

## Theory of charge nucleation in two dimensions

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Thermal nucleation of two-dimensional charges is studied. It is argued that the probability of  $N$  charge pairs to appear has a simple asymptotics for large  $N$ :  $p_N = [q(c, \beta, \mu)]^N / Z(\beta, \mu)$ , where  $q(c, \beta, \mu)$  is a function of charge concentration  $c$ , inverse temperature  $\beta$ , and chemical potential  $\mu$ , and  $Z(\beta, \mu)$  is the partition function. We present  $q(c, \beta, \mu)$  as a limit value of some functional integral and find an approximate value of this limit. This provides thermodynamic description of nucleation transition. The probability distribution of charge positions is studied within the same approximation. The behavior of the probability distribution indicates that for small charge concentration the transition is of Kosterlitz-Thouless type, i.e., the dipoles nucleated dissociate and form a neutral plasma, while at larger charge concentration the transition corresponds to nucleation of dipoles that may remain bounded. A transition with respect to chemical potential is observed, for  $\mu < \mu_{cr}$  the charge nucleation is a transition of infinite order, while for  $\mu > \mu_{cr}$  it becomes a first-order transition.

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### I. INTRODUCTION

A system of charges is a basic model for explaining various physical phenomena. We are going to discuss one feature of such a system: nucleation of two-dimensional charges due to thermal fluctuations. The key ideas in this area belong to Kosterlitz and Thouless [1]. They argued that below some critical temperature the charges are bound in dipoles. If temperature exceeds the critical value dipoles dissolve and form a neutral plasma. An enormous number of papers has contributed to studying this transition. We mention here only the review papers [2–4]. Most investigations follow Kosterlitz and Thouless and explore the ideas of the renormalization group method. In this paper we consider an alternative approach that is based on the direct asymptotic analysis of statistical characteristics exploring the presence of a large parameter, the number of charges. We give some arguments in favor of the following property of charge systems: the probability of  $N$  charge pairs to appear,  $p_N$ , has a simple asymptotics for large  $N$ :

$$p_N = \frac{1}{Z(\beta, \mu)} [q(c, \beta, \mu)]^N, \quad (1.1)$$

where  $q(c, \beta, \mu)$  is a function of charge concentration  $c$  (the area occupied by all charges divided by the specimen area), inverse temperature  $\beta$ , and chemical potential  $\mu$ , and  $Z(\beta, \mu)$  is the partition function. Charge concentration  $c$  plays the role of an order parameter of nonequilibrium configurations. Note that  $N$  appears in two places in the right hand side of Eq. (1.1): in the power and in the charge concentration.

Formula (1.1) implies a possibility of phase transition. To make this obvious let us consider a simplified situation when Eq. (1.1) is true for all admissible values of  $N$ ,  $0 \leq N \leq N_{\max}$ , and  $q$  does not depend on  $c$ . The partition function  $Z(\beta, \mu)$  is determined from the condition

$$\sum_{N=0}^{N_{\max}} p_N = 1$$

and is equal to

$$Z(\beta, \mu) = \sum_{N=0}^{N_{\max}} [q(\beta, \mu)]^N = \frac{1 - [q(\beta, \mu)]^{N_{\max}+1}}{1 - q(\beta, \mu)}.$$

Then the probability of  $N$  charge pairs to appear is given by a simple relation

$$p_N = \frac{1 - q(\beta, \mu)}{1 - [q(\beta, \mu)]^{N_{\max}+1}} [q(\beta, \mu)]^N. \quad (1.2)$$

The dependence of probabilities  $p_N$  on  $N$  changes qualitatively if, in the course of temperature variation, the function  $q(\beta, \mu)$  passes the value  $q(\beta, \mu) = 1$ . Indeed, for  $q < 1$ ,  $N_{\max} \gg 1$ ,

$$p_N \approx (1 - q)q^N$$

while for  $q > 1$

$$p_N \approx \frac{q - 1}{q^{N_{\max} - N}}.$$

Qualitative graphs of  $p_N$  in two different cases  $q < 1$  and  $q > 1$  are shown in Fig. 1. Obviously, for  $q < 1$  charge nucleation is impeded while for  $q > 1$  a large number of charges should be observed. Dependence of  $q$  on  $c$  may change the

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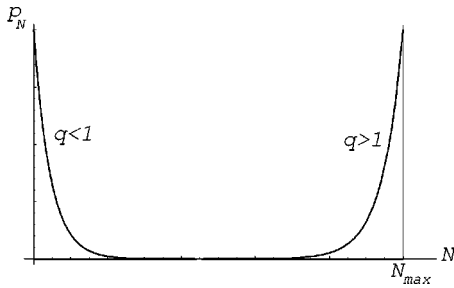


FIG. 1. Qualitative graphs of  $p_N$  in two cases  $q < 1$  and  $q > 1$ .

shape of curves in Fig. 1. A more accurate discussion given below confirms that there is a charge nucleation transition.

In order to justify formula (1.1) we present  $p_N$  as a functional integral. This integral contains a large parameter  $N$ . The large parameter appears in the form that suggests using Laplace’s method to evaluate the asymptotics of the integral as  $N$  goes to infinity. In accordance with Laplace’s method, the leading contribution to the asymptotics is provided by the integrals over vicinities of the stationary points of the integrand. We use this idea to evaluate the integral and obtain an explicit formula for  $q(c, \beta, \mu)$ . The computation of the functional integral gives the limit value of  $[p_N Z(\beta, \mu)]^{1/N}$ , which is independent of  $N$ . Although this does not prove the existence of the limit of  $[p_N Z(\beta, \mu)]^{1/N}$  as  $N \rightarrow \infty$ , one may expect that this limit exists. In any case, we obtain a lower bound for  $[p_N Z(\beta, \mu)]^{1/N}$  of the form

$$[p_N Z(\beta, \mu)]^{1/N} \geq \tilde{q}(c, \beta, \mu) \tag{1.3}$$

with explicitly determined function  $\tilde{q}(c, \beta, \mu)$ . This bound enables one to outline the region in  $(\beta, \mu)$  plane where the nucleation transition does occur. It remains valid independently on the validity of Eq. (1.1). There is also an upper bound

$$[p_N Z(\beta, \mu)]^{1/N} \leq \left( \frac{2e^{1+\beta\mu}}{c} \right)^2, \tag{1.4}$$

which is less informative.

Determining all stationary points of the functional integrand is an open problem, and it remains unclear whether the stationary point that we took into account leads to the correct asymptotics (some discussion on this issue will be given further). We therefore view the formula for  $q(c, \beta, \mu)$  as approximate. We discuss the outcomes of the approximate theory as if it captured correctly the true features of the charge system. It should be borne in mind, though, that some of these features may be the artifacts of the approximation.

Some of our conclusions on the physical nature of the phenomenon are similar to those obtained previously from different reasonings (see Refs. [2,5,6] and references therein).

In summary, nucleation of charges is characterized by the following features. There is a critical value of chemical potential  $\mu_{cr}$  separating two ranges of chemical potential  $\mu < \mu_{cr}$  and  $\mu > \mu_{cr}$ , where nucleation of charges is qualitatively different. The range  $\mu < \mu_{cr}$  includes the case of small fugacity  $e^{\beta\mu}$  (note that  $\mu_{cr} < 0$ ). For  $\mu < \mu_{cr}$  the nucleation transition is a transition of infinite order, i.e., thermodynamic potential and all its derivatives with respect to temperature are continuous while thermodynamic potential is not an analytical function at the transition point. A typical phase diagram in  $(c, T)$  plane is shown in Fig. 2(a). In this figure the horizontal and vertical axes correspond to the dimensionless temperature  $T$  and the charge concentration  $c$ , respectively. The thin curve is the curve  $q(c, \beta, \mu) = 1$ . It separates two regions. Region  $q(c, \beta, \mu) < 1$  corresponds to impeded charge nucleation, region  $q(c, \beta, \mu) > 1$  to massive charge nucleation. For each temperature one may compute the probability that charges appear in concentration  $c$ . The probability distribution in the  $(c, T)$  plane is highly nonuniform. In the region  $q(c, \beta, \mu) > 1$  the probability has a steep ridge on the curve  $\bar{c}(T)$  [the thick curve in Fig. 2(a)],  $\bar{c}$  being the average concentration. The ridge becomes a declining plateau away from the curve  $\bar{c}(T)$ . The plateau has a sharp drop at the curve  $q(c, \beta, \mu) = 1$ . In the region  $q(c, \beta, \mu) < 1$ , the average number of charges is finite and remain finite if the size of the specimen increases. Thus, in thermodynamic limit the average concentration is zero. For  $\mu > \mu_{cr}$  (fugacity is not necessarily small) the situation changes: the nucleation transition

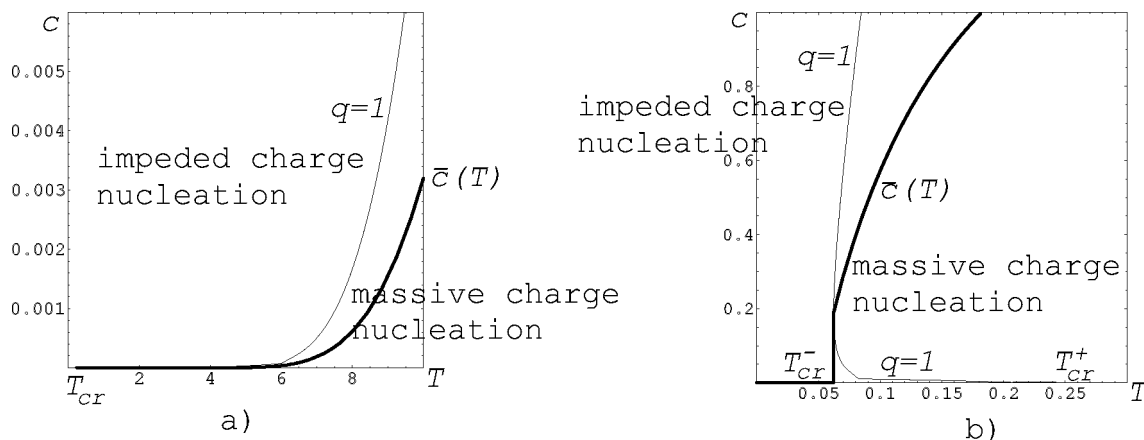


FIG. 2. Phase diagram in the  $(c, T)$  plane: (a)  $\mu < \mu_{cr}$ , (b)  $\mu > \mu_{cr}$

becomes a first-order transition. The critical temperature splits in low critical temperature  $T_{cr}^-$  and upper critical temperature  $T_{cr}^+$ . A typical phase diagram for  $\mu > \mu_{cr}$  is shown in Fig. 2(b). The thin curve in Fig. 2(b) separates the regions of impeded and massive charge nucleation. The meaning of the low critical temperature  $T_{cr}^-$  and the upper critical temperature  $T_{cr}^+$  is seen from the diagram. If  $T < T_{cr}^-$  there is a finite average number of charges in the specimen, which remains finite if the specimen size grows. If  $T > T_{cr}^+$  the system abounds in charges. Although all concentrations of charges are virtually possible, the most probable is the average concentration  $\bar{c}(T)$  shown by the thick line. As in case  $\mu < \mu_{cr}$ , if one moves from region  $q > 1$  to region  $q < 1$  the probability sharply drops at the boundary  $q = 1$ . This emphasizes a peculiar behavior of the system between  $T_{cr}^-$  and  $T_{cr}^+$ : the diagram shows that the nucleation of charges is a collective phenomenon—for  $T_{cr}^- < T < T_{cr}^+$  the probability of small concentrations of charges (in the region beneath the curve  $q = 1$ ) is much smaller than the probability of a little bit higher concentrations of charges (above the curve  $q = 1$ ).

Usually, the term “phase diagram” is used for graphs in the plane “average concentration-temperature.” The average concentration that is, in fact, also the most probable concentration, is in one-to-one correspondence with the chemical potential or the fugacity. Therefore phase diagrams are often shown in the plane “fugacity-temperature.” We use the term phase diagram also for transitions shown in the plane “order parameter-temperature.” Phase diagrams in the usual sense are presented in Sec. VII.

The nucleation transition may differ from the Kosterlitz-Thouless transition of dipole debonding, because the charges in the right region may be bound in dipoles. In order to clarify this issue we explicitly found the probability distribution of charge positions within the same approximation as for  $p_N$ . It turns out that at low charge concentrations the nucleation transition is also the Kosterlitz-Thouless transition, i.e., the dipoles nucleated dissociate. At finite concentrations, however, the charges may remain bounded if no external field is applied.

The paper is organized as follows. In Sec. II we specify the model. Our approach is outlined in Sec. III. We relate this to the previously established results on the probability distribution of energy in Sec. IV. In Sec. V we explain how functional integrals appear in our consideration. In Sec. VI the asymptotics of these integrals is considered and formulas for  $q$  in terms of  $(c, \beta, \mu)$  or  $(c, T, \mu)$  are obtained. In Sec. VII we calculate thermodynamic potential and present phase diagrams. In Sec. VIII an upper bound for phase diagrams is obtained. We analyze in Sec. IX the type of transition by studying the  $N$ -point distribution function. Probability distribution in  $(c, T)$  plane is derived in Sec. X. This is followed by Appendixes with auxiliary explanations.

## II. ENERGY

To specify the physical model we choose, following Kosterlitz and Thouless, screw dislocations in a crystal as “charges.” Let Burgers’ vectors of dislocations be directed

along the  $x_3$ -axis. The position of a dislocation is described by a point  $r$  in the  $(x_1, x_2)$ -plane. Dislocations deform the surrounding crystal lattice and create elastic stresses. The stress tensor has two independent nonzero components  $\sigma_{13}$  and  $\sigma_{23}$ . The equilibrium equations lead to the existence of a stress function  $\psi$  so that  $\sigma_{13} = \partial\psi/\partial x_2$ ,  $\sigma_{23} = -\partial\psi/\partial x_1$ . Consider first the crystal containing one dislocation positioned at the point  $r$ . The compatibility condition that requires the existence of a displacement field connecting the perfect and the imperfect lattices, combined with Hooke’s law, yields the equation for the stress function

$$\frac{1}{G} \Delta \psi = -b \delta(x-r), \quad (2.1)$$

where  $b$  is the  $x_3$ -component of Burgers’ vector,  $G$  the shear modulus,  $\delta(x)$  the two dimensional (2D)  $\delta$  function, and  $\Delta$  Laplace’s operator.

Denote by  $C$  the cross section of the crystal by planes  $x_3 = \text{const}$ . If the boundary  $\partial C$  of the region  $C$  is traction-free then

$$\psi = 0 \quad \text{at } \partial C. \quad (2.2)$$

The density of elastic energy of the crystal is  $(\nabla\psi)^2/2G$ . The total elastic energy is given by the integral

$$E = \frac{h}{2G} \int_C (\nabla\psi)^2 d^2x, \quad (2.3)$$

with  $h$  being the crystal thickness in the  $x_3$ -direction.

Energy (2.3) is infinite for the solution of Eqs. (2.1) and (2.2) due to divergence at the point  $x = r$ . Thus, a regularization is needed. Various regularizations are possible. We will regularize the energy by introducing higher derivatives in Eq. (2.3),

$$\begin{aligned} E(\psi) &= \frac{h}{2G} \int_C [(\nabla\psi)^2 + \epsilon^2(\nabla\nabla\psi)^2] d^2x \\ &= \frac{h}{2G} \int_C \left\{ \left( \frac{\partial\psi}{\partial x_1} \right)^2 + \left( \frac{\partial\psi}{\partial x_2} \right)^2 + \epsilon^2 \left[ \left( \frac{\partial^2\psi}{\partial x_1^2} \right)^2 \right. \right. \\ &\quad \left. \left. + 2 \left( \frac{\partial^2\psi}{\partial x_1 \partial x_2} \right)^2 + \left( \frac{\partial^2\psi}{\partial x_2^2} \right)^2 \right] \right\} d^2x. \end{aligned} \quad (2.4)$$

The small parameter  $\epsilon$  has the dimension of length and plays the role of an “effective size” of the dislocation core.

Modification of energy yields modification of Eq. (2.1) since  $\psi$  must be the minimizer of the energy functional

$$I(\psi) = E(\psi) - hb\psi(r). \quad (2.5)$$

The minimum is sought over all smooth functions  $\psi$  obeying the boundary condition (2.2). There is an additional boundary condition for  $\psi$  due to the dependence of the energy on higher derivatives, but we do not need its explicit form. The minimizer  $\check{\psi}$  satisfies the equation

$$\frac{1}{G}(\Delta\check{\psi} - \epsilon^2\Delta^2\check{\psi}) = -b\delta(x-r).$$

The minimum value of the functional  $I(\psi)$  is equal to the negative energy

$$\min_{\psi \in (2.2)} I(\psi) = -E(\check{\psi}). \quad (2.6)$$

The relations of statistical mechanics contain the product  $-\beta E$ . It is therefore convenient to rewrite the variational problem in terms of this product. It follows from Eqs. (2.4), (2.5), and 2.6 that

$$-\beta E = \min_{\psi \in (2.2)} \left[ \frac{\beta h}{2G} (A\psi, \psi) - \beta h b \psi(r) \right], \quad (2.7)$$

where

$$(A\psi, \psi) = \int_C [(\nabla\psi)^2 + \epsilon^2(\nabla\nabla\psi)^2] d^2x. \quad (2.8)$$

In order to explicitly perform further computations we will use the periodic boundary conditions instead of the traction-free boundary conditions. We expect that such a replacement will not change the results qualitatively. So, in what follows  $C$  is a square of the size  $a$ ,  $|x_1| \leq a/2$ ,  $|x_2| \leq a/2$ , and  $P$  is the subspace of functions that are double periodic and having double periodic first- and second-order partial derivatives. It is convenient to change the unknown function  $\psi \rightarrow u$ :  $\psi = \sqrt{G/h\beta}u$ . Then the variational problem takes the form

$$-\beta E = \min_{u \in P} \left[ \frac{1}{2} (Au, u) - \sqrt{\beta_*} u(r) \right], \quad (2.9)$$

where  $\beta_*$  is the dimensionless inverse temperature,  $\beta_* = \beta G b^2 h$ .

Variational problem (2.9), in contrast to Eq. (2.7), requires an additional constraint. The quadratic functional  $(Au, u)$  is invariant with respect to shifts of function  $u$  by a constant, while the linear functional  $\sqrt{\beta_*}u(r)$  is not. The periodic boundary conditions, in contrast to the boundary condition (2.2), do not eliminate such shifts. Therefore, in order to have a well-posed variational problem with the energy functional bounded below, we have to impose an additional constraint eliminating the shifts. We put

$$\langle u \rangle \equiv \frac{1}{a^2} \int_C u d^2x = 0. \quad (2.10)$$

Variational problem (2.9) with the additional constraint (2.10) is well posed.

Energy  $E$  is the sum of the elastic energy of the lattice surrounding the dislocation plus the energy of the dislocation core found within the regularization (2.4). The latter can differ from the true energy of the dislocation core. The correction of the energy is a constant that does not depend on the

dislocation position. We denote it by  $e_0$ . Thus, the total energy of a crystal containing one dislocation is

$$H = E + e_0.$$

The relation between  $e_0$ ,  $\epsilon$ , and the dislocation core energy in the limit  $\epsilon \rightarrow 0$  is established in Appendix B.

Let the crystal contain  $N_1$  dislocations with Burgers' vector  $b$  and  $N_2$  dislocations with Burgers' vector  $-b$ . The dislocations are positioned at the points  $r^+ = (r_1^+, \dots, r_{N_1}^+)$  and  $r^- = (r_1^-, \dots, r_{N_2}^-)$ . Then

$$-\beta H_N(r^+, r^-) = \min_{u \in P} \left[ \frac{1}{2} (Au, u) - (l, u) \right] - (N_1 + N_2) e_0 \beta, \quad (2.11)$$

where

$$(l, u) = \sqrt{\beta_*} \left( \sum_{a=1}^{N_1} u(r_a^+) - \sum_{a=1}^{N_2} u(r_a^-) \right). \quad (2.12)$$

We focus mostly on the case of neutral systems,  $N_1 = N_2 = N$ , with

$$(l, u) = \sqrt{\beta_*} \sum_{a=1}^N [u(r_a^+) - u(r_a^-)]. \quad (2.13)$$

For neutral systems the constraint (2.10) can be dropped without losing well posedness of the variational problem, because the linear part (2.13) of the functional is also invariant under shifts of  $u$  by a constant. Nevertheless, we will keep this constraint to maintain the nondegeneracy of the quadratic functional  $(Au, u)$ .

The variational principle for energy, besides its key role in the functional integral formulation of the problem to be considered further, gives important qualitative information about the system. We mention here a few useful facts. First, for zero  $e_0$ ,

$$\beta H_N \geq 0, \quad (2.14)$$

and for nonzero  $e_0$ ,

$$-\beta H_N \leq -(N_1 + N_2) e_0 \beta. \quad (2.15)$$

Inequality (2.14) follows from Eq. (2.11) if we choose  $u = 0$  as a trial function. Note that the self-energies of charges are included in  $H_N$ , otherwise Eq. (2.14) does not hold. Second, if one increases  $\epsilon$ ,  $-\beta H_N$  increases also since the quadratic form  $(Au, u)$  grows. Third, if one change the model by adding the term  $\kappa \int u^2 d^2x$  into the quadratic functional  $(Au, u)$ ,  $-\beta H_N$  increases (for  $\kappa > 0$ ) and grows monotonically with  $\kappa$  since the functional to be minimized increases. Fourth,  $-\beta H_N$  found for the periodic boundary conditions  $-\beta H_N|_{\text{pc}}$  does not exceed  $-\beta H_N$  found for the traction-free boundary conditions  $-\beta H_N|_{\text{fc}}$  if  $\epsilon$  is small:

$$-\beta H_N|_{\text{pc}} \leq -\beta H_N|_{\text{fc}}. \quad (2.16)$$



Indeed, if  $\epsilon$  is small, one may change in Eq. (2.11) the set  $P$  of periodic functions with periodic derivatives by the wider set  $P_0$  of periodic functions: this causes the reduction in  $-\beta H_N$  of the order  $o(\epsilon)$ . Then, choosing as a trial function in the variational problem on  $P_0$  the solution of the variational problem for traction-free boundary condition and neglecting the  $o(\epsilon)$  correction, one obtains Eq. (2.16).

### III. NUCLEATION CRITERION

Consider a crystal placed in a heat bath at a given temperature. Suppose that only neutral systems of dislocations may appear due to thermal fluctuations. The probability of a set of  $N$  dislocation pairs to appear at the positions  $(r_1^+, r_1^-), \dots, (r_N^+, r_N^-)$  is assumed to be grand canonical:

$$f_N(r^+, r^-) = \frac{1}{Z} \frac{e^{2N\beta\mu_1}}{(N!)^2} e^{-\beta H_N(r^+, r^-)}, \quad (3.1)$$

where  $\mu_1$  is a parameter. The partition function  $Z$  is determined by the normalization condition.

We redefine energy and parameter  $\mu_1$  by including the additive term of energy  $-2N\beta e_0$  in  $2N\beta\mu_1$ . Then Eq. (3.1) takes the form

$$f_N(r^+, r^-) = \frac{1}{Z} \frac{e^{2N\beta\mu}}{(N!)^2} e^{-\beta H_N(r^+, r^-)}, \quad (3.2)$$

where the energy  $H_N$  is determined by the variational problem

$$\begin{aligned} & -\beta H_N(r^+, r^-) \\ &= \min_{u \in P} \left\{ \frac{1}{2} (Au, u) - \sqrt{\beta_*} \sum_{a=1}^N [u(r_a^+) - u(r_a^-)] \right\}, \quad (3.3) \end{aligned}$$

and  $\mu = \mu_1 - e_0$ .

The grand canonical distribution describes an equilibrium exchange of particles of a small system embedded in a large bath. In that case, parameter  $\mu$  has the sense of chemical potential of the bath. We will also call  $\mu$  chemical potential though the physical situation under consideration is quite different. The physical meaning of  $\mu$  is discussed in Appendix A.

Possible values of  $N$  range from zero to some maximum possible number of dislocation pairs  $N_{\max}$ . The probability that there are  $N$  dislocation pairs in the crystal is

$$p_N = \frac{1}{Z(\beta, \mu)} \sum_{r^+, r^-} \frac{e^{2N\beta\mu}}{(N!)^2} e^{-\beta H_N(r^+, r^-)}. \quad (3.4)$$

By definition,  $H_N = 0$  for  $N = 0$ . Therefore, the probability that there are no dislocations in the crystal is

$$p_0 = \frac{1}{Z(\beta, \mu)}. \quad (3.5)$$

The probability that dislocations do appear is obviously

$$p = 1 - \frac{1}{Z(\beta, \mu)}. \quad (3.6)$$

The normalization condition  $\sum_{N=0}^{N_{\max}} p_N = 1$  yields the value of the partition function

$$Z(\beta, \mu) = \sum_{N=0}^{N_{\max}} \sum_{r^+, r^-} \frac{e^{2N\beta\mu}}{(N!)^2} e^{-\beta H_N(r^+, r^-)}. \quad (3.7)$$

Vectors  $r_a^+, r_a^-$  run over a piece of a 2D discrete lattice enclosed in the box  $C$ . The lattice spacing is identified with the magnitude of Burgers' vector  $b$ . States with coinciding positions of a positive and a negative dislocation are not allowed since this yields an annihilation of two dislocations; such states have been taken into account in the sum with  $N - 1$  dislocation pairs. The coincidence of dislocations of the same sign is possible: this corresponds to a dislocation with a larger Burgers' vector. Such states, however, should carry the factor that differs from  $1/(N!)^2$ . To avoid the latter complication we assume that dislocations with Burgers' vectors of a magnitude larger than  $b$  do not appear.

Let us represent  $p_N$  in the form

$$p_N = \frac{1}{Z(\beta, \mu)} (q_N)^N, \quad (3.8)$$

where

$$q_N = e^{2\beta\mu} \left[ \sum_{r^+, r^-} \frac{1}{(N!)^2} e^{-\beta H_N(r^+, r^-)} \right]^{1/N}. \quad (3.9)$$

We argue that, for large  $N$ ,  $q_N$  depends on  $N$  in the thermodynamic limit only through the dislocation concentration  $c = 2Nb^2/a^2$ . More precisely, let  $N$  and  $a$  tend to infinity in such a way that  $c$  remains constant. Then  $q_N$  tends to some limit value  $q$  that depends on concentration  $c$ , inverse temperature  $\beta$ , and chemical potential  $\mu$ :

$$q = q(c, \beta, \mu).$$

The values of parameters for which

$$q(c, \beta, \mu) = 1$$

are critical in the following sense: If, for some  $c$  and a given  $\beta$ ,  $q(c, \beta, \mu) > 1$ , then the sum

$$Z(\beta, \mu) = \sum_{N=0}^{N_{\max}} (q_N)^N \quad (3.10)$$

contains many big terms and is very large. Therefore, the probability (3.6) that dislocations do appear is about unity. In contrary, if, at a given  $\beta$ ,  $q(c, \beta, \mu) \leq q_* < 1$  for all  $c$ , then the sum (3.10) does not exceed a constant independent on  $N_{\max}$ , and there is a finite probability that dislocations do not appear.

Our analysis is based on the replacement of the sum in Eq. (3.9) by the integral

$$q_N = e^{2\beta\mu} \left[ \frac{1}{(N!)^2} \int_C \cdots \int_C e^{-\beta H_N(r^+, r^-)} \frac{d^2 r_1^+}{b^2} \cdots \frac{d^2 r_N^-}{b^2} \right]^{1/N}, \quad (3.11)$$

where each variable  $r_1^+, \dots, r_N^-$  runs over the entire square  $C$ . Allowing each variable  $r_1^+, \dots, r_N^-$  to run over  $C$  we neglect the condition that dislocation positions do not coincide. The error caused by this is small if the concentration  $c$  is small. In the next two sections we compute the integral in Eq. (3.11) approximately and find out that the right hand side of Eq. (3.11) does not depend on  $N$ . In this indirect way, we support the assumption that it has a limit as  $N \rightarrow \infty$ . We use the formula obtained for the limit to discuss the dislocation nucleation for all  $c$ , including finite  $c$ . The conclusions for finite  $c$  require further investigation because the expression (3.11) is no longer valid in this case.

Note an essential feature of the expression (3.11): it contains big factors  $b^{-2}$ . These factors stem from the ‘‘space discretization.’’ In a sense, the space quantum  $b$  is analogous to the de Broglie length (compare with the expression for the partition function in Ref. [4]). To appreciate the contribution of the factors  $b^{-2}$  let us write Eq. (3.11) in the form

$$q_N = e^{2\beta\mu} \left[ \frac{(a^2/b^2)^{2N}}{(N!)^2} J_N \right]^{1/N}, \quad (3.12)$$

where

$$J_N = \int_C \cdots \int_C e^{-\beta H_N(r^+, r^-)} \frac{d^2 r_1^+}{a^2} \cdots \frac{d^2 r_N^-}{a^2}. \quad (3.13)$$

The ratio  $a^2/b^2$  is equal to the number of atoms  $N_a$  in the area  $C$ . The number  $N!$  can be approximated by Stirling’s formula:  $\ln N! = N \ln N - N$ . Therefore,

$$\frac{(a^2/b^2)^{2N}}{(N!)^2} = e^{2N \ln N_a - 2N \ln N + 2N} = e^{2N[1 - \ln(c/2)]}. \quad (3.14)$$

Obviously,  $c \leq 1$  and  $1 - \ln(c/2) > 0$ . Thus, the number (3.14) is very big: the ratio  $(a^2/b^2)^N$  outweighs  $N!$ . The third factor in Eq. (3.12),  $J_N$ , is always less than unity, due to (2.14)  $e^{-\beta H_N} \leq 1$ , hence  $J_N \leq 1$ .

So, in Eq. (3.12) we have a competition of two factors: very big number (3.14) and presumably very small number  $J_N$ . Quantity  $q_N$  may be larger than unity only due to the big factor (3.14) that is caused by the ‘‘space quantization.’’ Note that the elementary estimate (1.4) follows immediately from Eqs. (3.12)–(3.14) and (2.15).

Our next goal is to study the integral  $J_N$ .

#### IV. DISTRIBUTION OF ENERGY

The integral  $J_N$  admits the following probabilistic interpretation. Let us regard  $r_1^+, \dots, r_N^-$  as statistically independent

vectors homogeneously distributed over  $C$ . Then  $H_N(r^+, r^-)$  is the random function depending on these random vectors. The integral in Eq. (3.13) is the mathematical expectation of  $\exp[-\beta H_N(r^+, r^-)]$ .

Let  $f_N(E)$  be the probability density function of the energy  $H_N$ . Then

$$J_N = \int_C \cdots \int_C e^{-\beta H_N(r^+, r^-)} \frac{d^2 r_1^+}{a^2} \cdots \frac{d^2 r_N^-}{a^2} = \int_0^\infty e^{-\beta E} f_N(E) dE. \quad (4.1)$$

The energy  $H_N$  possesses a special feature: according to Eq. (2.11) it is the negative minimum value of a quadratic functional. The probability density function of minimum values of random quadratic functionals of this type was obtained in Ref. [7]. It is easy to see that, after removing self-energies, the energy variance is of the order  $N^2$ . Thus, one may expect that the ratio  $H_N/N$  has a limit probability distribution. Indeed, it was shown that the probability distribution function of the ratio  $h = H_N/N$ ,  $g_N(h)$ , after a self-energy shift, has a limit,  $g_\infty(h)$ , as  $N \rightarrow \infty$ , and an analytical form of  $g_\infty(h)$  was obtained. Function  $g_\infty(h)$  was investigated further in Ref. [8] for the case of two-dimensional charges in a periodic box, it was found that the analytical formula for  $g_\infty(h)$  is in good agreement with the numerical simulations conducted in Ref. [9]. We consider in this paper an approximation of the integral  $J_N$ , which corresponds to replacing the function  $f_N(E)$  in Eq. (4.1) by  $g_\infty(NE)$ . In order to better understand the error introduced by such change we repeat the argument from Ref. [7] in the following section and reduce the evaluation of  $J_N$  to studying the asymptotics in  $N$  of some functional integral.

#### V. FUNCTIONAL INTEGRAL

The idea of representing the partition function as a functional integral is widely used in statistical physics (see, for example, Refs. [10,11]). We will follow it in our treatment [7].

The starting point is the following identity: for any positive definite quadratic form  $(Au, u)_m = \sum_{i,j=1}^m A_{ij} u_i u_j$  and linear form  $(l, u)_m = \sum_{j=1}^m l_j u_j$ ,

$$\sqrt{\frac{\det A_m}{(2\pi)^m}} \int e^{-(1/2)(Au, u)_m - i(l, u)_m} d^m u = e^{-(1/2)(A^{-1}l, l)_m}, \quad (5.1)$$

where  $\det A_m$  is the determinant of the matrix  $\|A_{ij}\|$ ;  $(A^{-1}l, l)_m = \sum_{i,j=1}^m A_{ij}^{-1} l_i l_j$ ,  $A_{ij}^{-1}$  being the component of the inverse matrix, and  $i^2 = -1$ .

Since

$$\min_u \left[ \frac{1}{2}(Au, u)_m - (l, u)_m \right] = -\frac{1}{2}(A^{-1}l, l)_m, \quad (5.2)$$

we can write the identity (5.1) in the form

$$\begin{aligned}
& e_u^{\min[(1/2)(Au,u)_m - (l,u)_m]} \\
&= \sqrt{\frac{\det A_m}{(2\pi)^m}} \int e^{-(1/2)(Au,u)_m - i(l,u)_m} d^m u.
\end{aligned} \tag{5.3}$$

Note here that, due to Eq. (2.11),  $-\beta H_N$  is the minimum value of the quadratic functional. Making a finite-dimensional truncation in the variational problem (2.11), one can evaluate the energy with any desirable accuracy. The truncated variational problem has the form (5.2) where  $(Au,u)_m$  and  $(l,u)_m$  are the  $m$ -dimensional truncations of the functionals  $(Au,u)$  and  $(l,u)$ . Therefore

$$\begin{aligned}
e^{-\beta H_N(r^+, r^-)} &= \lim_{m \rightarrow \infty} e_u^{\min[(1/2)(Au,u)_m - (l,u)_m]} \\
&= \lim_{m \rightarrow \infty} \sqrt{\frac{\det A_m}{(2\pi)^m}} \int e^{-(1/2)(Au,u)_m - i(l,u)_m} d^m u.
\end{aligned}$$

We write this limit symbolically as

$$e^{-\beta H_N(r^+, r^-)} = \int e^{-(1/2)(Au,u) - i(l,u)} \mathcal{D}u, \tag{5.4}$$

where the ‘‘volume element’’  $\mathcal{D}u$  is specified by the condition

$$\int \mathcal{D}u e^{-(1/2)(Au,u)} = 1. \tag{5.5}$$

Integrating Eq. (5.4) over  $r^+, r^-$  we have

$$J_N = \int e^{-(1/2)(Au,u) - i(l,u)} \mathcal{D}u \frac{d^2 r_1^+}{a^2} \dots \frac{d^2 r_N^-}{a^2}.$$

This formula can be simplified due to a special form of the functional  $(l,u)$  (2.13). We obviously have

$$\begin{aligned}
J_N &= \int \mathcal{D}u e^{-(1/2)(Au,u)} [Q(u)]^N \\
&= \int \mathcal{D}u e^{-(1/2)(Au,u) + N \ln Q(u)},
\end{aligned} \tag{5.6}$$

where

$$Q(u) = \int_C \int_C e^{-i\sqrt{\beta_*} [u(r) - u(r')]} \frac{d^2 r}{a^2} \frac{d^2 r'}{a^2}. \tag{5.7}$$

The integral  $J_N$  depends on the large parameter  $N$ . We need to find its asymptotics as  $N \rightarrow \infty$ .

## VI. ASYMPTOTICS OF THE FUNCTIONAL INTEGRAL

The integral (5.6) resembles integrals studied by Laplace’s method, since it contains the large parameter  $N$ . The similarity is, to some extent, misleading: the parameter  $N$  is hidden also in the operator  $A$  and the volume element

$\mathcal{D}u$  that depend on  $\epsilon \sim a/\sqrt{N}$ . Nevertheless, we proceed ignoring this fact and hoping that, due to Eq. (5.5), we capture approximately the behavior of the integral. One may say that we unbound  $\epsilon$  and  $N$  and, for a fixed  $\epsilon$ , tends  $N$  to infinity. Then, at a final stage, the link between  $\epsilon$  and  $N$  is taken into account. More on the ‘‘real asymptotics’’ of  $J_N$  will be said in Sec. VIII.

From Eq. (5.7)

$$Q(u) = \left( \int_C \cos \sqrt{\beta_*} u \frac{d^2 x}{a^2} \right)^2 + \left( \int_C \sin \sqrt{\beta_*} u \frac{d^2 x}{a^2} \right)^2.$$

The functional  $Q(u)$  is real and does not exceed unity. Thus, the integral (5.6) converges absolutely. We seek the stationary points of  $Q(u)$ . The stationary points obey the equation

$$-\sin \sqrt{\beta_*} u \cos \sqrt{\beta_*} \alpha + \cos \sqrt{\beta_*} u \sin \sqrt{\beta_*} \alpha = 0, \tag{6.1}$$

where  $\alpha$  is a constant depending on  $u$ :  $\sqrt{Q(u)} \cos \sqrt{\beta_*} \alpha = \int_C \cos \sqrt{\beta_*} u d^2 x / a^2$ . Putting Eq. (6.1) in the form

$$\sin \sqrt{\beta_*} [u(x) - \alpha] = 0, \tag{6.2}$$

we see that  $u(x)$  is a piecewise constant function taking the values  $\alpha + \pi k / \sqrt{\beta_*}$ ,  $k = 0, \pm 1, \pm 2, \dots$ . Functions  $u$  with a finite value of energy  $(Au,u)$  are continuous. There is only one continuous function  $u(x) = 0$ , which satisfies Eqs. (6.2) and (2.10). Other stationary points existing in  $m$ -dimensional truncations tend to infinity in the space  $P$  with the energy norm  $(Au,u)^{1/2}$  as  $m \rightarrow \infty$ . Thus, one may expect that  $u = 0$  is the only stationary point that should be taken into account.

In the vicinity of the point  $u = 0$  the functional  $Q(u)$  takes the form

$$Q(u) = 1 - \frac{\beta_*}{a^2} \int_C u^2 d^2 x \tag{6.3}$$

and, within the same approximation,

$$\ln Q(u) = - \frac{\beta_*}{a^2} \int_C u^2 d^2 x.$$

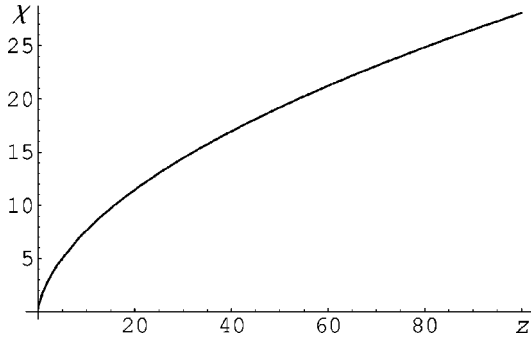
Note that the approximation of the functional  $Q(u)$  by formula (6.3) may also be viewed as a high temperature expansion.

In the approximation (6.3)

$$\begin{aligned}
J_N &= \int \mathcal{D}u \exp \left\{ - \frac{1}{2} \int_C [\nabla u^2 + \epsilon^2 (\nabla \nabla u)^2] d^2 x \right. \\
&\quad \left. - \frac{\beta_* N}{a^2} \int_C u^2 d^2 x \right\}.
\end{aligned} \tag{6.4}$$

Computation of this elementary integral gives (see Appendix C)

$$J_N = \frac{1}{\sqrt{\Phi_\epsilon(\beta_* N / 2\pi^2)}}, \tag{6.5}$$

FIG. 3. Function  $\chi(z)$ .

where  $\Phi_\varepsilon(z)$  is expressed in terms of the eigenvalues of energy  $\lambda_k$ ,

$$\Phi_\varepsilon(z) = \prod_{k \in \mathbb{Z}'_2} \left( 1 + \frac{z}{\lambda_k} \right), \quad \lambda_k = |k|^2 + \varepsilon^2 |k|^4, \quad \varepsilon = 2\pi\epsilon/a. \quad (6.6)$$

In this infinite product  $k$  runs over  $\mathbb{Z}'_2$  that is the 2D square lattice with unit spacing and with the origin  $k=0$  being excluded.

It is convenient to write  $\Phi_\varepsilon(z)$  in the form  $\Phi_\varepsilon(z) = e^{-2h_\varepsilon(z)}$ , where

$$h_\varepsilon(z) = -\frac{1}{2} \ln \Phi_\varepsilon(z) = -\frac{1}{2} \sum_{k \in \mathbb{Z}'_2} \ln \left( 1 + \frac{z}{|k|^2 + \varepsilon^2 |k|^4} \right). \quad (6.7)$$

Combining Eqs. (5.6), (6.5), and (3.14) we get

$$q_N = e^{2[1 - \ln(c/2)] + h_\varepsilon(\beta_* N/2\pi^2)/N + 2\mu\beta}. \quad (6.8)$$

In the thermodynamic limit the function  $h_\varepsilon(\beta_* N/2\pi^2)/N$  converges to the function (see Appendix D)  $-\chi(\beta_*\rho)/4\pi\rho$ , where

$$\chi(z) = \int_0^\infty \ln \left( 1 + \frac{z}{u+u^2} \right) du, \quad (6.9)$$

and  $\rho$  is the density of dislocation cores:  $\rho = 2N\epsilon^2/a^2$ . Function  $\chi(z)$  is positive, monotone increasing, and concave for real  $z > 0$ . At the end points function  $\chi(z)$  has the following asymptotic behavior

$$\chi(z) \sim -z \ln z + z \quad \text{as } z \rightarrow 0; \quad \chi(z) \sim \pi\sqrt{z} \quad \text{as } z \rightarrow \infty, \quad (6.10)$$

(see Appendix D). The graph of  $\chi(z)$  for real positive  $z$  is plotted in Fig. 3.

From Eq. (6.8)

$$q = e^{2[1 - \ln(c/2)] - 1/4\pi\rho\chi(\beta_*\rho) + 2\mu\beta}. \quad (6.11)$$

To present this result in the dimensionless form we introduce the dimensionless chemical potential  $\mu_*$  by the relation  $\mu_*\beta_* = \mu\beta$ , i.e.,  $\mu_* = \mu/Gb^2h$ , and the dimensionless dislocation core radius  $\lambda = \epsilon/b$ , so that  $\rho = c\lambda^2$ . Thus, finally,

$$\ln q = 2 \left( 1 - \ln \frac{c}{2} \right) - \frac{1}{4\pi\lambda^2 c} \chi(\beta_* c \lambda^2) + 2\mu_* \beta_*. \quad (6.12)$$

Note that, besides  $c$ ,  $\beta_*$ , and  $\mu_*$ , the function  $q$  also depends on the parameter  $\lambda$  of the Hamiltonian as it is clearly seen from Eq. (6.12), but we do not emphasize this in our notation.

Defining the dimensionless temperature  $T$  as  $T = 2\pi/\beta_*$  we obtain  $q$  in terms of  $c$  and  $T$ ,

$$\ln q = 2 \left( 1 - \ln \frac{c}{2} \right) - \frac{1}{4\pi\lambda^2 c} \chi \left( \frac{2\pi\lambda^2 c}{T} \right) + \frac{4\pi\mu_*}{T}. \quad (6.13)$$

## VII. THERMODYNAMIC POTENTIAL AND PHASE DIAGRAMS

The thermodynamic potential  $\Omega$  is defined by the formula

$$\Omega(\beta, \mu) = -\frac{1}{N_a} \ln Z. \quad (7.1)$$

As follows from Eq. (3.7), the average dislocation density can be expressed in terms of the derivative of  $\Omega(\beta, \mu)$ :

$$\begin{aligned} \bar{c} &\equiv \sum_{N=0}^{N_{\max}} \frac{2N}{N_a} p_N = \frac{1}{\beta N_a} \frac{\partial \ln Z}{\partial \mu} = -\frac{1}{\beta} \frac{\partial \Omega(\beta, \mu)}{\partial \mu} \\ &= -\frac{1}{\beta_*} \frac{\partial \Omega(\beta_*, \mu_*)}{\partial \mu_*}. \end{aligned} \quad (7.2)$$

Let us find  $\Omega$  explicitly within the approximation of Sec. VI. Consider the partition function (3.10). Since, for large  $N$ ,  $q_N \approx q$ , the partition function is finite if  $q(c, \beta, \mu) < 1$  for all  $c$ . Therefore, in the limit  $N_a \rightarrow \infty$  the thermodynamic potential  $\Omega$  (7.1) is zero and  $\bar{c} = 0$ , in this case.

If  $q(c, \beta, \mu) > 1$  for some  $c$ , then we compute the partition function in the following way. Consider the sum

$$Z = \sum_{N=0}^{N_{\max}} (q_N)^N.$$

Since  $Z$  is very large, and there is only a finite number of terms for which  $q_N$  differ from  $q$  considerably, we may write

$$Z \approx N_a \sum_{N=0}^{N_{\max}} \left[ q \left( \frac{2N}{N_a}, \beta, \mu \right) \right]^N \frac{1}{N_a}.$$

The last sum may be approximated by the integral

$$\begin{aligned} \sum_{N=0}^{N_{\max}} \left[ q \left( \frac{2N}{N_a}, \beta, \mu \right) \right]^N \frac{1}{N_a} &\approx \int_0^{N_{\max}} \left[ q \left( \frac{2N}{N_a}, \beta, \mu \right) \right]^N \frac{dN}{N_a} \\ &= \frac{1}{2} \int_0^{c_{\max}/2} [q(c, \beta, \mu)]^{cN_a/2} dc. \end{aligned}$$

Finally,



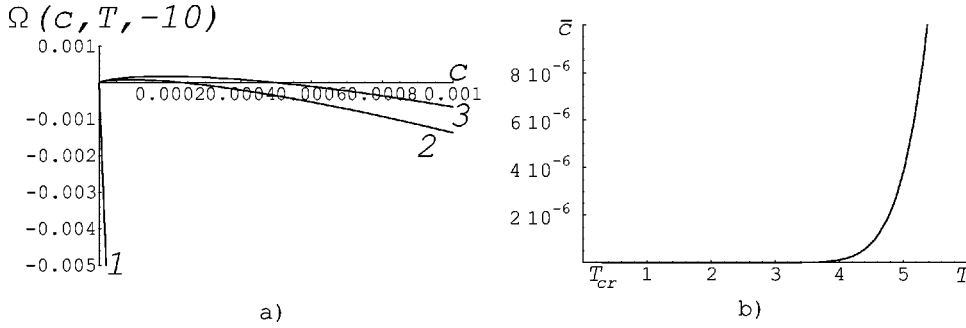


FIG. 4. (a)  $\Omega(c, T, \mu_*)$  as function of  $c$  for  $\lambda = 1$ ,  $\mu_* = -10$ ; curve 1:  $T = 1/4$ , curve 2:  $T = 6.5$ , curve 3:  $T = 7$ . (b) Average dislocation density  $\bar{c}$  as function of  $T$  for  $\lambda = 1$ ,  $\mu_* = -10$ .

$$Z = \frac{N_a}{2} \int_0^{c_{\max}^2} e^{(1/2)N_a c \ln q(c, \beta, \mu)} dc. \quad (7.3)$$

Denote by  $\Omega(c, \beta, \mu)$  the function

$$\Omega(c, \beta, \mu) = \frac{1}{2} c \ln q(c, \beta, \mu). \quad (7.4)$$

Let us show that thermodynamic potential is given by the formula

$$-\Omega(\beta, \mu) = \max_c \Omega(c, \beta, \mu). \quad (7.5)$$

According to this formula, function  $\Omega(c, \beta, \mu)$  plays the role of nonequilibrium thermodynamic potential, while  $c$  is an order parameter.

Assume that, for each  $\beta, \mu$ , the function  $\Omega(c, \beta, \mu)$  of  $c$  is smooth and bounded above [the bound (1.4) is too rough to guarantee that]. Denote the point where the maximum value of  $\Omega(c, \beta, \mu)$  is reached by  $\hat{c}$ . Consider first the case that  $\hat{c}$  is an internal point of the integration interval. At this point  $\partial\Omega/\partial c = 0$ . Assume that  $\partial^2\Omega/\partial c^2 \neq 0$ . Obviously,  $\partial^2\Omega/\partial c^2 < 0$ . The asymptotics of  $Z$  can be found from Eq. (7.3) by Laplace's method:

$$Z = \frac{N_a}{2} e^{-(1/2)N_a \Omega(\hat{c}, \beta, \mu)} \left[ -\pi N_a \frac{\partial^2 \Omega(\hat{c}, \beta, \mu)}{\partial^2 c} \right]^{-1/2}. \quad (7.6)$$

Formula (7.5) follows from Eqs. (7.6) and (7.1). Note also that the point  $\hat{c}$  coincides with the average dislocation density  $\bar{c}$ .

Formula (7.5) holds true also if  $\hat{c} = 0$  and  $\Omega(0, \beta, \mu) \neq 0$ : we still have the exponential asymptotics of the type (7.6) (with a different factor). The last option to consider is  $\hat{c} = 0$  and  $\Omega(0, \beta, \mu) = 0$ . In this case the asymptotics of  $Z$  changes:  $Z$  grows slower than any exponential function of  $N_a$  [under some physically nonrestrictive assumptions satisfied, in particular, for function  $q(c, \beta, \mu)$  of Eq. (6.12)]. Therefore function (7.1) is zero. On the other hand,  $\max_c \Omega(c, \beta, \mu) = 0$  and again Eq. (7.5) is valid.

Consider now the nonequilibrium thermodynamic potential within the approximation (6.12) in terms of temperature that is defined as  $T = 2\pi/\beta$ ,

$$\Omega(c, T, \mu) = c \left[ 1 - \ln \frac{c}{2} - \frac{1}{8\pi\lambda^2 c} \chi \left( \frac{2\pi\lambda^2 c}{T} \right) + \frac{2\pi\mu_*}{T} \right]. \quad (7.7)$$

Let  $c$  tends to zero. Keeping only the leading terms in Eq. (7.7) as  $c \rightarrow 0$  in accordance with Eq. (6.10), we have

$$\Omega(c, T, \mu) = \left( \frac{1}{4T} - 1 \right) c \ln c. \quad (7.8)$$

We see that there is a critical value of temperature  $T_{\text{cr}} = 1/4$ , where the behavior of the system changes: for  $T < T_{\text{cr}}$ , the function  $\Omega(c, T, \mu)$  has a local maximum at  $c = 0$ , for  $T > T_{\text{cr}}$  its local maximum is attained at some positive value of  $c$ . Whether function  $\Omega(c, T, \mu)$  has a global maximum at  $\hat{c} = 0$  or at  $\hat{c} > 0$  depends on the value of chemical potential  $\mu_*$ . Some conclusion can be drawn from the analysis of function  $\Omega(c, T, \mu)$  for small  $c$  and small temperature deviations from the critical value. Expanding  $\Omega$  with respect to small  $c$  and  $T' = (T - T_{\text{cr}})/T$  and keeping only the leading terms, we have

$$\Omega(c, T, \mu) = c [-T' \ln c + 8\pi(\mu_* - \mu_{\text{cr}}) + AT'], \quad (7.9)$$

where  $\mu_{\text{cr}} = -\ln(16\pi\lambda^2)/8\pi$ , and  $A$  is some coefficient whose value is not essential for what follows. Let  $T'$  be much smaller than  $\mu_* - \mu_{\text{cr}}$ . Equating  $\partial\Omega/\partial c$  to zero we have

$$-T' \ln c + 8\pi(\mu_* - \mu_{\text{cr}}) = 0. \quad (7.10)$$

This equation has a solution  $\hat{c}$  that does not exceed unity only if  $\mu_* < \mu_{\text{cr}}$ . The solution is

$$\hat{c} = e^{8\pi(\mu_* - \mu_{\text{cr}})/T'}. \quad (7.11)$$

For  $\lambda = 1$  the critical value of chemical potential is equal to  $\mu_{\text{cr}} = -0.1559$ .

Numerical analysis of function (7.7) shows that the above mentioned features established for small values of  $c$  and  $T'$  are, in fact, the global features of the thermodynamic potential. The global features are illustrated in Figs. 4–5. Figure 4(a) shows the dependence of  $\Omega(c, T, \mu_*)$  on  $c$  for  $\mu_* = -10$  and  $T = T_{\text{cr}} = 1/4$ ,  $T = 6.5$ ,  $T = 7$ . Figure 4(b) shows the corresponding dependence of  $\bar{c}$  on  $T$ . Note that all derivatives of function  $\bar{c}(T)$  vanish at  $T = T_{\text{cr}}$ . Thermodynamic potential  $\Omega(T, \mu_*)$  is continuous at  $T = T_{\text{cr}}$  along with all its

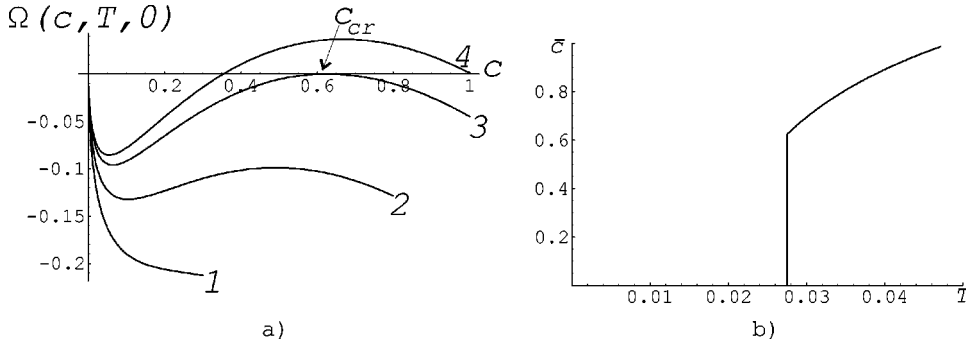


FIG. 5. (a)  $\Omega(c, T, \mu_*)$  as function of  $c$  for  $\lambda=1, \mu_*=0$ ; curve 1:  $T=0.02$ , curve 2:  $T=0.024$ , curve 3:  $T=0.02757$ , curve 4:  $T=0.029$ . (b) Average dislocation density  $\bar{c}$  as function of  $T$  for  $\lambda=1, \mu_*=0$

derivatives with respect to  $T$ . Indeed, from Eqs. (7.9) and (7.11),  $\Omega = AT' \exp[8\pi(\mu_* - \mu_{cr})/T']$  and all derivatives of  $\Omega$  with respect to  $T$  vanishes at  $T = T_{cr}$ . Thus, the transition is of infinite order.

The situation changes if  $\mu$  becomes greater than  $\mu_{cr}$ . A typical graph is shown in Fig. 5(a) for the case  $\mu_* = 0, \lambda = 1$ . At low temperatures (curve 1)  $\Omega(c, \beta, \mu)$  is monotonically decreasing, it has the only maximum at the end point  $c=0$ . As temperature rises a new local maximum appears (curve 2), but it is still smaller than that at the end point  $c=0$ , and the average dislocation density is still equal to zero. The value of  $\Omega(c, \beta, \mu)$  at the new maximum becomes equal to the value at the end point  $c=0$  when temperature reaches the low critical value  $T_{cr}^-$  (curve 3). For  $T > T_{cr}^-$  the maximum is greater than 0 and attained at a point  $\bar{c} > c_{cr}$  (curve 4). At the instant when temperature passes the point  $T_{cr}^-$ , the average dislocation density jumps from zero to  $c_{cr}$ . At  $T = T_{cr}^-$  thermodynamic potential has a jump of the derivative with respect to  $\mu_*$ , and the transition is the first-order phase transition. The corresponding graph of the average dislocation density as function of  $T$  is shown in Fig. 5(a). The transition takes place at  $T = T_{cr}^- \approx 0.02757$ , at which  $\bar{c}$  jumps from zero to 0.626.

The closer the value of  $\mu_*$  to  $\mu_{cr}$ , the smaller the jump of average concentration  $\bar{c}$ . For  $\lambda=1, \mu_* = -0.01$  the plot of  $\bar{c}(T)$  is shown in Fig. 6(a) [the jump in  $\bar{c}(T)$  is  $\approx 0.19$  and  $T_{cr}^- \approx 0.0622$ ]. This plot corresponds to the phase diagram shown in Fig. 1(b). For  $\lambda=1, \mu_* = -0.02$  the plot of  $\bar{c}(T)$  is shown in Fig. 6(b).

The point  $(\bar{c}, T_{cr}^-)$  where the jump occurs coincides with the point on the curve  $q(c, T, \mu) = 1$  in the  $(c, T)$ -plane where it has the vertical tangent line. Indeed, differentiating function (7.4) with respect to  $c$  we have  $\ln q + cq^{-1} \partial q / \partial c = 0$ .

The above mentioned point obeys this equation since at this point  $q=1$  and  $\partial q / \partial c = 0$ . This fact along with the property of the curve  $q=1$ , which will be discussed in Sec. X, make the graphs of these curves quite instructive. These curves are shown in Fig. 7 for various values of parameters.

Figure 7(a) illustrates the dependence of the curve  $q=1$  on parameter  $\lambda$ . Increase of  $\lambda$  corresponds to increase of the dislocation core size  $\epsilon$ . As was mentioned in Sec. II,  $-\beta H_N$  grows if  $\epsilon$  increases. Thus,  $J_N$  and, hence,  $q$ , must grow. This corresponds to motion of the curves  $q=1$  to the left in Fig. 7(a). Accordingly, the low critical temperature  $T_{cr}^-$  decreases as  $\lambda$  increases.

Decrease of  $\mu_*$  yields decrease of  $q$ . Therefore the curves  $q=1$  move to the right as shown in Fig. 7(b). Accordingly, the low critical temperature grows. The influence of  $\mu_*$  is especially important for low temperature since the last term in Eq. (6.13) becomes dominant as  $T \rightarrow 0$ . The level curve  $q=1$  is plotted in Fig. 2(b) for  $\lambda=1, \mu_* = -0.01$ . One can see that the critical temperature  $T_{cr}^- \approx 0.0622$  is larger than that obtained in the case  $\mu_* = 0$ . At the same time, the corresponding dislocation density  $c_{cr} \approx 0.19$  is lower than that for  $\mu_* = 0$ , for which  $c_{cr} \approx 0.626$ . As  $\mu_* \rightarrow \mu_{cr}$  from above ( $\mu_{cr} \approx -0.1559$  for  $\lambda=1$ ) the low critical temperature  $T_{cr}^-$  approaches  $T_{cr}$ , while the critical dislocation density  $c_{cr}$  approaches zero [see Fig. 7(c)].

Figure 8(a) shows the phase diagram in the  $(T, \mu_*)$ -plane. The low critical temperature  $T_{cr}^-$  increases monotonically as  $\mu_*$  decreases down to the critical value  $\mu_{cr}$ , from there on  $T_{cr}^- = T_{cr} = 1/4$ . The corresponding phase diagram in the  $(T, z)$ -plane, with  $z = e^{2\pi\mu_*/T}$  being the fugacity, is shown in Fig. 8(b).

## VIII. UPPER BOUND FOR PHASE DIAGRAMS

In this section we construct a lower bound for the function  $q(c, T, \mu)$ , i.e., a function  $\tilde{q}(c, T, \mu)$  such that

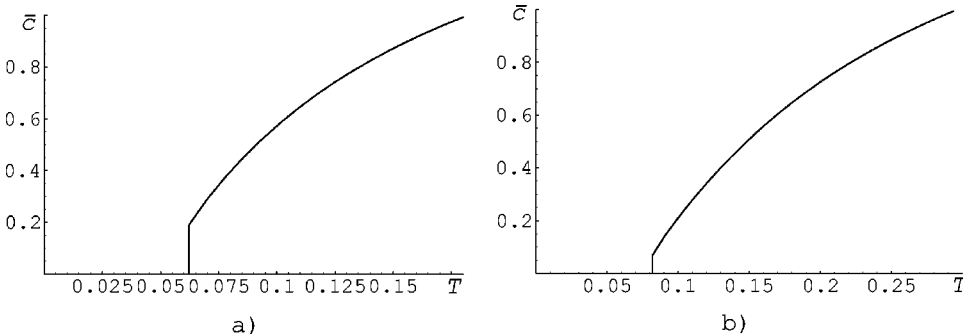


FIG. 6. Average dislocation density  $\bar{c}$  as function of  $T$  for  $\lambda=1$  and (a)  $\mu_* = -0.01$ , (b)  $\mu_* = -0.02$ .

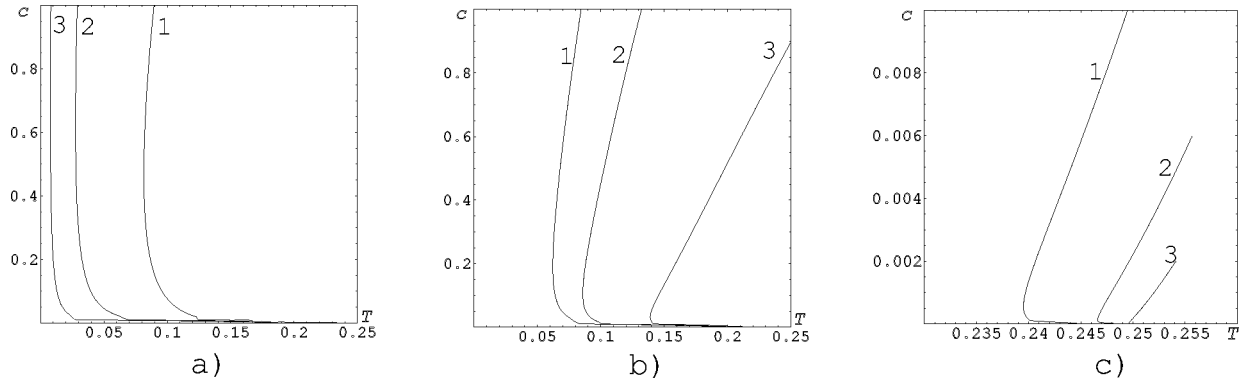


FIG. 7. Level curves  $q=1$  for different  $\lambda$  and  $\mu_*$ . (a)  $\mu_*=0$ ; curve 1:  $\lambda=0.5$ , curve 2:  $\lambda=1$ , curve 3:  $\lambda=2$ . (b)  $\lambda=1$ ; curve 1:  $\mu_*=-0.01$ , curve 2:  $\mu_*=-0.02$ , curve 3:  $\mu_*=-0.05$ . (c)  $\lambda=1$  ( $\mu_{cr}\approx-0.1559$ ); curve 1:  $\mu_*=-0.14$ , curve 2:  $\mu_*=-0.15$ , curve 3:  $\mu_*=-0.155$ .

$$\tilde{q}(c, T, \mu) \leq q(c, T, \mu). \quad (8.1)$$

If  $\tilde{q} > 1$ , then  $q > 1$ , and the nucleation transition occurs. Since the level curve  $q=1$  separates the  $(c, T)$ -plane into two regions, that on the right corresponding to  $q > 1$  and that on the left corresponding to  $q < 1$ , the level curve  $\tilde{q}=1$  should lie in the right region. Thus,  $\tilde{q}=1$  outlines the region where massive nucleation of charges does occur.

Consider the integral  $J_N$

$$J_N = \int e^{-(1/2)(Au, u)} [Q(u)]^N \mathcal{D}u. \quad (8.2)$$

We are going to show that

$$J_N \geq \tilde{J}_N = \text{const} \sqrt{N} e^{NS(c, \beta_*)}, \quad (8.3)$$

where  $S(c, \beta_*)$  is determined by the variational problem

$$S(c, \beta_*) = \max_{0 \leq \eta \leq 1} \min_{0 \leq z \leq 1} \left[ \ln(1 - \eta) + z \eta - \frac{1}{4\pi c \lambda^2} \chi(\beta_* c \lambda^2 z) \right], \quad (8.4)$$

and  $\chi(z)$  is the function (6.9). From Eqs. (8.3) and (3.12), for large  $N$ , an estimate follows

$$q_N \geq 2 \left( 1 - \ln \frac{c}{2} \right) + S(c, \beta_*) + 2\mu_* \beta_*.$$

We start with the derivation of Eq. (8.3).

Denote by  $g(\xi)$  the function

$$g(\xi) = \int_{Q(u) \leq \xi} e^{-(1/2)(Au, u)} \mathcal{D}u, \quad (8.5)$$

where  $Q(u)$  is the functional (5.7). The functional  $Q(u)$  is positive and does not exceed unity since

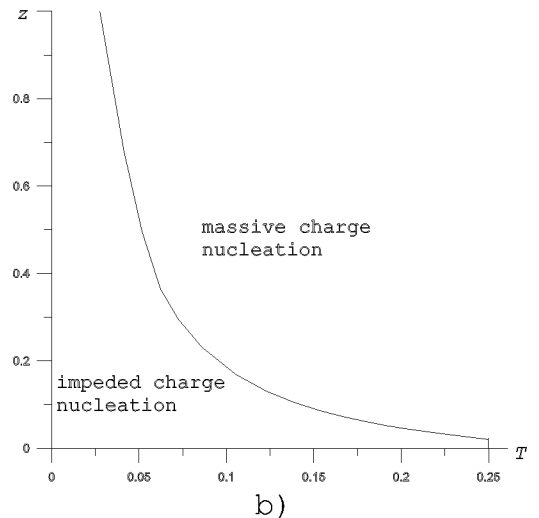
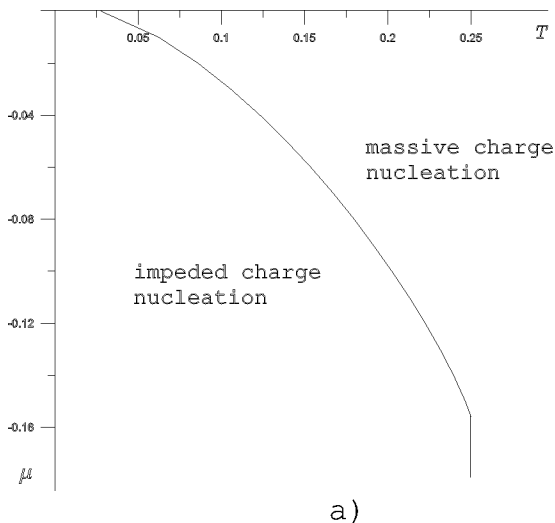


FIG. 8. Phase diagram for  $\lambda=1$  in (a)  $(T, \mu_*)$  plane, (b)  $(T, z)$  plane, with  $z$  being fugacity.

$$\begin{aligned}
 Q(u) &= \left( \int_C \cos \sqrt{\beta_*} u \frac{d^2x}{a^2} \right)^2 + \left( \int_C \sin \sqrt{\beta_*} u \frac{d^2x}{a^2} \right)^2 \\
 &\leq \int_C \frac{d^2x}{a^2} \int_C \cos^2 \sqrt{\beta_*} u \frac{d^2x}{a^2} \\
 &\quad + \int_C \frac{d^2x}{a^2} \int_C \sin^2 \sqrt{\beta_*} u \frac{d^2x}{a^2} = 1.
 \end{aligned}$$

Therefore,  $g(\xi) = 0$  if  $\xi \leq 0$ ,  $g(\xi) = 1$  if  $\xi \geq 1$ , and  $g(\xi)$  increases monotonically as  $\xi$  grows from 0 to 1. Obviously  $J_N = \int_0^1 \xi^N dg(\xi)$ . Integrating by parts we obtain

$$J_N = N \int_0^1 \xi^{N-1} [g(1) - g(\xi)] d\xi. \tag{8.6}$$

The function  $G(\xi) \equiv g(1) - g(\xi)$  can be written as

$$\begin{aligned}
 G(\xi) &= \int_{Q(u) \leq 1} e^{-(1/2)(Au,u)} \mathcal{D}u - \int_{Q(u) \leq \xi} e^{-(1/2)(Au,u)} \mathcal{D}u \\
 &= \int_{Q(u) \geq \xi} e^{-(1/2)(Au,u)} \mathcal{D}u. \tag{8.7}
 \end{aligned}$$

It is convenient to introduce the variable  $\eta = 1 - \xi$  and write Eqs. (8.6) and (8.7) in the form

$$J_N = N \int_0^1 (1 - \eta)^{N-1} G(1 - \eta) d\eta,$$

$$G(1 - \eta) = \int_R e^{-(1/2)(Au,u)} \mathcal{D}u,$$

where  $R$  is the following region  $R = \{u | 1 - Q(u) \leq \eta\}$ . Consider also the region

$$\tilde{R} = \left\{ u \left| \frac{\beta_*}{a^2} \int_C u^2 d^2x \leq \eta \right. \right\}.$$

The region  $R$  is wider than the region  $\tilde{R}$ . Indeed,

---


$$\begin{aligned}
 1 - Q(u) &= 1 - \left( \int_C \cos \sqrt{\beta_*} u \frac{d^2x}{a^2} \right)^2 - \left( \int_C \sin \sqrt{\beta_*} u \frac{d^2x}{a^2} \right)^2 \\
 &= \left( 1 - \int_C \cos \sqrt{\beta_*} u \frac{d^2x}{a^2} \right) \left( 1 + \int_C \cos \sqrt{\beta_*} u \frac{d^2x}{a^2} \right) - \left( \int_C \sin \sqrt{\beta_*} u \frac{d^2x}{a^2} \right)^2 \\
 &= \left( 1 - \int_C \cos \sqrt{\beta_*} u \frac{d^2x}{a^2} \right) \left( 2 - 1 + \int_C \cos \sqrt{\beta_*} u \frac{d^2x}{a^2} \right) - \left( \int_C \sin \sqrt{\beta_*} u \frac{d^2x}{a^2} \right)^2 \\
 &= 2 \left( 1 - \int_C \cos \sqrt{\beta_*} u \frac{d^2x}{a^2} \right) - \left( 1 - \int_C \cos \sqrt{\beta_*} u \frac{d^2x}{a^2} \right)^2 - \left( \int_C \sin \sqrt{\beta_*} u \frac{d^2x}{a^2} \right)^2 \\
 &< 2 \int_C (1 - \cos \sqrt{\beta_*} u) \frac{d^2x}{a^2} \\
 &< \frac{\beta_*}{a^2} \int_C u^2 d^2x.
 \end{aligned}$$

In the last inequality we took into account that  $1 - \cos x \leq x^2/2$ . Therefore, if  $u \in \tilde{R}$  then  $u \in R$  and, hence,  $\tilde{R} \subset R$ . Thus,  $G(1 - \eta) \geq \tilde{G}(\eta) \equiv \int_{\tilde{R}} e^{-(1/2)(Au,u)} \mathcal{D}u$ , and

$$J_N \geq \tilde{J}_N \equiv N \int_0^1 (1 - \eta)^{N-1} \tilde{G}(\eta) d\eta.$$

The asymptotics of the integral  $\tilde{J}_N$  as  $N \rightarrow \infty$  can be found explicitly. To this end we put  $\tilde{J}_N$  in the form

---


$$\begin{aligned}
 \tilde{J}_N &= N \int_0^1 (1 - \eta)^{N-1} \int_{\beta_* / a^2 \int_C u^2 d^2x < \eta} e^{-(1/2)(Au,u)} \mathcal{D}u d\eta \\
 &= N \int (1 - \eta)^{N-1} \frac{dz}{2\pi iz} \exp \left[ z\eta - \frac{z\beta_*}{a^2} \int_C u^2 d^2x \right. \\
 &\quad \left. - \frac{1}{2}(Au,u) \right] \mathcal{D}u d\eta.
 \end{aligned}$$

Here we used a presentation of the step function  $\theta(E)$

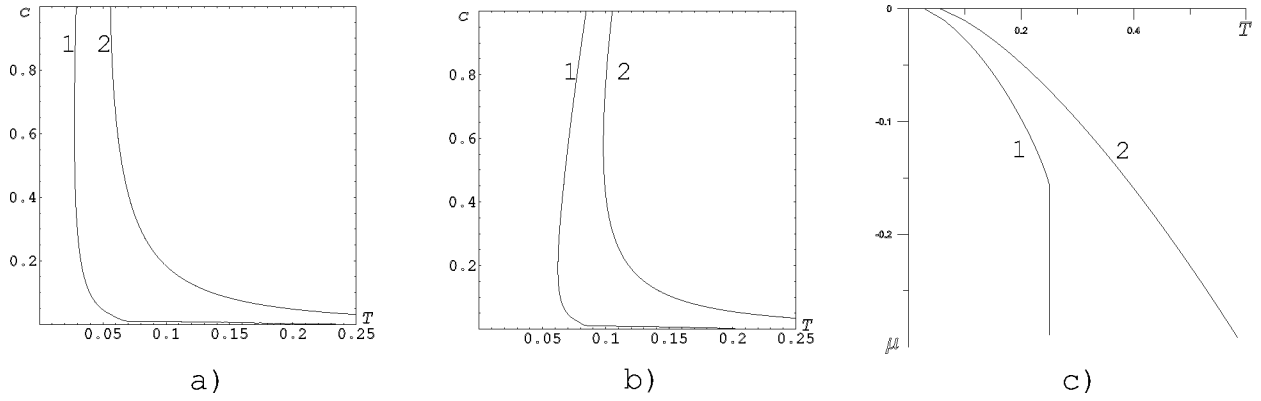


FIG. 9. Lower bound for function  $q$  at  $\lambda=1$ . (a)  $\mu_* = 0$ ; curve 1:  $q=1$ , curve 2:  $\tilde{q}=1$ . (b)  $\mu_* = -0.01$ ; curve 1:  $q=1$ , curve 2:  $\tilde{q}=1$ . (c) Upper bound for phase diagram: curve 1 (solid line), phase diagram of approximate theory from Fig. 8; curve 2 (dash line): exact upper bound.

$= \int e^{Fz} dz / 2\pi iz$ . The integral is taken over the line  $[a - i\infty, a + i\infty]$  in the complex  $z$  plane,  $a > 0$ . Changing  $z$  to  $Nz$  we obtain

$$\tilde{J}_N = N \int \frac{dz d\eta}{2\pi iz} e^{N[\ln(1-\eta) + z\eta]} \int_P \exp\left[-\frac{1}{2}(Au, u) - \frac{z\beta_* N}{a^2} \int_C u^2 d^2x\right] \mathcal{D}u.$$

As shown in Appendix C, the integral over  $P$  is equal to  $[\Phi_\varepsilon(z\beta_* N/2\pi^2)]^{-1/2}$ . The function  $\Phi_\varepsilon(z\beta_* N/2\pi^2)$  converges in the thermodynamic limit to  $\exp[N\chi(\beta_* \rho z)/2\pi\rho]$ , where  $\chi(z)$  is given by Eq. (6.9). Thus,

$$\tilde{J}_N = N \int_0^1 \int_{a-i\infty}^{a+i\infty} \frac{dz d\eta}{2\pi iz} e^{N[\ln(1-\eta) + z\eta - (1/4\pi\rho)\chi(\rho\beta_* z)]}.$$

The asymptotics of this integral is given by Eqs. (8.3) and (8.4).

Denote by  $\tilde{q}(c, T, \mu_*)$  the function

$$\tilde{q}(c, T, \mu_*) = 2 \left(1 - \ln \frac{c}{2}\right) + S(c, 2\pi/T) + 4\pi\mu_*/T.$$

The level curves  $\tilde{q}=1$  are shown in Figs. 9(a,b) for various values of parameters.

Figure 9(c) shows the upper bound of the phase diagram in the plane  $(T, \mu_*)$ . The dash line corresponds to  $\tilde{T}_{cr}^-$  versus  $\mu_*$ , where  $\tilde{T}_{cr}^-$  is the critical temperature determined from the curve  $\tilde{q}=1$ . The solid line on this figure corresponds to our approximate theory.

### IX. DIPOLE STATE VERSUS PLASMA STATE

The phase transition described above corresponds to a nucleation transition if the temperature is high enough for the dislocations to appear. Now we are going to examine whether the positive and negative dislocations are bound in dipoles or form a neutral plasma. Unfortunately, the moment

$m = \langle (r_1^+ - r_1^-)^2 \rangle$ , being a simple characteristic, does not serve as an indicator of the dipole-plasma transition because  $m$  is always of the order  $a^2$ . Indeed, in the plasma state,  $m$  is obviously of the order  $a^2$ ; in the dipole state,  $r_1^+$  may be bound with, say,  $r_2^-$  and  $r_1^-$  with  $r_2^+$  while  $r_1^+$  and  $r_1^-$  run over the whole specimen, therefore, again  $m \sim a^2$ . One needs a more subtle characteristics. As such we consider the probability density of position of the first negative dislocation under the condition that there are  $N$  dislocation pairs in the specimen and the positions of all positive dislocations  $r_1^+, \dots, r_N^+$  are fixed. Denote this function of  $r_1^-$  by  $f_N(r_1^- | r_1^+, \dots, r_N^+)$ . In the dipole state the function  $f_N(r_1^- | r_1^+, \dots, r_N^+)$  has strong local maxima at the points  $r_1^+, \dots, r_N^+$ . Otherwise the system is in the plasma state.

According to Eq. (3.1)

$$f_N(r_1^- | r_1^+, \dots, r_N^+) = \frac{1}{Z_N} \int e^{-\beta H_N(r_1^-, \dots, r_N^-)} d^2 r_2^- \dots d^2 r_N^- \quad (9.1)$$

Note that all factors that do not depend on  $r_1^-$  can be included in the normalizing factor  $Z_N$ . In particular, one can use formula (3.3) for  $-\beta H_N$ . Using Eqs. (2.11) and (5.3) we write Eq. (9.1) as a functional integral

$$f_N(r_1^- | r_1^+, \dots, r_N^+) = \int \exp\left[-\frac{1}{2}(Au, u) + i\sqrt{\beta_*} u(r_1^-) - i\sqrt{\beta_*} \sum_{a=1}^N u(r_a^+)\right] \times \left(\int_C e^{i\sqrt{\beta_*} u(x)} d^2x\right)^{N-1} \frac{\mathcal{D}u}{Z_N}. \quad (9.2)$$

Integration with respect to  $u$  is taken over the subspace extracted by the constraint (2.10). Since  $N$  is large, we may replace the power  $(N-1)$  in Eq. (9.2) by  $N$  and write Eq. (9.2) in the form



$$f_N(r_1^- | r_1^+, \dots, r_N^+) = \frac{1}{Z_N} \int e^{-(1/2)(Au, u) + i\sqrt{\beta_*}u(r_1^-) + Ns(u)} \mathcal{D}u, \quad (9.3)$$

where

$$s(u) = -\frac{i\sqrt{\beta_*}}{N} \sum_{a=1}^N u(r_a^+) + \ln \int_C e^{i\sqrt{\beta_*}u(x)} d^2x. \quad (9.4)$$

Note that functional (9.4) is invariant with respect to shifts of  $u$  by a constant.

Let the positive charges be distributed more or less homogeneously and  $u(x)$  be a smooth function. Then  $\sum_{a=1}^N u(r_a^+)/N \approx \int_C u(x) d^2x/a^2$ , and the first term in Eq. (9.4) vanishes due to Eq. (2.10). The only smooth stationary point of Eq. (9.4) is  $u=0$ . This suggests an approximation of the second term in Eq. (9.4) by the functional

$$\begin{aligned} \ln \int_C e^{i\sqrt{\beta_*}u} d^2x &\approx \ln \left( \int_C d^2x - \frac{\beta_*}{2} \int_C u^2 d^2x \right) \\ &\sim -\frac{\beta_*}{2a^2} \int_C u^2 d^2x. \end{aligned}$$

Here we dropped the constant  $\ln a^2$  redefining  $Z_N$ . Finally, we put

$$s(u) = -\frac{i\sqrt{\beta_*}}{N} \sum_{a=1}^N u(r_a^+) - \frac{\beta_*}{2a^2} \int_C u^2 d^2x. \quad (9.5)$$

One can regard Eq. (9.5) as the first terms of the high temperature (small  $\beta_*$ ) expansion of  $s$ . In this approximation  $f_N(r_1^- | r_1^+, \dots, r_N^+)$  can be found explicitly. Indeed,

$$\begin{aligned} Z_N f_N(r_1^- | r_1^+, \dots, r_N^+) &= \int e^{-(1/2)(Au, u) + i\sqrt{\beta_*}u(r_1^-) + Ns(u)} \mathcal{D}u \\ &= e^{\min_u I(u, r_1^- | r_1^+, \dots, r_N^+)}, \end{aligned} \quad (9.6)$$

$$\begin{aligned} I(u, r_1^- | r_1^+, \dots, r_N^+) &= \frac{1}{2}(Au, u) \\ &\quad + \frac{\beta_* N}{2a^2} \int u^2 d^2x + \sqrt{\beta_*}u(r_1^-) \\ &\quad - \sqrt{\beta_*} \sum_{a=1}^N u(r_a^+). \end{aligned}$$

Here we use again Eq. (5.3). Note that, due to the presence of the term  $\beta_* N \langle u^2 \rangle / 2$  that is positive definite, the functional  $I$  is bounded below in  $P$ . Therefore the constraint  $\langle u \rangle = 0$  can be removed in the minimization problem (9.6), for this changes  $\min I$  by a constant that can be included in the normalizing factor.

Denote by  $G(x, x')$  the periodic solution of the equation

$$\Delta G - \epsilon^2 \Delta^2 G - \frac{\beta_* N}{a^2} G = -\delta(x - x'). \quad (9.7)$$

Obviously,  $G(x, x')$  is a function of the difference  $x - x'$ . At  $x = x'$  the function  $G$  is finite; denote its value by  $G_0$ .

We have

$$\begin{aligned} \min I = & -\frac{\beta_*}{2} \left[ \sum_{a,b=1}^N G(r_a^+, r_b^+) + G(r_1^-, r_1^-) \right. \\ & \left. - 2 \sum_{a=1}^N G(r_a^+, r_1^-) \right]. \end{aligned} \quad (9.8)$$

Since  $G(r_1^-, r_1^-) = G_0$  is a constant, the only terms depending on  $r_1^-$  are  $\sum_a G(r_a^+, r_1^-) = \sum_a G(r_1^- - r_a^+)$ . Keeping only these terms and redefining  $Z_N$  accordingly, we obtain

$$f_N(r_1^- | r_1^+, \dots, r_N^+) = \text{const} \exp \left[ \beta_* \sum_{a=1}^N G(r_1^- - r_a^+) \right]. \quad (9.9)$$

So the dipole-plasma transition is determined by the behavior of the solution of Eq. (9.7). Solution of Eq. (9.7) in scaled coordinates  $x/\epsilon$  depends only on the parameter  $\kappa = 4\pi\lambda^2 c/T$ . For finite  $\kappa$  the solution of Eq. (9.7) is concentrated around the point  $x'$ . Thus, the negative charge  $r_1^-$  is located in the vicinity of a positive charge with overwhelming probability. For small  $\kappa$  the solution of Eq. (9.7) spreads over the cell, and the system is in the plasma state. Small  $\kappa$  corresponds to small concentrations. This suggests that the nucleation transition at small concentrations is accompanied by dipole debonding while the dipoles nucleated at high concentrations may remain bounded.

## X. PROBABILITY DISTRIBUTION

In this section we consider some features of probability distribution  $p_N$ .

First, let temperature and chemical potential be such that  $q(c, \beta, \mu) < 1$  for all  $c$ . Then the sum

$$Z = \sum_{N=0}^{N_{\max}} (q_N)^N \quad (10.1)$$

is finite in thermodynamic limit because its tail is approximated by the converging series  $\sum q^N$ . In thermodynamic limit we may put in Eq. (10.1),  $N_{\max} = \infty$ . The average number of charges

$$\bar{N} = \sum_{N=0}^{\infty} N p_N$$

is finite, since for large  $N$  the terms of the sum decay exponentially as  $Nq^N/Z = Ne^{N \ln q/Z}$ ,  $\ln q < 0$ . We conclude that in the zone of ‘‘impeded charge nucleation’’ the average number of charges does not depend on the specimen size.

If function  $q(c, \beta, \mu) > 1$  for some  $c, \beta$ , and  $\mu$ , the situation changes drastically. In this case, in accordance with Eq. (7.6),

$$Z = \text{const } e^{-(1/2)N_a \Omega(\beta, \mu)} \quad (10.2)$$

is exponentially large since  $\Omega(\beta, \mu) < 0$ . The average concentration  $\bar{c}$  is finite, and the average number of charges grows proportionally to the specimen size. In this case it is better to regard probability  $p_N$  as a function of  $c$ ,  $p = p(c)$ . Probability  $p(c)$  reaches its maximum at the point  $\bar{c}$ . Indeed, for a given  $c$ ,  $N$  tends to infinity as  $N_a \rightarrow \infty$ . Thus, one can replace in Eq. (3.8)  $q_N$  by  $q$  and write

$$p(c) = \frac{q^{(1/2)cN_a}}{Z}. \quad (10.3)$$

From Eqs. (10.3), (10.2), and (7.4)

$$p(c) = \text{const exp} \left( \frac{1}{2} N_a \left\{ c \ln q(c, \beta, \mu) - \max_c [c \ln q(c, \beta, \mu)] \right\} \right). \quad (10.4)$$

Obviously, the maximum value of  $p(c)$  is reached at the point  $c = \bar{c}$ . Function  $p(c)$  decays exponentially away from the point  $c = \bar{c}$ .

Additional drops of function  $p(c)$  occur at points  $c = c_*$  where  $q(c, \beta, \mu) = 1$ . Indeed, from Eq. (10.4)

$$\begin{aligned} & \frac{p(c_* + \Delta c)}{p(c_* - \Delta c)} \\ &= \exp \left\{ \frac{1}{2} N_a \left[ (c_* + \Delta c) \ln q(c_* + \Delta c, \beta, \mu) - (c_* - \Delta c) \ln q(c_* - \Delta c, \beta, \mu) \right] \right\} \\ &= e^{N_a (dq/dc_*) \Delta c}. \end{aligned}$$

We see that probability in the region  $q > 1$  is exponentially larger than probability in the region  $q < 1$ . This phenomenon can be hidden by the large values of  $Z$ : probability near the curve  $q = 1$  is exponentially small. An exception is the singular point where the curves  $\bar{c}(T)$  and  $q = 1$  cross.

#### ACKNOWLEDGMENTS

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#### APPENDIX A: CHEMICAL POTENTIAL

In this Appendix we discuss the physical meaning of chemical potential in the problem under consideration. De-

note by  $x_i$  the position of atoms of a 2D crystal, where  $i = 1, \dots, N_a$ ,  $N_a$  is the total number of atoms. Let  $H(x_1, \dots, x_{N_a})$  be the potential energy of the atom configuration  $x_1, \dots, x_{N_a}$ . The probability of atoms to occupy the positions  $x_1, \dots, x_{N_a}$  is assumed to be Gibbsian  $f(x_1, \dots, x_{N_a}) = e^{-\beta H(x_1, \dots, x_{N_a})} / Z_0$ . Various equilibrium states of the crystal correspond to local minima of function  $H$ . There are local equilibrium states that correspond to the presence of dislocations in the crystal. The  $2N_a$ -dimensional configurational space of all possible atom positions can be split into subregions that correspond to no dislocations, to the presence of one dislocation positioned at point  $r_1$ , two dislocations positioned at points  $r_1, r_2$ , etc. The probability that there is a dislocation at the point  $r_1$  is given by the integral  $f(r_1) = \int e^{-\beta H(x_1, \dots, x_{N_a})} d^2 x_1 \dots d^2 x_{N_a} / Z_0$ , which is taken over the subregion of the configurational space corresponding to this dislocation position. Denote this subregion by  $A(r_1)$ . Then

$$\begin{aligned} f(r_1) &= e^{-\beta H(r_1)} \\ &\times \int_{A(r_1)} \frac{1}{Z_0} e^{-\beta [H(x_1, \dots, x_{N_a}) - H(r_1)]} d^2 x_1 \dots d^2 x_{N_a}, \end{aligned} \quad (A1)$$

where  $H(r_1)$  is the energy of the crystal containing one dislocation at the point  $r_1$ . We introduce the parameter  $\mu_1$  by the formula

$$\int_{A(r_1)} \frac{1}{Z_0} e^{-\beta [H(x_1, \dots, x_{N_a}) - H(r_1)]} d^2 x_1 \dots d^2 x_{N_a} = \frac{e^{\beta \mu_1}}{Z}, \quad (A2)$$

where  $Z$  was defined in Sec. III. Moreover, we assume that for states with two dislocations positioned at points  $r_1, r_2$ ,

$$\begin{aligned} & \int_{A(r_1, r_2)} \frac{1}{Z_0} e^{-\beta [H(x_1, \dots, x_{N_a}) - H(r_1, r_2)]} d^2 x_1 \dots d^2 x_{N_a} \\ &= \frac{e^{2\beta \mu_1}}{Z}, \end{aligned} \quad (A3)$$

and that similar relations are valid for a larger number of dislocations.

Formulas (A2), (A3) determine the physical meaning of the parameter  $\mu_1$ . It is clear that  $\mu_1$  may depend on temperature. Besides, Eq. (A3) may hold only if dislocations are far apart, otherwise  $\mu_1$  in Eq. (A3) may depend on the distance between dislocations.

#### APPENDIX B: ENERGY OF ONE DISLOCATION

In order to find the energy created by one dislocation we have to solve variational problem (2.9) subject to constraint (2.10). Changing variables  $x \rightarrow y = 2\pi x/a$  we have

$$\beta H_0 = -\min_{u \in P} \left\{ \frac{1}{2} \int_{\bar{C}} [(\nabla u)^2 + \varepsilon^2 (\nabla \nabla u)^2] d^2 y - \sqrt{\beta_*} [u(r) - \langle u \rangle] \right\}, \quad (\text{B1})$$

with  $\nabla$  and  $\langle \cdot \rangle$  being the gradient and the averaging operators with respect to  $y$ , respectively,  $\bar{C} = (0, 2\pi) \times (0, 2\pi)$ . Denote by  $G$  the periodic solution (the Green's function) of the equation

$$\Delta G - \varepsilon^2 \Delta^2 G = -\sqrt{\beta_*} \left[ \delta(y-r) - \frac{1}{(2\pi)^2} \right], \quad \langle G \rangle = 0. \quad (\text{B2})$$

Obviously,  $G$  is a function of the difference  $y-r$ . At  $y=r$  the function  $G$  is finite; denote its value by  $G_0$ .

Each periodic function  $u(y)$  with zero mean can be presented as a series

$$u(y) = \sum_{k \in \mathbb{Z}'_2} u_k e^{ik \cdot y}. \quad (\text{B3})$$

Here  $u_k = u'_k + i u''_k$  are some complex numbers, the Fourier coefficients. For real-valued functions  $u(y)$  the Fourier coefficients obey the condition  $\bar{u}_k = u_{-k}$ , where  $\bar{u}$  denotes the complex conjugate of  $u$ . This condition means that  $u_k$  and  $u_{-k}$  are not independent. To deal with independent coefficients we may choose any subset of  $\mathbb{Z}'_2$ , which does not contain points  $k$  and  $-k$  simultaneously. As such we take the set  $\mathbb{Z}'_2^+$  that consists of points  $k = (k_x, k_y)$  with  $k_x \geq 1$ ,  $k_y$  any, and  $k_x = 0$ ,  $k_y \geq 1$ . Then

$$\begin{aligned} u(y) &= 2 \operatorname{Re} \sum_{k \in \mathbb{Z}'_2^+} u_k e^{ik \cdot y} \\ &= 2 \sum_{k \in \mathbb{Z}'_2^+} [u'_k \cos(k \cdot y) - u''_k \sin(k \cdot y)]. \end{aligned}$$

The  $\delta$  function can be presented (symbolically) as a series

$$\delta(y) - \frac{1}{(2\pi)^2} = \sum_{k \in \mathbb{Z}'_2} \frac{1}{(2\pi)^2} e^{ik \cdot y}. \quad (\text{B4})$$

From Eqs. (B2) and (B4) we obtain

$$G(y) = \sum_{k \in \mathbb{Z}'_2} \frac{\sqrt{\beta_*}}{(2\pi)^2 (|k|^2 + \varepsilon^2 |k|^4)} e^{ik \cdot y}.$$

Thus, the energy of the lattice created by one dislocation multiplied by  $\beta$  is given by

$$\begin{aligned} \beta H_0 &= \frac{1}{2} \int_{\bar{C}} [(\nabla G)^2 + \varepsilon^2 (\nabla \nabla G)^2] d^2 y \\ &= \frac{1}{2} \int_{\bar{C}} (\nabla G \nabla \bar{G} + \varepsilon^2 \nabla \nabla G \nabla \nabla \bar{G}) d^2 y \\ &= \frac{\beta_*}{2} \int_{\bar{C}} \sum_{k, m \in \mathbb{Z}'_2} \frac{(k \cdot m + \varepsilon^2 (k \cdot m)^2) e^{ik \cdot y} e^{-im \cdot y}}{(|k|^2 + \varepsilon^2 |k|^4)(|m|^2 + \varepsilon^2 |m|^4)} \\ &\quad \times d^2 y \\ &= \frac{\beta_*}{8\pi^2} \sum_{k \in \mathbb{Z}'_2} \frac{1}{|k|^2 + \varepsilon^2 |k|^4}. \end{aligned} \quad (\text{B5})$$

Since the series in Eq. (B5) converges slowly, we calculate it by summing up the terms with  $k$  inside a circle of radius  $\varrho$  ( $|k| < \varrho$ ) and approximating the rest of the series by a double integral,

$$\sum_{|k| > \varrho} \frac{1}{|k|^2 + \varepsilon^2 |k|^4} \approx \int_{|k| > \varrho} \frac{1}{|k|^2 + \varepsilon^2 |k|^4} d^2 k = \pi \ln \frac{1 + \varepsilon^2 \varrho^2}{\varepsilon^2 \varrho^2}. \quad (\text{B6})$$

For small  $\varrho$  the integral (B6) is approximately equal to  $2\pi \ln(1/\varepsilon)$ . Starting from small  $\varrho$  and increasing  $\varrho$  we obtain convergence of the series (B5) to

$$\beta H_0 \approx \frac{\beta_*}{4\pi} \ln \frac{1}{\varepsilon} + \beta_* \tilde{e}, \quad (\text{B7})$$

where  $\tilde{e}$  does not depend on  $\varepsilon$ . The calculations show that  $\tilde{e} \approx 0.0327386$ . Formula (B7) gives the sum of the dislocation core energy and the energy of surrounding lattice. Separation of the dislocation core energy from this sum is a matter of convention. If we, following Ref. [12], interpret the term  $(1/4\pi) \ln 1/\varepsilon$  as the elastic energy of the lattice surrounding the dislocation, then  $\tilde{e}$  can be regarded as the energy of the dislocation core found within the regularization (2.3).

### APPENDIX C: FUNCTIONAL INTEGRAL

In this Appendix we will evaluate the functional integral

$$I = \int e^{-(1/2)(Au, u) - \nu \langle u^2 \rangle} \mathcal{D}u, \quad (\text{C1})$$

where  $(Au, u)$  is the quadratic functional (2.8), the integral is taken over all functions  $u \in P$  with  $\langle u \rangle = 0$ , and  $\mathcal{D}u$  is defined by the condition

$$\int e^{-(1/2)(Au, u)} \mathcal{D}u = 1. \quad (\text{C2})$$

We show that  $I = 1/\sqrt{\Phi_\varepsilon(\nu/2\pi^2)}$ , where  $\Phi_\varepsilon(z)$  is the function (6.6).

Denote the coordinates of the function  $u(y)$  in the orthogonal basis  $e^{ik \cdot y}$  by  $u_k$  (see Appendix B). Due to the orthogonality of  $e^{ik \cdot y}$  it is easy to see that

$$\begin{aligned} \langle u^2 \rangle &= \langle u \bar{u} \rangle = \left\langle \sum_{k, m \in \mathbb{Z}'_2} u_k \bar{u}_m e^{i(k-m) \cdot y} \right\rangle \\ &= \sum_{k \in \mathbb{Z}'_2} |u_k|^2 = 2 \sum_{k \in \mathbb{Z}_2^+} |u_k|^2. \end{aligned}$$

Similarly

$$\begin{aligned} (Au, u) &= \int [(\nabla u)^2 + \varepsilon^2 (\nabla \nabla u)^2] d^2 y \\ &= 2(2\pi)^2 \sum_{k \in \mathbb{Z}_2^+} (|k|^2 + \varepsilon^2 |k|^4) |u_k|^2. \end{aligned}$$

Since  $|u_k|^2 = (u'_k)^2 + (u''_k)^2$ , and  $(u'_k, u''_k)$  with  $k \in \mathbb{Z}_2^+$  characterize fully periodic functions with zero mean, we shall project  $P$  onto the space of  $u'_k$  and  $u''_k$ . Denote by  $du_k = du'_k du''_k$ . Then

$$\begin{aligned} I &= \int \exp \left\{ - \sum_k [(2\pi)^2 \lambda_k + 2\nu] |u_k|^2 \right\} \\ &\quad \times \prod_{k \in \mathbb{Z}_2^+} \frac{2(2\pi)^2 \lambda_k}{2\pi} \prod_{k \in \mathbb{Z}_2^+} du_k \\ &= \prod_{k \in \mathbb{Z}_2^+} \frac{2(2\pi)^2 \lambda_k}{2(2\pi)^2 \lambda_k + 4\nu} = \frac{1}{\sqrt{\Phi_\varepsilon(\nu/2\pi^2)}}. \end{aligned}$$

#### APPENDIX D: FUNCTION $\chi$

Consider the function

$$\frac{1}{N} h_\varepsilon \left( \frac{zN}{2\pi^2} \right) \equiv - \frac{1}{2N} \sum_{k \in \mathbb{Z}'_2} \ln \left( 1 + \frac{zN}{2\pi^2 (|k|^2 + \varepsilon^2 |k|^4)} \right). \quad (\text{D1})$$

We are going to find its limit as  $N \rightarrow \infty$ ,  $\varepsilon \rightarrow 0$  in such a way that  $\rho = 2N\varepsilon^2/a^2 = N\varepsilon^2/2\pi^2$  remains constant. Let us rewrite Eq. (D1) in the form

$$\frac{1}{N} h_\varepsilon \left( \frac{z}{2\pi^2} N \right) = - \frac{1}{2N\varepsilon^2} \sum_{k \in \mathbb{Z}'_2} \varepsilon^2 \ln \left( 1 + \frac{zN\varepsilon^2/2\pi^2}{\varepsilon^2 |k|^2 + \varepsilon^4 |k|^4} \right). \quad (\text{D2})$$

The sum in Eq. (D2) may be considered as a sum over the lattice with spacing  $\varepsilon$ . Then the sum is an integral sum for the integral over 2D plane

$$\int_{\mathbb{R}_2} \ln \left( 1 + \frac{zN\varepsilon^2/2\pi^2}{|x|^2 + |x|^4} \right) d^2 x.$$

Therefore

$$\begin{aligned} \frac{1}{N} h_\varepsilon \left( \frac{z}{2\pi^2} N \right) \\ \xrightarrow{N \rightarrow \infty, \varepsilon \rightarrow 0} - \frac{1}{4\pi^2 \rho} \int_{\mathbb{R}_2} \ln \left( 1 + \frac{\rho z}{|x|^2 + |x|^4} \right) d^2 x. \end{aligned}$$

In the polar coordinates the latter expression reduces to  $-\chi(\rho z)/4\pi\rho$ , with  $\chi(z)$  given by Eq. (6.9). So,  $\Phi_\varepsilon(Nz) = e^{-2h_\varepsilon(Nz)}$  behaves as  $e^{N\chi(2\pi^2\rho z)/2\pi\rho}$  for large  $N$  and small  $\varepsilon$ .

Note that the integral (6.9) is elementary and can be found exactly. In the interval  $0 < z < 1/4$ , the function  $\chi(z)$  has the form

$$\chi(z) = \frac{1}{2} \sqrt{1-4z} \ln \frac{1-\sqrt{1-4z}}{1+\sqrt{1-4z}} - \frac{1}{2} \ln z. \quad (\text{D3})$$

For  $z \geq 1/4$  function  $\chi(z)$  is given by

$$\chi(z) = \sqrt{4z-1} \arctan \sqrt{4z-1} - \frac{1}{2} \ln z. \quad (\text{D4})$$

Formulas (6.10) follow from Eqs. (D3) and (D4).

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