), and along the line connecting the center of a triangle and the middle point of its edge for the small- d phase ($d < 0.48$).

[this appears as a cusp in Fig. 1(a) where the absolute value of V_p is plotted]. At this value of d , these two dipole positions become equal in energy, and the pinning is determined by a small barrier between them. Therefore the complete vanishing of the pinning energy at $d=0.29$ in Fig. 1(a) is an artifact of our definition of V_p : in the close vicinity of this point V_p does not characterize the actual pinning barrier.

In addition to the height of the pinning barrier V_p , we also studied another important characteristic, namely, the maximum pinning force F_p shown in Fig. 1(b) as a function of d . This quantity is related to the threshold value of an external electrical field at which depinning of the crystal occurs. We calculated F_p as a maximum gradient of the energy when the donor is adiabatically shifted parallel to the plane along the easiest path connecting two equivalent ground-state positions. For $d > 0.48$ (or $d < 0.29$) this path is the line connecting two lattice sites (or centers of adjacent triangles). In the interval $0.29 < d < 0.48$ the ground state of the dipole donor electron is at a triangle edge center, and the easiest path is a curve connecting two adjacent ground states. The middle point of this curve is very close to the center of the triangle. Moreover, in the finite interval of d at $d > 0.29$ where the triangle center remains a local minimum of the energy, this curve degenerates to a broken line with two segments going through the triangle center. For this reason, in the entire interval $0.29 < d < 0.48$, we calculated the maximum pinning force along the line connecting edge and triangle centers. The step in F_p at $d=0.29$ appears because the path of the donor reverses its direction at this point: it is from the edge to the triangle center at $d > 0.29$, and from the center to the edge at $d < 0.29$. The values of F_p at both sides of the step result from different slopes of a small barrier existing between these two equienergetic positions.

Apart from the peculiarity at $d=0.29$, the dependence $F_p(d)$ is almost identical to $V_p(d)$ in the whole range of donor-crystal distances d [Figs. 1(a) and 1(b)]. This suggests that, at least for $d > 0.48$, the profile of the pinning potential (unlike its magnitude) depends very weakly on d . Hence this profile should be close to the simple form given by Eq. (9), which was obtained for very large d and predicts the energy change

$$V(s) = \frac{V_p}{2} \cos \frac{2\pi s}{a} \quad (28)$$

when the donor is shifted by a distance s along the line connecting two lattice sites. To check this point we calculated the ratio F_p/V_p for $d > 0.48$, which varies in the interval 2.9–3.5. This is close to the value $F_p = \pi V_p/a = 2.9 V_p$ derived from Eq. (28). In the small- d phase, $d < 0.48$, the overall pinning profile certainly cannot be approximated by Eq. (9) because its minima form a honeycomb lattice in contrast to the triangular lattice symmetry of Eq. (9). We find, however, that, at least at $d < 0.25$, the ratio F_p/V_p is also almost constant and equals to 5. This is very close to the value given by Eq. (28) if one replaces a by $a/\sqrt{3}$, which, in this regime, is the distance between adjacent ground-state positions

(triangle centers).

An analogous computation was done for an acceptor. In this case, the transition between the large- and small- d phases, described in Sec. III, takes place at $d=0.68$. In the large- d phase, we defined the pinning energy V_p in the same way as for the donor: the barrier height between two adjacent equivalent ground-state positions. Here the ground state is reached when the acceptor is against a triangle center. For $d < 0.68$, this is not appropriate because the acceptor is built into the lattice, and the pinning potential is not periodic. Instead, we calculated the Hook constant k_p of the acceptor-lattice coupling at small displacements of the acceptor from the potential minimum (k_p does not depend on the displacement direction due to hexagonal symmetry). We define the characteristic pinning energy as $V_p = k_p a^2/8$.

The entire V_p vs d dependence is shown in Fig. 2(a) for different sizes of the system. As we expected, the pinning in the large- d phase is very weak. In contrast, at small values of d , the pinning energy V_p is large. Another feature of the small- d phase is a very strong size effect. Unlike the large- d phase, where the size corrections become small already at $m \geq 10$, this size effect never disappears when the system is enlarged. The reason for that is a finite elasticity of the electron lattice which is deformed as a whole when the acceptor is shifted by a small distance from a lattice site. The lattice deformability can be estimated as the Hook constant k_l of an elastic film with a size $R = am$, when a force is applied at its center in a small region of order of the lattice constant a . The value of k_l is given by (see Appendix)

$$k_l = \frac{4\pi\mu}{\ln(\gamma R/a)}, \quad (29)$$

where μ is the shear modulus of the film [for the Wigner crystal, $\mu=0.245$ (Ref. 15)], and $\gamma \sim 1$ is a numerical coefficient which can vary depending on the shape of the film and details of the force distribution. To find the size dependence $V_p(m) = k_p(m)a^2/8$, we model the system by two springs connected in series: one with a constant $k_l(m)$ and the other with a constant k_{p0} , which describes the local interaction of the acceptor with neighboring electrons and does not depend on m . Using Eq. (29) with $\gamma = 1$, we obtain

$$\frac{1}{V_p(m,d)} = \frac{1}{V_{p0}(d)} + \frac{2}{\pi\mu a^2} \ln m. \quad (30)$$

The dependences $1/V_p$ vs $\ln m$ found in our simulation for different d are shown in Fig. 2(b). All of them perfectly fit straight lines with the slope calculated from Eq. (30). Unfortunately, the dependence $V_{p0}(d)$, which can be found by this fitting, does not have an exact meaning because it depends on our choice of the numerical coefficient γ in the argument of the logarithm which we put to be 1.

Note that this problem with lattice elasticity does not appear for the donor nor for the acceptor at large d . Indeed, in these two cases, the interaction energy was calculated only for the impurity situated against symmetry points of the lattice, the net force acting on the lattice be-

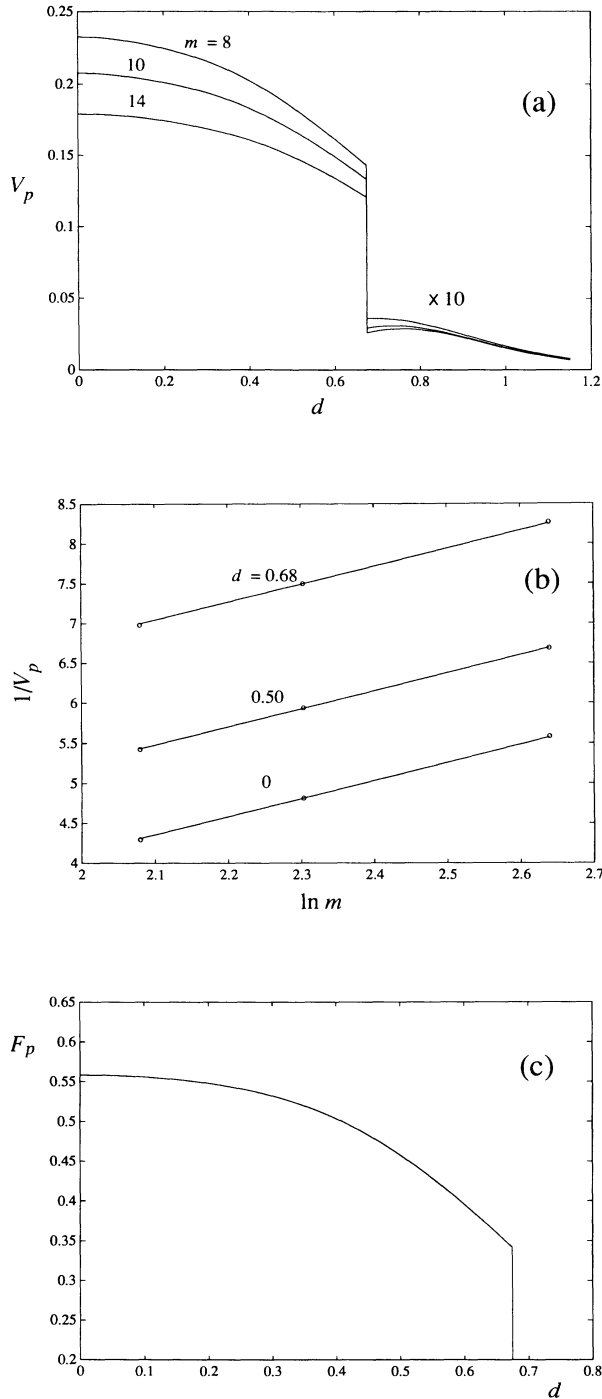


FIG. 2. (a) Pinning energy V_p for an acceptor as a function of the distance d from the crystal plane for sizes $m=8, 10,$ and 14 . The abrupt step at $d=0.68$ reflects the transition from the large- d to the small- d phase. At $d < 0.68$, V_p is defined by $V_p = k_p a^2 / 8$, where k_p is the effective Hook constant of the system for small displacements of the acceptor from a lattice site. At $d > 0.68$, the actual values of V_p are multiplied by 10. (b) Size dependence of V_p for an acceptor at three different values of d . Results of numerical calculations are shown by circles. The slope of the lines is calculated using Eq. (30), their absolute positions are found by a trivial fit to the numerical results. (c) Maximum coupling force F_p of an acceptor at distances $d < 0.68$ for a lattice size $m=12$ (115 mobile electrons).

ing equal to zero.

In order to find the maximum pinning force F_p for the acceptor at $d < 0.68$, we moved it adiabatically from its site along the easiest direction, which is the bisector of a lattice triangle, and calculated the force acting on it. The force as a function of the acceptor coordinate has a maximum, which we define to be the value of F_p , and then changes its sign twice. The second zero corresponds to a local potential minimum which appears after the acceptor passes between two electrons neighboring to its initial position. This metastable state represents a short pair interstitial vacancy. If one continues to move the acceptor, increasing the pair length, new potential barriers appear. However, they are not important because the corresponding forces are smaller than F_p . (We note that our adiabatic procedure permits one only to find the maximum external force acting on acceptor at which equilibrium is still maintained and cannot describe the dynamics if this maximum is exceeded.) The resulting dependence $F_p(d)$ for the small- d phase is shown in Fig. 2(c). Though the acceptor coordinate at which the force is maximum varies with the system size, the corresponding value F_p is practically size independent at $m \geq 10$. This shows that the maximum coupling force F_p is an intrinsic characteristic and is determined by the local interaction of the acceptor with neighboring electrons.

V. PINNING BY MANY IMPURITIES

The pinning strength of a single charged impurity studied in preceding sections permits one, in principle, to predict properties of the Wigner crystal pinned by many random impurities. The main observable parameters are the threshold electrical field E_{th} , at which depinning of the crystal occurs, and the static correlation length ξ_c . The latter represents the spatial scale where both the long-range order and the translational symmetry are broken. This manifests itself in the low-frequency oscillation spectrum of the crystal as a characteristic pinning frequency⁶ $\omega_p = \pi s / \xi_c$, where s is the sound velocity of the acoustic mode. Below we shall estimate ξ_c and E_{th} for donors and acceptors in a model where they are uniformly distributed in the space near the plane of the crystal.

In order to express ξ_c and E_{th} in terms of the pinning potential of a single impurity one should know, first of all, the pinning regime. If the crystal is soft with respect to the pinning strength of an individual impurity, it will adjust its local phase to the position of *each* impurity, so that $\xi_c \sim n_i^{-1/2}$, where n_i is the 2D impurity concentration (the strong pinning limit). If the crystal is, on the contrary, rigid enough, the long-range order will be broken at much larger distances: $\xi_c \gg n_i^{-1/2}$ (the weak pinning limit). In order to find a criterion for strong pinning we estimate the deformation energy per impurity and compare it to the pinning energies calculated in the previous section.

Consider *strong* (attracting) pinning centers distributed randomly with a concentration n_i in a δ -doped layer at some distance d from the plane of the crystal. In equilibrium, one of the lattice sites in the neighborhood of each

impurity will be displaced in order to coincide with the impurity projection in the plane. The deformation energy of the crystal per impurity ϵ_{def} is given by

$$\epsilon_{\text{def}} = k \langle \mathbf{u}_m^2 \rangle / 2, \quad (31)$$

where k is the effective Hook constant of a region with size of the order of $n_i^{-1/2}$, and $\langle \mathbf{u}_m^2 \rangle$ is the mean-square crystal displacement near the m th impurity. The Hook constant k is given by Eq. (29) with $\mu = 0.245e^2n^{3/2}/\kappa$.¹⁵ Note that details of boundary conditions, such as fluctuations of the effective film radius R from one impurity to another around the value $n_i^{-1/2}$, affect only the coefficient γ in the argument of the logarithm in Eq. (29) which is assumed to be large: $n_i a^2 \ll 1$ (below we put $\gamma = 1$). Next, we find the averaged square displacement $\langle \mathbf{u}_m^2 \rangle$ assuming that the deformed ground state in the presence of impurities is reached by making each impurity coincide with the site which was *closest* to it in the undeformed state. In this approximation, all \mathbf{u}_m are independent and randomly distributed within the Wigner-Seitz cell of the lattice; this yields

$$\langle \mathbf{u}_m^2 \rangle = \frac{5a^2}{36} = \frac{5}{18\sqrt{3}n}, \quad (32)$$

where n is the electron concentration in the lattice. Substituting Eqs. (31), (32), and the shear modulus μ into Eq. (29) yields

$$\epsilon_{\text{def}} = \frac{0.25}{\ln(R/a)} \frac{e^2 n^{1/2}}{\kappa}. \quad (33)$$

For reasonable values $R/a = 10-1000$, this formula gives $\epsilon_{\text{def}} = (0.11-0.036)e^2 n^{1/2}/\kappa$. As we have seen in the preceding section, the height of the pinning barrier V_p for donors peaks at the distance $d = 0.48n^{-1/2}$ between the δ -doped layer and the crystal, where $V_p = 0.06e^2 n^{1/2}/\kappa$. Thus, at $d \approx 0.5n^{-1/2}$, both energies ϵ_{def} and V_p are of the same order, and we are in the intermediate pinning regime. Nevertheless, the strong pinning seems to be a better description in this case, because the weak pinning approach makes sense only if the *strong* inequality $V_p \ll \epsilon_{\text{def}}$ is satisfied. The last condition can be met, of course, for other values of d where pinning is much weaker. Formula (33) is valid also for acceptors at $d < 0.68n^{-1/2}$, when they substitute electrons in lattice sites (cf. Secs. III and IV). Obviously, acceptors in this case provide strong pinning (and very weak pinning at larger d). The best indication of that is a strong size effect of the energy change at small displacements of an acceptor from a lattice site (see Fig. 2). This shows that even at small sizes the crystal is soft in comparison with the strength of the acceptor-lattice coupling.

Suppose now that acceptors and donors are randomly distributed above the plane of the crystal with 3D concentrations N_A and N_D , respectively. As shown in Figs. 2(a) and 1(a), the pinning is dominated by acceptors at distances $d < 0.68n^{-1/2}$ and by donors at $d \approx 0.5n^{-1/2}$. The correlation length is given by the effective interimpurity distance R :

$$\xi_c \sim R = (n_A + n_D)^{-1/2},$$

where $n_{A,D}$ is the effective 2D concentration of corresponding impurities. For acceptors, the latter is equal to $n_A = 0.68n^{-1/2}N_A$; for donors, it can be roughly estimated as $n_D = 0.1n^{-1/2}N_D$, where $0.1n^{-1/2}$ is the half width of the peak in Fig. 1(a).¹⁶

Consider now the threshold electric field E_{th} at which the static equilibrium disappears and the crystal begins to slide as a whole. In the strong pinning regime when deformation effects are small, E_{th} can be estimated as

$$E_{\text{th}} = \frac{F_p n_i}{en}, \quad (34)$$

where n_i is the 2D concentration of impurities (we return here, for a while, to a δ -doped layer of equivalent impurities). We assumed here that at the threshold *each* impurity acts on the crystal with its maximum coupling force F_p , and therefore Eq. (34) is an upper bound for the threshold field. An analogous formula can be written for donors uniformly distributed in space with a concentration N_D :

$$E_{\text{th}} = \frac{N_D}{en} \int F_p(d) dd = 0.1 \frac{eN_D}{\kappa n^{1/2}}, \quad (35)$$

where the dependence $F_p(d)$ is shown in Fig. 1(b).

Although acceptors at $d < 0.68n^{-1/2}$ are definitely strong pinning centers, the estimate given by the first equality in Eq. (35) cannot be used for them. In an infinite system, the threshold field for the acceptors is smaller than this value by at least two orders of magnitude. The reason is that the potential of coupling between the lattice and built-in acceptors is not periodic. After an acceptor is forced to leave the lattice site (leaving a vacancy behind), it becomes an interstitial and its coupling to the lattice is extremely small (Secs. III and IV). In what follows below we assume that this coupling is exactly zero. Thus an acceptor is equivalent to a nail which is broken when a force acting on it exceeds some maximum value F_p . (This is not the case for a periodic pinning potential when an impurity continues to interact with the crystal even after its pinning barrier was bent out by an external force, and the impurity shifted by a few lattice constants.) It is easy to demonstrate that, in a system of "nails," the crystal begins to slide starting from very sparse fluctuations—large regions where nails are absent.

Consider an empty region with area M/n_A which corresponds on average to M acceptors ($M \gg 1$). The force acting on the boundary of this region is equal to $(Mn/n_A)eE$ and is distributed over approximately $M^{1/2}$ boundary acceptors. The threshold electric field E_{th} for this region is hence given by

$$E_{\text{th}} \sim \frac{n_A F_p}{enM^{1/2}} \quad (36)$$

and vanishes in the limit of large M . After the threshold value of the electric field is exceeded for the largest empty region in the system, the nails on the region boundary are broken, and the region begins to grow. Since the force per one boundary impurity increases as $M^{1/2}$, this growth

never stops. (The situation is different for periodically coupled impurities: the force is being redistributed over *all* the impurities whose barrier was bent out, until the region of these impurities stops to grow. Hence fluctuations of impurities are not of crucial importance in this case.) One can conclude that pinning does not exist in an infinitely large system of nails. In a large but finite system with area S , M corresponding to the largest empty region is given by

$$(Sn_A)e^{-M} \sim 1, \quad (37)$$

where $\exp(-M)$ is the Poisson probability of the region formation. Substituting M from Eq. (37) into (36) yields

$$E_{\text{th}} \sim \frac{n_A F_p}{en \ln^{1/2}(Sn_A)}, \quad (38)$$

which differs from (34) by a large logarithm in the denominator. Thus the threshold field for acceptors turns out to decrease with the size of the system. The approximate nature of equality (37) means that M fluctuates within an ensemble of equivalent samples by $\delta M \sim 1$. This results in fluctuations of E_{th} , as given by $\delta E_{\text{th}} \sim E_{\text{th}}/2 \ln(Sn_A)$.

Expression (38) can be generalized for the case of spatially distributed acceptors with concentration N_A by substituting into it the effective 2D concentration $n_A = (0.7n^{-1/2})N_A$ and the average pinning force $F_p = \langle F_p \rangle$ given by

$$\langle F_p \rangle = \frac{1}{0.7n^{-1/2}} \int F_p(d) dd = 0.52 \frac{e^2 n}{\kappa},$$

where the integral is evaluated over the function $F_p(d)$ plotted in Fig. 2(c).

An important sign of the depinning mechanism described above for acceptors is a long-time hysteresis of the current-voltage characteristic at low temperatures T . Suppose the voltage is gradually increased starting from zero. After the threshold is exceeded, the system switches from the ground state when acceptors are at lattice sites to a metastable one: acceptors become interstitials interacting very weakly with the lattice. Vacancies decoupled from acceptors are carried away to the lead together with the sliding lattice. If the applied voltage is now *quickly* decreased far below the threshold value, the conductance remains high until the ground state for acceptors is restored. This relaxation process is thermally activated and can be very long at low temperatures. The following scenario of relaxation can be suggested. The acceptors at interstitials interchange their positions with neighboring electrons by means of activated hops and become sites of the lattice. These electron interstitials diffuse to the crystal boundary and are built into the lattice. The hysteresis does not appear if the time of the voltage decrease is longer than the relaxation time.

VI. CONCLUSION

We have studied the distance dependence of the magnitude of the pinning potential V_p for two types of charged impurities—donors and acceptors. Results are extremely

asymmetric with respect to the impurity charge: acceptors pin effectively only in a layer of a finite width adjacent to the electron plane, whereas donors have a sharp maximum of pinning energy at some distance from this plane. In addition, pinning by acceptors is much stronger. If residual acceptors are distributed uniformly in the spacer, they always are in the strong pinning regime. Donors, depending on their concentration, create either strong or intermediate pinning. Thus, for a uniform distribution of charged impurities, we did not find a regime where the weak pinning approximation applies. The correlation length ξ_c and the depinning field E_{th} are estimated in the case of strong pinning. Since the concentration of residual impurities is usually unknown, we did not try to compare expressions for ξ_c and E_{th} with experiment. A direct verification could be done in experiments on samples with additional δ layer of impurities inside the spacer at a given distance from the electron plane.

We have shown that the strongest pinning centers—close acceptors display an unusual behavior. They are built into the electron lattice and do not interact with it in a periodic way. The conventional model of pinning based on a periodic lattice-impurity coupling¹⁷ is not valid in this case. Instead, an acceptor can be considered as a nail which is broken after a force acting on it exceeds some critical value F_p . The consequences of this are a long-time hysteresis of the current-voltage dependence and a decrease of the depinning field E_{th} with the system size. This was shown under the assumption that, after the maximum force F_p acting on an acceptor is exceeded, it appears in an interstitial and *goes away* from the vacancy left (or, better to say, the vacancy is carried away with the lattice from the acceptor). Though the last statement seems very likely, it is not proven here. Another logical possibility is that the vacancy and the acceptor travel together. If this were the case, acceptors would not behave like “nails,” and the size-dependent logarithm in the denominator of Eq. (38) for E_{th} would disappear. We cannot rule this out in the framework of the computational method used here. Our simulation was adiabatic: electrons had time to relax at each position of a slowly moving acceptor. This permits one to obtain successive equilibrium states (and, particularly, the maximum coupling force F_p), but does not describe the motion of the acceptor with respect to the crystal when an external force exceeds F_p . The last problem is essentially dynamical and can be solved by molecular-dynamics methods, for example, assuming the presence of strong damping.

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APPENDIX

We calculate the effective Hook constant of an elastic film of radius R with fixed boundaries with respect to a

force \mathbf{F} applied at its center in a small region $r \ll R$. The local displacement $\mathbf{u}(\rho)$, where ρ is the 2D radius vector, satisfies the standard equation

$$K \text{grad div } \mathbf{u} + \mu \Delta \mathbf{u} = -h(\rho)\mathbf{F}, \quad (\text{A1})$$

where K and μ are “bulk” and shear moduli, respectively, and the function $h(\rho)$ which decays at $|\rho| \sim r$ describes the force distribution. First, we solve Eq. (A1) at $R \rightarrow \infty, r \rightarrow 0$; in the final answer, we shall take finite values r and R into account. Replacing $h(\rho)$ by a δ function and taking the Fourier transform of Eq. (A1) one gets

$$K \mathbf{q}(\mathbf{q} \cdot \mathbf{u}_q) + \mu q^2 \mathbf{u}_q = \mathbf{F}, \quad (\text{A2})$$

whence

$$\mathbf{u}_q = \frac{1}{\mu q^2} \left[\mathbf{F} - \frac{K \mathbf{q}(\mathbf{F} \cdot \mathbf{q})}{(K + \mu)q^2} \right], \quad (\text{A3})$$

where \mathbf{u}_q is the Fourier transform of $\mathbf{u}(\rho)$. In the limit of

an incompressible film, $K \gg \mu$, Eq. (A3) takes a form

$$\mathbf{u}_q = \frac{1}{\mu q^2} \left[\mathbf{F} - \frac{\mathbf{q}(\mathbf{F} \cdot \mathbf{q})}{q^2} \right]. \quad (\text{A4})$$

The displacement at the center of the film $\rho=0$ is found from Eq. (A4), as given by

$$\mathbf{u}(0) = \frac{1}{(2\pi)^2} \int d^2q \mathbf{u}_q = \frac{\mathbf{F}}{4\pi\mu} \int_0^\infty \frac{dq}{q}. \quad (\text{A5})$$

The last integral diverges logarithmically and should be truncated at small and large values of q at $q_{\min} \sim 1/R$ and $q_{\max} \sim 1/r$, respectively. Finally, for the effective Hook constant $k = F/u(0)$ one obtains

$$k = \frac{4\pi\mu}{\ln(\gamma R/r)}, \quad (\text{A6})$$

where $\gamma \sim 1$ is a numerical coefficient which depends on the form of the force distribution $h(\rho)$.

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¹⁶The last expression underestimates the correlation length ξ_c since dominating donors at moderate concentrations N_D are in the intermediate regime. On the other hand, at very small N_D , when the deformation energy (32) is small so that dominating donors are in the strong pinning regime, their effective number n_D may be larger than given by this estimate. Namely, $n_D = N_D \Delta$, where the effective width Δ is found from the self-consistent approximate equation $V_p(0.48n^{-1/2} + \Delta) \sim \epsilon_{\text{def}}$, which separates strong and weak pinning centers. The function $V_p(d)$ is plotted in Fig. 1(a), and ϵ_{def} as a function of R is given by Eq. (32).
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