Reentrant melting in solid films with quenched random impurities

David R. Nelson

Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138 (Received 24 August 1982)

Crystalline films with a quenched distribution of impurities are studied. These materials are stable only over a finite band of temperatures. At sufficiently low temperatures, thermally excited dislocation pairs are broken apart by the random impurity potential. The hexatic phase which results can persist down to T=0. For large impurity concentrations, the solid phase is destroyed entirely. These conclusions are consistent with recent studies of vibrating binary ball-bearing arrays, and could be tested experimentally in a variety of other systems with quenched disorder.

I. INTRODUCTION

In contrast to extensive theoretical investigations of quenched randomness in spin systems,¹ relatively little is known about disorder in crystalline solids. Many theoretical investigations of random magnets are an offshoot of the renormalization-group approach to critical phenomena in pure systems.² Recently, similar methods have led to analytical theories of melting in two-dimensional solids³⁻⁶ based on a dislocation model proposed by Kosterlitz and Thouless.⁷ It is interesting to extend these investigations to account for disorder in thin crystalline films.

In this paper we discuss solid films with quenched impurities. This kind of disorder is illustrated in Fig. 1, which shows an isolated large atom imbedded in a crystalline matrix composed of smaller particles. Such impurities are a source of local dilations and compressions of the crystalline lattice. Although the defect is free to participate in longwavelength phonon excitations, its average position within the surrounding solid matrix is fixed in the sense that it cannot exchange places with a neighboring host atom. This sort of quenching requires small impurity diffusion constants which are readily obtainable at low temperatures. We shall assume that dislocations in the film are in thermodynamic equilibrium. At low temperatures this condition requires equilibration times such that dislocations are able to diffuse by gliding⁸ across the entire crystalline solid.

Our results are conveniently presented within the framework of continuum elastic theory.⁹ The fluctuating phonon displacement field $\vec{u}(\vec{r})$ interacting with quenched impurity fluctuations is described by the free energy (see Sec. II)

$$F = \frac{1}{2} \int d^2 r \left(2\mu u_{ij}^2 + \lambda u_{kk}^2 - 2w \delta c u_{kk} \right) , \qquad (1.1)$$

where $u_{ii}(\vec{r})$ is the symmetrized strain tensor

$$u_{ij}(\vec{\mathbf{r}}) = \frac{1}{2} \left[\partial_i u_j(\vec{\mathbf{r}}) + \partial_j u_i(\vec{\mathbf{r}}) \right], \qquad (1.2)$$

and $\delta c(\vec{r})$ is a fluctuation in the local concentration of impurities. The function $\delta c(\vec{r})$ can also contain contributions from frozen-in vacancies and interstitials associated with the host lattice. The quantities μ and λ are the usual isotropic elastic constants characterizing a triangular solid and w parametrizes the coupling between the local elastic dilation $\nabla \cdot \vec{u} = u_{kk}$ and the quenched-in volume fluctuations



FIG. 1. Disorder introduced into a crystalline matrix by an impurity. Large shaded atom causes a local dilation of the lattice. Square lattice is shown for simplicity, although we shall be primarily interested in impurities imbedded in triangular solids.

27

2902

©1983 The American Physical Society

due to the impurities. An estimate of w is given in Sec. II. We shall assume that a given configuration $\delta c(\vec{r})$ occurs with probability

$$\mathscr{P}[\delta c(\vec{r})] \propto \exp\left[-\frac{1}{2\sigma} \int d^2 r [\delta c(\vec{r})]^2\right].$$
(1.3)

Small deviations from Gaussian distribution (1.3) turn out to be unimportant at long wavelengths. As usual in problems with *quenched* disorder, we assume that it is the free energy rather than the partition function which should be averaged over this probability distribution.

Important effects due to impurity quenching follow from the harmonic free energy (1.1), even in the absence of thermally activated defects like dislocations: Translational order in a solid is conveniently measured via a translational order parameter,⁵

$$\rho_{\vec{\mathbf{G}}}(\vec{\mathbf{r}}) = e^{i \vec{\mathbf{G}} \cdot \vec{\mathbf{u}}(r)}, \qquad (1.4)$$

where \vec{G} is a reciprocal-lattice vector. It is well known that conventional long-range translational order is impossible in two-dimensional (2D) solids at finite temperatures in the sense that correlations of $\rho_{\vec{G}}(\vec{r})$ decay algebraically to zero.¹⁰ In the presence of quenched impurities, this decay takes the form (see Appendix A)¹¹

$$\mathscr{C}_{\vec{G}}(r) \equiv [\langle \rho_{\vec{G}}(\vec{r}) \rho_{\vec{G}}^{*}(\vec{0}) \rangle]_{\mathscr{P}}$$

~1/r^{\$\eta_{\vec{G}}\$}, (1.5a)



FIG. 2. Dislocation pair interacting in a medium of quenched random impurities of various sizes (dark atoms). Atoms associated with the surrounding crystalline matrix are not shown.

where

$$\eta_{\vec{G}} = \left[\frac{k_B T (3\mu + \lambda)}{4\pi\mu(2\mu + \lambda)} + \frac{\sigma w^2}{4\pi(2\mu + \lambda)^2}\right] |\vec{G}|^2.$$
(1.5b)

The angle brackets in Eq. (1.5a) indicate a conventional thermal average weighted by e^{-F/k_BT} with a fixed distribution of impurities. The square brackets and subscript \mathscr{P} mean a subsequent average over the defect probability distribution (1.3). Because the defects are quenched there is a contribution to the algebraic decay embodied in Eqs. (1.5) even at T=0.¹² Extending this calculation to *d* dimensions, one finds that d=2 is a kind of lower critical dimension where arbitrarily small concentrations of quenched impurities first destroy long-range translational order in classical crystalline solids at T=0. The parameter σ can be viewed as a frozen-in "temperature" characterizing the quenched defect distribution.

Just as in pure systems it is important to allow for thermally activated dislocations characterized by a nonvanishing contour integral of the displacement field⁸

$$\oint d\vec{\mathbf{u}} = a_0 \vec{\mathbf{b}} . \tag{1.6}$$

The quantity \vec{b} is a dimensionless Burgers vector, and a_0 is the lattice constant of the solid in the presence of impurities. In addition to the usual logarithmic interaction between dislocations,⁸ we must account for interactions between dislocations and impurities. It is straightforward^{8,13} to show that the energy associated with a dislocation with Burgers vector \vec{b} and position \vec{r} , and an impurity at the origin is (see Sec. II)

$$E_{\rm int} = \frac{\mu w a_0}{\pi (2\mu + \lambda)} \frac{\hat{z} \cdot (\vec{b} \times \vec{r})}{r^2} , \qquad (1.7)$$



FIG. 3. Solid, liquid, and hexatic phases as a function of temperature and the degree of disorder σ . Translational correlation length diverges along the paths marked by arrows.

where \hat{z} is a unit vector perpendicular to the plane of the film. In pure systems melting is triggered by an unbinding of logarithmically bound dislocation pairs.⁷ As illustrated in Fig. 2, we must now understand how the quenched random strains generated by the impurities affect the polarizability of dislocation dipoles.

Our conclusion for this simple model of interacting dislocations and impurities are sketched in Fig. 3. As discussed in Sec. II the randomness parameter σ is an increasing function of impurity concentration. For sufficiently small σ there is the usual⁷ dislocation-mediated continuous melting transition at a temperature $T_m^+(\sigma)$. As pointed out in Refs. 4 and 5, this transition cannot be into an isotropic liquid, but must instead lead to a "hexatic" phase with residual sixfold-bond orientational order. A second transition $T_i(\sigma)$ is necessary to destroy orientational order and complete the melting process. In contrast to defect-free solids, we also find a reentrant dislocation unbinding transition at a lower temperature $T_m^-(\sigma)$. Even though the quenched impurity array is unable to respond to strains induced by dislocation pairs, impurities do make it easier for thermally excited dislocations to separate. At low temperatures we find that dislocation pairs are ripped apart by a quenched random impurity potential which is a superposition of terms like Eq. (1.7). At intermediate temperatures (and small σ) there are enough thermal-dislocation pairs to screen out this potential.

It is only over this intermediate temperature range that the behavior indicated in Eq. (1.5) is qualitatively correct. Outside this range, we expect that translational order decays exponentially. At impurity concentrations such that

$$\sigma > \sigma_c \approx a_0^2 / 64\pi \Omega_0^2 , \qquad (1.8)$$

where Ω_0 is the change in area associated with a single impurity, the solid phase is destroyed entirely. In pure systems (or solids with *annealed* impurities), there is a combination of renormalized elastic constants which approaches a universal value at T_m ,^{4,7}

$$\lim_{T \to T_m} \frac{\mu_R(\mu_R + \lambda_R)a_0^2}{(2\mu_R + \lambda_R)k_BT} = 4\pi$$
(for pure systems). (1.9a)

This universality is destroyed in the presence of quenched random impurities; the limit becomes σ dependent. Just below the point marked by a dot on the melting curve in Fig. 3 we find that

$$\frac{\mu_R(\mu_R + \lambda_R)a_0^2}{(2\mu_R + \lambda_R)k_BT} = 8\pi .$$
(1.9b)

As one approaches the solid phase on the paths indicated by arrows in Fig. 3 the translational correlation length diverges exponentially,

 $\xi_T \sim \exp(\operatorname{const} / |T - T_m^{\pm}|^{\overline{\nu}(\sigma)}) . \qquad (1.10)$

The exponent \overline{v} is σ dependent, and decreases to zero as σ approaches σ_c from below.

In the simple model of impurity disorder considered here the hexatic fluid surrounding the bubble of solid phase in Fig. 3 appears to persist down to T=0. The phase below $T_m^-(\sigma)$ need not be an equilibrium hexatic in real materials, however. As the translational correlation length begins to drop just below the lower melting temperature the impurities may become sufficiently mobile to allow for new processes like phase separation. If, on the other hand, the lower transition occurs sufficiently close to zero temperature, impurity diffusion times will remain large and could eventually become even larger than in the solid. Ultimately, it may become impossible for dislocations to equilibrate as well; the result would be a quenched hexatic "glass" with a nonzero shear modulus on experimental time scales. The crystal could, of course, become unstable at low temperatures via some other mechanism like proliferation of grain boundaries, possibly leading to an isotropic liquid.¹⁴ It cannot remain stable down to T = 0, however.

The results summarized in Fig. 3 are qualitatively similar to those obtained recently by Rubinstein *et al.*¹⁵ for 2D XY magnets with random Dzyaloshinskii-Moriya interactions. Here, random contributions to the exchange coupling between sites in an XY magnet dephase the spins in a way reminiscent of the coupling w in Eq. (1.1). This paper adapts the techniques developed in Ref. 15 to a physically different but mathematically rather similar problem.

A number of recent investigations have focused on the effect of random symmetry-breaking fields on 2D XY magnetism.¹⁶ One motivation of these studies was to eventually understand phase pinning by impurities in solid films. It should be emphasized that the impurities considered here are different. Because our defects are allowed to move with the solid matrix the underlying free energy (1.1) is invariant under a uniform translation,

$$\vec{u}(\vec{r}) \rightarrow \vec{u}(\vec{r}) + \vec{u}_0 . \tag{1.11}$$

Disorder like that considered in Ref. 16, however, breaks translational invariance, and would be obtained by "gluing" the impurities to the substrate. Analogous disorder would occur in physiadsorbed monolayers on a glassy substrate. This random broken translational symmetry is rather like the symmetry disruption in an XY magnet with a random magnetic field. Long-range order is destroyed below *four* dimensions in such systems.¹⁷

It may be possible to find a number of experimental thin-film systems which satisfy the assumptions of this paper. The experimental time scale t_{exp} must be such that

$$L^2/D_g \ll t_{\exp} \ll a_0^2/D_{imp}$$
, (1.12)

where L is a characteristic crystallite size, D_g is the diffusion constant for dislocation glide, and D_{imp} is the impurity diffusion constant. In a classical solid D_g is of order $\omega_0 a_0^2$, where ω_0 is a characteristic zone-boundary phonon frequency⁸; this diffusion constant is typically, in units of cm²/sec,

$$D_g \sim 10^{-4} - 10^{-5}$$
 (1.13)

(Glide diffusion eventually becomes more difficult when the temperature drops below its Debye value.) Impurity diffusion in solids is usually mediated by vacancy motion; the corresponding diffusion constant is roughly

$$D_{\rm imp} \sim D_0 e^{-\epsilon_{\rm imp}/k_B T}, \qquad (1.14)$$

where D_0 is a 2D liquid diffusion constant $(D_0 \sim 10^{-6} \text{ cm}^2/\text{sec})$, and ϵ_{imp} is an impurity activation energy. Since ϵ_{imp} is typically several times the melting temperature T_m , D_{imp} is usually of order $10^{-10} \text{ cm}^2/\text{sec}$ even at T_m .¹⁸ Because of the Arrhenius temperature dependence in Eq. (1.14), impurity diffusion constants such that

$$D_{\rm imp} \le 10^{-17}$$
, (1.15)

in units of cm²/sec, are readily obtainable at low temperatures $(D_{\rm imp} \sim 10^{-17} \text{ cm}^2/\text{sec}$ means that the impurity diffuses ~10 Å in 15 min). Because $D_{\rm imp} \ll D_g$, it appears possible to satisfy the inequalities (1.12) at low temperature and impose simultaneously the important requirement that $L \gg a_0$.

Systems which could be doped to produce the kind of disorder studied here include lipid monolayers on water¹⁹ and polystyrene spheres at a water-air interface.²⁰ Electrons on the surface of helium²¹ could also be studied, but the incompressibility of the electron lattice complicates the application of the theory. Another possible experimental system is incommensurate rare-gas monolayers physiadsorbed on a periodic substrate like graphite.²² Although an additional orientational elastic constant is required to describe these materials,⁵ we still expect reentrant melting at low temperatures provided the solid remains incommensurate. Strongly chemisorbed impurities on the same substrate would create random fields like those studied in Ref. 16, while physiadsorbed defects would lead to the kind

of disorder studied here. Of course, physiadsorbed impurities could also drive transitions into commensurate phases which become more prevalent at low temperatures. One must also insure that impurities cannot diffuse rapidly via evaporation into and condensation from a coexisting bulk vapor phase.

A recent investigation of translational and orientational order in randomly packed ball-bearing arrays¹² supports the theoretical conclusions reached here. When a dilute concentration of large ball bearings imbedded in an otherwise uniform array is subjected to mechanical vibrations, a macroscopic analog of the equilibrium hexatic phase can appear.¹² Dislocations become trapped on a finite subset of the large-sphere inhomogeneities. The resulting structure is just what we would expect in the lowtemperature hexatic region of Fig. 3. Of course, mechanical vibrations are only a crude approximation to the fluctuations present in thermal equilibrium and experiments on lipids, polystyrene spheres, and rare-gas atoms would be highly desirable. Depending on the ratio of sphere sizes some of the ball-bearing arrays in Ref. 12 were disrupted by a network of grain boundaries, suggesting another way in which solids can accommodate impurity disorder.

In Sec. II we develop a model of solids with quenched impurities and introduce dislocations explicitly. The polarizability of dislocations in a quenched random potential is discussed in Sec. III. In Sec. IV we derive and discuss renormalizationgroup recursion relations. Disruption of translational order by harmonic phonons and quenched impurities is discussed in an Appendix.

II. THE MODEL

A. Harmonic theory

In the presence of a frozen array of defects the continuum elastic free energy of a crystalline solid may be written

$$\mathcal{F} = \frac{1}{2} \int d^2 r (2\mu u_{ij}^2 + \lambda u_{kk}^2) - \int d^2 r \, \sigma_{ij}^{imp} u_{ij} , \qquad (2.1)$$

where $\sigma_{ij}^{imp}(\vec{r})$ is the stress due to the impurities. Assuming for simplicity that an isolated impurity acts like a localized region of expansion or compression in an otherwise rigid matrix, we find a contribution to $\sigma_{ij}^{imp}(\vec{r})$ of the form¹³

$$(\mu + \lambda)\Omega_0 \delta_{ii} \delta(\vec{r} - \vec{r}_i) , \qquad (2.2)$$

where \vec{r}_i is the impurity position and Ω_0 is the change in crystal area due to the defect. The quantity Ω_0 , of course, can be of either sign. Adding up the stresses associated with a concentration

$$c(\vec{r}) \equiv \sum_{i} \delta(\vec{r} - \vec{r}_{i})$$
(2.3)

of impurities at positions \vec{r}_i , we find that \mathscr{F} may be written

$$\mathcal{F} = \frac{1}{2} \int d^2 r (2\mu u_{ij}^2 + \lambda u_{kk}^2) - (\mu + \lambda) \Omega_0 \int d^2 r \, c \, (\vec{r}) u_{kk}(\vec{r}) \,.$$
(2.4)

At sufficiently long wavelengths we should be able to replace $c(\vec{r})$ by a smooth function of \vec{r} and ignore the discreteness implied by (2.3). It is convenient to measure this smoothed defect concentration from its value averaged over the area of the crystal, and define

$$\delta c(\vec{r}) \equiv c(\vec{r}) - c_0 , \qquad (2.5a)$$

where

$$c_0 = [c(\vec{\mathbf{r}})]_{\mathscr{P}} \,. \tag{2.5b}$$

When we use (2.5a) to eliminate $c(\vec{r})$ from Eq. (2.4), the term proportional to c_0 acts like a uniform hydrostatic pressure. This pressure term can be eliminated by dilating the underlying crystalline lattice,

$$\vec{u}(\vec{r}) \rightarrow \vec{u}(\vec{r}) + c_0 \Omega_0 \vec{r} . \qquad (2.6)$$

Suppressing a constant contribution we find that

$$\mathcal{F} = \frac{1}{2} \int d^2 r (2\mu u_{ij}^2 + \lambda u_{kk}^2) - (\mu + \lambda) \Omega_0 \int d^2 r \, \delta c u_{kk} , \qquad (2.7)$$

which has the form (1.1) quoted in the Introduction with

$$w = (\mu + \lambda)\Omega_0 . \tag{2.8}$$

As mentioned in the Introduction we shall assume that impurity fluctuations $\delta c(\vec{r})$ are described by a quenched Gaussian probability distribution. Since the maximum fluctuation $(\delta c)_{max}$ should be of order δc in a region of a defect-free lattice, we expect that the variance σ entering Eq. (1.3) is of order

$$\sigma \sim \frac{1}{2}c_0 \tag{2.9}$$

for small impurity concentrations. Inserting expression (2.8) for w into the exponent (1.5b) governing the algebraic decay of order-parameter correlations, we find that

$$\eta_{\vec{G}} = \frac{|\vec{G}|^2}{4\pi(2\mu+\lambda)} \left[\frac{k_B T (3\mu+\lambda)}{\mu} + \frac{\sigma(\mu+\lambda)^2 \Omega_0^2}{2\mu+\lambda} \right]. \quad (2.10)$$

One might expect quenched impurity fluctuations to become important at temperatures such that the second term in Eq. (2.10) becomes comparable to the first, i.e., when

$$k_B T \leq \frac{\sigma \mu (\mu + \lambda)^2 \Omega_0^2}{(3\mu + \lambda)(2\mu + \lambda)} . \tag{2.11}$$

B. Dislocation free energy

At low temperatures we expect that the statistical mechanics associated with the free energy (1.1) will be dominated by extremal configurations of strains u_{ii}^* satisfying

$$\partial_i [2\mu u_{ij}^*(\vec{\mathbf{r}}) + \lambda \delta_{ij} u_{kk}^*(\vec{\mathbf{r}}) - w \delta_{ij} \delta c(\vec{\mathbf{r}})] = 0.$$
(2.12)

In the absence of dislocations it is easy to check that the strains associated with a fixed configuration of impurity fluctuations are

$$u_{ij}^{*}(\vec{r}) = \frac{w}{2\mu + \lambda} \partial_i \partial_j \int d^2 r' \, \delta c \, (\vec{r}\,') G \, (\vec{r} - \vec{r}\,') , \qquad (2.13)$$

where $G(\vec{r})$ is a Green's function satisfying

$$\nabla^2 G(\vec{r}) = \delta(\vec{r}) . \qquad (2.14)$$

For large r, we have

$$G(r) \approx \frac{1}{2\pi} \ln(r/a) , \qquad (2.15)$$

where a is of order a lattice constant. Dislocations can be included in the usual way, 3,5,7,8 by requiring that Eq. (2.12) hold almost everywhere, except at a set of dislocation position $\{\vec{r}_j\}$ where Eq. (1.6) holds with Burgers vectors $\{\vec{b}^j\}$. The total contribution to the extremal strain is

$$u_{ij}^{*}(\vec{\mathbf{r}}) = \frac{w}{2\mu + \lambda} \partial_{i} \partial_{j} \int d^{2}r' \,\delta c \,(\vec{\mathbf{r}}') G(\vec{\mathbf{r}} - \vec{\mathbf{r}}') + \frac{2(\mu + \lambda)}{2\mu + \lambda} \left[\epsilon_{ik} \epsilon_{jl} \partial_{k} \partial_{l} - \frac{\lambda \delta_{ij}}{2(\mu + \lambda)} \nabla^{2} \right] \int d^{2}r' \,a_{0} b_{m}(\vec{\mathbf{r}}') \widetilde{G}_{m}(\vec{\mathbf{r}} - \vec{\mathbf{r}}') , \qquad (2.16)$$

2906

where ϵ_{ij} is the antisymmetric 2×2 matrix,

 $\epsilon_{xy} = -\epsilon_{yx} = 1$, and $G_m(\vec{r})$ is a Green's function satisfying

$$\nabla^4 \widetilde{G}_m(\vec{\mathbf{r}}) = -\epsilon_{mn} \partial_n \delta(\vec{\mathbf{r}}) . \qquad (2.17)$$

For large r, we have

$$\widetilde{G}_m(\vec{r}) \approx \frac{-1}{4\pi} \epsilon_{mn} r_n \ln(r/a)$$
 (2.18)

The continuum vector dislocation "charge" density $\vec{b}(\vec{r})$ entering Eq. (2.16) is related to the dimensionless Burgers vectors \vec{b}^{j} characterizing a discrete set of point dislocations via

$$\vec{\mathbf{b}}(\vec{\mathbf{r}}) = \sum_{j} \vec{\mathbf{b}}^{j} \delta(\vec{\mathbf{r}} - \vec{\mathbf{r}}_{j}) .$$
(2.19)

At this point, we decompose $u_{ij}(\vec{r})$ into $u_{ij}^*(\vec{r})$ and a smooth deviation $\phi_{ij} = \partial_i \phi_j + \partial_j \phi_i$ from this extremal complexion

$$u_{ij}(\vec{r}) = u_{ij}^{*}(\vec{r}) + \phi_{ij}(\vec{r}) . \qquad (2.20)$$

After some tedious but straightforward manipulations²³ the free energy (1.1) becomes

$$\mathcal{F} = \mathcal{F}_0 + \mathcal{F}_D + \mathcal{F}_{\text{int}} , \qquad (2.21)$$

where

$$\mathcal{F}_{0} = \frac{1}{2} \int d^{2}r (2\mu\phi_{ij}^{2} + \lambda\phi_{kk}^{2} - 2w\delta c\phi_{kk}), \quad (2.22)$$

and

$$\frac{\mathscr{F}_{D}}{k_{B}T} = \frac{K}{8\pi} \sum_{i \neq j} \left[\vec{\mathbf{b}}^{i} \cdot \vec{\mathbf{b}}^{j} \ln(r_{ij}/a) - \frac{(\vec{\mathbf{b}}^{j} \cdot \vec{\mathbf{r}}_{ij})(\vec{\mathbf{b}}^{j} \cdot \vec{\mathbf{r}}_{ij})}{r_{ij}^{2}} \right] + \frac{E_{c}}{k_{B}T} \sum_{j} |\vec{\mathbf{b}}^{j}|^{2}. \qquad (2.23a)$$

The quantity \mathscr{F}_D is the usual dislocation free energy³⁻⁸ containing a phenomenological core energy E_c and an important dimensionless coupling

$$K = \frac{4a_0^2 \mu(\mu + \lambda)}{k_B T (2\mu + \lambda)} .$$
 (2.23b)

The term \mathcal{F}_{int} comes entirely from the second part of Eq. (1.1) and may be written

$$\mathcal{F}_{\text{int}} = \frac{\mu w a_0}{\pi (2\mu + \lambda)} \int d^2 r \sum_j \delta c(\vec{r}) \\ \times \frac{\hat{z} \cdot [\vec{b}^{\ j} \times (\vec{r} - \vec{r}_j)]}{|\vec{r} - \vec{r}_j|^2}$$
(2.24)

in agreement with the impurity-dislocation interaction energy quoted in the Introduction. We have suppressed an unimportant contribution to \mathcal{F} of order $[\delta c(\vec{r})]^2$ (this term drops out of quenched averages), and require that

$$\sum_{j} \vec{\mathbf{b}}^{j} = 0 \tag{2.25}$$

to insure that the total free energy is finite. The contribution \mathcal{F}_0 to the total free energy decouples from the dislocation part and allows us to recover results like Eq. (1.5) in the absence of dislocations. The remaining terms in Eq. (2.20) lead to a partition sum associated with a fixed configuration of impurities, namely

$$Z[\delta c(\vec{\mathbf{r}})] = \operatorname{Tr}'_{\{\overrightarrow{b}^{j}\}} e^{-(\mathscr{F}_{D} + \mathscr{F}_{\mathrm{int}})/k_{B}T}, \qquad (2.26)$$

where Tr' means a sum over dislocation configurations satisfying (2.25). The macroscopic free energy is obtained by averaging $\ln Z$ over the distribution (1.3).

III. SCREENING

A. Dielectric function

In Sec. II it was shown that solids with quenched random impurities may be understood in terms of a set of logarithmically interacting dislocations subject to a quenched random potential. The relevant free energy is

$$\frac{\mathscr{F}_{\text{eff}}}{k_B T} \equiv \frac{\mathscr{F}_D}{k_B T} + \frac{\mathscr{F}_{\text{int}}}{k_B T} = \frac{-K}{8\pi} \sum_{i \neq j} \left[\vec{\mathbf{b}}^{\,i} \cdot \vec{\mathbf{b}}^{\,j} \ln(r_{ij}/a) - \frac{(\vec{\mathbf{b}}^{\,i} \cdot \vec{\mathbf{r}}_{ij})(\vec{\mathbf{b}}^{\,j} \cdot \vec{\mathbf{r}}_{ij})}{r_{ij}^2} \right] + \frac{E_c}{k_B T} \sum_j |\vec{\mathbf{b}}^{\,j}|^2 + \frac{K}{4\pi} \left[\frac{\Omega_0}{a_0} \right] \int d^2 r \sum_j \delta c(\vec{\mathbf{r}}) \frac{\hat{z} \cdot [\vec{\mathbf{b}}^{\,j} \times (\vec{\mathbf{r}} - \vec{\mathbf{r}}_j)]}{|\vec{\mathbf{r}} - \vec{\mathbf{r}}_j|^2} ,$$
(3.1)

where we have used the expression (2.8) for w. As in most charged systems, screening (and, in particular, the "insulator-to-metal" transition from bound to unbound dislocation pairs) is conveniently described in terms of a dielectric function.^{7,24} We imagine that the system is perturbed by a small external charge density $\vec{b}^{\text{ext}}(\vec{r})$ and define an associate external potential $\vec{\phi}^{\text{ext}}(\vec{r})$ by the relation

$$-\nabla^2 \phi_i^{\text{ext}}(\vec{\mathbf{r}}) \equiv \mathscr{P}_{ij} b_j^{\text{ext}}(\vec{\mathbf{r}}) , \qquad (3.2)$$

where \mathcal{P}_{ij} is the transverse projection operator

$$\mathscr{P}_{ij} = \delta_{ij} - \frac{\partial_i \partial_j}{\nabla^2} . \tag{3.3}$$

It can be shown in a straightforward manner that the resulting change in free energy is given by

$$\frac{\mathscr{F}_{\text{eff}}}{k_B T} \rightarrow \frac{\mathscr{F}_{\text{eff}}}{k_B T} - K \int d^2 r \, \vec{\phi}^{\text{ext}}(\vec{r}) \cdot \vec{b}(\vec{r}) , \qquad (3.4)$$

where $\vec{b}(\vec{r})$ is the dislocation charge density defined by Eq. (2.19). Although there is also a contribution from the interaction of the external charges with the quenched impurities, this drops out of the dielectric function considered below.

By expanding in the weak external potential $\vec{\phi}^{\text{ext}}(\vec{r})$, it is easy to show that the induced dislocation charge in thermal equilibrium is

$$\langle b_i(\vec{\mathbf{r}}) \rangle = \langle b_i(\vec{\mathbf{r}}) \rangle_0 - K \int d^2 r' \phi_j^{\text{ext}}(\vec{\mathbf{r}}') [\langle b_i(\vec{\mathbf{r}}) b_j(\vec{\mathbf{r}}') \rangle_0 - \langle b_i(\vec{\mathbf{r}}) \rangle_0 \langle b_j(\vec{\mathbf{r}}') \rangle_0], \qquad (3.5)$$

(3.8)

where $\langle \rangle_0$ means a thermal average with $\vec{\phi}^{\text{ext}}(\vec{r}) \equiv 0$. Because of statistical homogeneity and the charge neutrality constraint, we expect that $\langle b(\vec{r}) \rangle_0$ vanishes when averaged over the quenched randomness. Screening is included in a renormalized potential $\vec{\phi}(\vec{r})$ which is due to both $\vec{b}^{\text{ext}}(\vec{r})$ and $\langle \vec{b}(\vec{r}) \rangle$,

$$-\nabla^2 \phi_i(\vec{\mathbf{r}}) \equiv \mathscr{P}_{ij}[b_i^{\text{ext}}(\vec{\mathbf{r}}) + \langle b_j(\vec{\mathbf{r}}) \rangle] . \tag{3.6}$$

In terms of Fourier-transformed potentials $\vec{\phi}^{\text{ext}}(\vec{q})$ and $\vec{\phi}(\vec{q})$, the dielectric matrix $\epsilon_{ij}^{-1}(\vec{q})$ is defined, upon averaging over the randomness, by the relation

$$[\phi_i(\vec{q})]_{\mathscr{P}} \equiv \epsilon_{ij}^{-1}(\vec{q})\phi_j^{\text{ext}}(\vec{q}) . \qquad (3.7)$$

Passing to a Fourier representation we readily find by combining Eqs. (3.2) and (3.5)-(3.7) that

$$\epsilon_{ij}^{-1}(\vec{q}) = \delta_{ij} - \frac{q_i q_j}{q^2} - \frac{K}{q^2} \left[\delta_{ik} - \frac{q_i q_k}{q^2} \right] \\ \times [\langle \delta b_k(\vec{q}) \delta b_j(-\vec{q}) \rangle_0]_{\mathscr{P}},$$

where

$$\delta b_i(\vec{q}) = b_i(\vec{q}) - \langle b_i(\vec{q}) \rangle_0 . \qquad (3.9)$$

Since $\vec{\phi}_{j}^{\text{ext}}(\vec{q})$ and $\phi_{j}(\vec{q})$ are purely transverse, we can write

$$\epsilon_{ij}^{-1}(\vec{q}) \equiv \epsilon^{-1}(\vec{q}) \left[\delta_{ij} - \frac{q_i q_j}{q^2} \right] . \tag{3.10}$$

Upon taking the trace of both sides of Eq. (3.8), we find finally that

$$\epsilon^{-1}(q) = 1 - \frac{K}{q^2} \left[\delta_{ij} - \frac{q_i q_j}{q^2} \right] \\ \times \left[\left\langle \delta b_i(\vec{q}) \delta b_j(-\vec{q}) \right\rangle_0 \right]_{\mathscr{P}} . \quad (3.11)$$

Physically, $\epsilon^{-1}(\vec{q})$ describes how the potential between two dislocations is screened due to the remaining dislocations in a medium of random impurities. In Sec. IV we show explicitly that an exponential, "Debye-Hückel" screening of this potential occurs when the dislocations are unbound.

B. Perturbation theory in the dislocation fugacity

When dislocations are bound in pairs, we expect that the potential between distant dislocations has the same form as in Eq. (3.1) but with a renormalized interaction strength K_R . The ratio of K_R to K is determined by the dielectric function $e^{-1}(q)$,^{7,24}

$$\frac{K_R}{K} = \lim_{q \to 0} \epsilon^{-1}(q)$$

$$= 1 - \lim_{q \to 0} \frac{K}{q^2} \left[\delta_{ij} - \frac{q_i q_j}{q^2} \right]$$

$$\times [\langle \delta b_i(\vec{q}) \delta b_j(-\vec{q}) \rangle_0]_{\mathscr{P}} . \quad (3.12)$$

It is instructive to evaluate this formula via perturbation theory in the dislocation fugacity,

$$y = e^{-E_c/k_B T}$$
. (3.13)

As we shall see, a convergent perturbation expansion is only possible over an intermediate-temperature range.

To evaluate Eq. (3.12), we write

REENTRANT MELTING IN SOLID FILMS WITH QUENCHED...

$$\begin{split} [\langle \delta b_i(\vec{q}) \delta b_j(-\vec{q}) \rangle_0]_{\mathscr{P}} \\ = [\langle b_i(\vec{q}) b_j(-\vec{q}) \rangle_0]_{\mathscr{P}} \\ - [\langle b_i(\vec{q}) \rangle_0]_{\mathscr{P}} [\langle b_j(-\vec{q}) \rangle_0]_{\mathscr{P}}, \qquad (3.14) \end{split}$$

and note that $\langle b_i(\vec{q}) \rangle_0$ and $\langle b_j(-\vec{q}) \rangle_0$ are each of order y^2 . The only contribution at $O(y^2)$ to Eq. (3.12) comes from the first term of (3.14). Expanding the quantity

$$[\langle b_i(\vec{q})b_j(-\vec{q})\rangle_0]_{\mathscr{P}} = \int d^2r \, e^{i\vec{q}\cdot\vec{r}} \times [\langle b_i(\vec{r})b_j(\vec{0})\rangle_0]_{\mathscr{P}}$$
(3.15)

in \vec{q} , and making use of charge neutrality and inversion symmetry in \vec{r} we find that

$$\frac{K_R}{K} = 1 + K \lim_{q \to 0} \left[\delta_{ij} - \frac{q_i q_j}{q^2} \right] \frac{q_k q_l}{q^2}$$
$$\times \int d^2 r \, r_k r_l [\langle b_i(\vec{r}) b_j(\vec{0}) \rangle_0]_{\mathscr{P}} .$$
(3.16)

To leading order in y the thermal and random averages in Eq. (3.16) commute and we can simply integrate out the impurity fluctuations in Eq. (3.1)as if they were annealed. The effective free energy which results is just the nonrandom dislocation free energy (2.23) with the replacement

$$K \rightarrow \widehat{K} = K - \sigma \Omega_0^2 K^2 / a_0^2 . \qquad (3.17)$$

The angular part of the integral in Eq. (3.16) can now be evaluated following the methods of Refs. 5 and 6. The result is

$$\int d^2 r \, r_k r_l [\langle b_i(\vec{r}) b_j(\vec{0}) \rangle_0]_{\mathscr{P}}$$

$$= [A \, (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + B \delta_{ij} \delta_{kl}]$$

$$\times \int_a^\infty \frac{dr}{a} \left[\frac{r}{a} \right]^{3 - \hat{K}/4\pi}, \quad (3.18)$$

where

$$A = -\frac{3}{2}\pi y^2 e^{\hat{K}/8\pi} I_1(\hat{K}/8\pi) ,$$

$$B = -\frac{3}{2}\pi y^2 e^{\hat{K}/8\pi} [2I_0(\hat{K}/8\pi) - I_1(\hat{K}/8\pi)] ,$$
(3.19)

and $I_0(x)$ and $I_1(x)$ are Bessel functions. The remaining integral in Eq. (3.18) has been cut off by the dislocation core diameter. Combining Eqs. (3.18) and (3.16), we find that

$$K_{R} = K - \frac{3}{4}\pi y^{2} K^{2} e^{\hat{K}/8\pi} [2I_{0}(\hat{K}/8\pi) - I_{1}(\hat{K}/8\pi)] \\ \times \int_{a}^{\infty} dr \, r^{3 - \hat{K}/4\pi} + O(y^{3}) \,.$$
(3.20)

When $\sigma = 0$ so that all randomness is suppressed, one can show that Eq. (3.19) leads to the usual^{6,7} renormalization-group recursion relations in pure systems. Analogous recursion relations for random systems will be derived by a different method in Sec. IV. It is clear already that the perturbation expansion (3.19) is only sensible over a finite range of temperatures given by

$$\hat{K} = K - \sigma (\Omega_0 K/a)^2 > 16\pi$$
 (3.21)

Remembering that $K \propto 1/T$, we see that this inequality is violated at both high and low temperatures. For impurity concentrations such that

$$\frac{\sigma \Omega_0^2}{a_0^2} > \frac{1}{64\pi} , \qquad (3.22)$$

it is impossible to satisfy the inequality at any temperature.

IV. RENORMALIZATION GROUP

A. Recursion relations from replicas

Renormalization-group recursion relations for solids with quenched random impurities are conveniently constructed via the replica trick.²⁵ The method we use is adapted from work by Cardy and Ostlund on random spin systems.¹⁶ Although this approach involves an unjustified and problematic limiting procedure, it was shown for a similar problem in Ref. 15 that identical results can be obtained (somewhat more laboriously) without recourse to replicas.

We start with an expression for the average of the logarithm of Eq. (2.22) over the randomness

$$[\ln Z]_{\mathscr{P}} = \left[\lim_{n \to 0} \frac{Z^n - 1}{n}\right]_{\mathscr{P}}.$$
(4.1)

Assuming that we can interchange the random average and the limit $n \rightarrow 0$, we first integrate out the quenched impurity fluctuations. The "replicated" dislocation free energy F_r which results is

$$\frac{F_{r}}{k_{B}T} = -\frac{\hat{K}}{8\pi} \sum_{i \neq j} \sum_{\alpha} \left[\vec{b}_{\alpha}^{i} \cdot \vec{b}_{\alpha}^{j} \ln(r_{ij}/a) - \frac{(\vec{b}_{\alpha}^{i} \cdot \vec{r}_{ij})(\vec{b}_{\alpha}^{j} \cdot \vec{r}_{ij})}{r_{ij}^{2}} \right] \\
- \frac{\tilde{K}}{8\pi} \sum_{i,j} \sum_{\alpha \neq \beta} \left[\vec{b}_{\alpha} \cdot \vec{b}_{\beta} \ln(r_{ij}/a) - \frac{(\vec{b}_{\alpha}^{i} \cdot \vec{r}_{ij})(\vec{b}_{\beta}^{j} \cdot \vec{r}_{ij})}{r_{ij}^{2}} \right] + \frac{E_{c}}{k_{B}T} \sum_{i} \sum_{\alpha} |\vec{b}_{\alpha}^{j}|^{2},$$
(4.2)

where \hat{K} was defined in Eq. (3.17),

$$\widetilde{K} = -\sigma \Omega_0^2 K^2 / a_0^2 , \qquad (4.3)$$

and α is a replica index running from 1 to *n*.

Recursion relations for a rather general vector Coulomb gas have been obtained by Young.⁶ Applying his method to the free energy (4.2), we find

$$\frac{d\hat{K}(l)}{dl} = -[\hat{K}^2 + (n-1)\tilde{K}^2]y^2 f(\hat{K}) , \qquad (4.4a)$$

$$\frac{d\tilde{K}(l)}{dl} = -\left[2\hat{K}\tilde{K} + (n-2)\tilde{K}^2\right]y^2 f(\hat{K}) , \quad (4.4b)$$

$$\frac{dy(l)}{dl} = \left[2 - \frac{\hat{K}}{8\pi}\right] y + 2\pi y^2 e^{\hat{K}/16\pi} I_0(\hat{K}/16\pi) ,$$
(4.4c)

where

$$f(\hat{K}) = \frac{3\pi}{4} e^{\hat{K}/8\pi} [2I_0(\hat{K}/8\pi) - I_1(\hat{K}/8\pi)] .$$
(4.5)

The configurations of dislocations which lead to the renormalizations of \hat{K} and \hat{K} indicated in Eqs. (4.4a) and (4.4b) are shown in Fig. 4. The $O(y^2)$ renormalization of y occurs because two dislocations within the same replica can combine to form a third.³ The couplings \hat{K} , \tilde{K} , and y entering Eq. (4.4) are



FIG. 4. Renormalization of the interaction between distant dislocation pairs by another more tightly bound dipole. (a) and (b) lead to renormalizations of \hat{K} , while (c) and (d) renormalize \tilde{K} .

scale-dependent effective couplings which result from increasing the effective dislocation core diameter

$$a \rightarrow ae^{l}$$
 (4.6)

Upon taking the limit $n \rightarrow 0$ in Eq. (4.4), we can extract the following three basic recursion relations:

$$\frac{dK^{-1}}{dl} = \frac{3}{4}\pi e^{(K-\overline{\sigma}K^2)/8\pi} \{2I_0[(K-\overline{\sigma}K^2)/8\pi] -I_1[(K-\overline{\sigma}K^2)/8\pi]\}y^2,$$
(4.7a)

$$\frac{dy}{dl} = [2 - (K - \bar{\sigma}K^2)/8\pi]y + 2\pi e^{(K - \bar{\sigma}K^2)/16\pi} I_0 [(K - \bar{\sigma}K^2)/16\pi]y^2,$$

(4.7b)

$$\frac{d\overline{\sigma}}{dl} = 0 , \qquad (4.7c)$$

where

$$\bar{\sigma} \equiv \sigma \Omega_0^2 / a_0^2 . \tag{4.8}$$

Note that the randomness parameter $\overline{\sigma}$ is unrenormalized. A recursion relation identical to Eq. (4.7a) can be obtained from the perturbation expansion (3.20) for K_R , providing a useful check on the replica method used here. In the limit $\sigma \rightarrow 0$ we recover the renormalization equations appropriate for pure systems.^{5,6}

B. Hamiltonian flows

The Hamiltonian flows generated by Eqs. (4.7) are very similar to those found in Ref. 15, and are indicated schematically in Fig. 5. The two special points along the fixed line y = 0 where the flows are locally elliptical (K_{-}^{-1}) and hyperbolic (K_{+}^{-1}) are

$$K_{\pm}^{-1} = \frac{1}{32\pi} \left[1 \pm (1 - 64\pi\bar{\sigma})^{1/2} \right].$$
(4.9)

There is a special trajectory which leaves the fixed line at K_0^{-1} and enters again at K_+^{-1} , bounding a region of solid phase. At the two temperatures such that the locus of initial conditions (3.13) crosses this line, there are dislocation-unbinding transitions. In

2910

contrast to the result (1.9) for pure systems, we find that

$$\lim_{T \to T_m} \frac{\mu_R(\mu_R + \lambda_R)a^2}{(2\mu_R + \lambda_R)k_BT} = \frac{1}{4}K_+(\overline{\sigma}) , \qquad (4.10)$$

as this line is approached from the solid phase. Note that the limit is σ dependent. For

$$\overline{\sigma} > \overline{\sigma}_c = 1/64\pi , \qquad (4.11)$$

the fixed line is always unstable and the solid phase is destroyed entirely. As $\overline{\sigma}$ approaches 1/64 π from below, Eq. (4.10) goes over to the result (1.9b) quoted in the Introduction. In the solid phase the exponent $\eta_{\vec{G}}$ is given by Eq. (1.5b), evaluated with renormalized elastic constants. As the temperature is lowered from the upper melting temperature, $\eta_{\vec{G}}(T)$ initially decreases, and then begins to increase at a temperature of order K^{-1}_{-1} .

Outside the region of stable solid we expect that the translational correlation function $\mathscr{C}_{\vec{G}}(\vec{r})$ decays exponentially,

$$\mathscr{C}_{\vec{\mathsf{G}}}(\vec{\mathsf{r}}) \sim e^{-r/\xi_T} \,. \tag{4.12}$$

The translational correlational length ξ_T diverges exponentially as one approaches the solid phase,

$$\xi_T \sim \exp(\operatorname{const} / |T - T_m|^{\nu(\overline{\sigma})}), \qquad (4.13)$$

where the exponent $v(\overline{\sigma})$ depends on the behavior of the recursion relations near $K_{+}(\overline{\sigma})$.

To determine $\overline{v}(\sigma)$ we expand the recursion relations (4.7a) and (4.7b) about the point $y = 0, K_+^{-1}(\sigma)$. Upon expressing $K^{-1}(l)$ in terms of a small deviation x(l),

$$K^{-1}(l) = K^{-1}(\bar{\sigma})[1 + x(l)], \qquad (4.14)$$

we find that

$$\frac{dx(l)}{dl} \approx 12\pi^2 A(\overline{\sigma}) y^2 , \qquad (4.15a)$$

$$\frac{dy(l)}{dl} \approx 2C(\overline{\sigma})xy + 2\pi B_0 y^2, \qquad (4.15b)$$

where

$$A(\bar{\sigma}) = \frac{K_{+}(\bar{\sigma})}{16\pi} [2e^{2}I_{0}(2) - e^{2}I_{1}(2)]$$

$$\approx \frac{K_{+}(\bar{\sigma})}{16\pi} (21.937) , \qquad (4.16)$$

$$B_0 = e^1 I_0(2) \approx 6.1965 , \qquad (4.17)$$

and

$$C(\sigma) = 2 - \frac{K_+(\overline{\sigma})}{16\pi} . \tag{4.18}$$

The outgoing and incoming separatrices near $K_{+}^{-1}(\sigma)$ in Fig. 5 are given by solutions of the form

$$y(l) = m_{\pm} x(l)$$
 (4.19)

Substituting this expression in Eqs. (4.15) we find that the slopes m_{\pm} are

$$m_{\pm} = \frac{1}{12\pi A} \left[B \pm (B^2 + 24AC)^{1/2} \right] \,. \tag{4.20}$$

Since $K_{+}(\overline{\sigma})$ approaches 32π as $\overline{\sigma} \rightarrow \overline{\sigma}_{c}$ [see Eq. (4.9)], $c(\sigma)$ vanishes at this point. It follows that m_{-} tends to zero as $\overline{\sigma} \rightarrow \overline{\sigma}_{c}$, while m_{+} remains finite. This analysis is easily extended to obtain the exponent $\overline{v}(\overline{\sigma})$. Taking over the discussion in Refs. 3 and 5, we find that

$$\overline{\nu}(\overline{\sigma}) = \frac{6\pi^2 A(\overline{\sigma}) m_{-}^2(\overline{\sigma})}{1 + 6\pi^2 A(\overline{\sigma}) m_{-}^2(\overline{\sigma})} .$$
(4.21)

The exponent $\overline{v}(\overline{\sigma})$ entering the correlation length (4.13) decreases monotonically from its value for $\overline{\sigma}=0,^{4-6}$

$$\overline{v}(0) = 0.36963...$$
 (4.22)

to zero at $\overline{\sigma} = \overline{\sigma}_c$,

$$\overline{v}(\overline{\sigma}_c) = 0 . \tag{4.23}$$

C. Properties of the melted crystal

Outside the domain of attraction of the fixed line in Fig. 5, the Hamiltonian flows evidently lead towards high temperatures and large dislocation fugacities y. This instability presumably means that the



FIG. 5. Hamiltonian flows for solids with quenched impurities for fixed $\overline{\sigma} < \overline{\sigma}_c$. Locus of initial conditions is shown as a dashed line. Upper and lower melting temperatures are given by the intersection of this line with the heavy trajectory leaving K_0^{-1} and terminating at K_+^{-1} . Shaded portion corresponds to a stable solid phase.

crystal is melted by a proliferation of unbound dislocations. Although perturbation theory in y breaks down in this limit, we can resort instead to an approximate Debye-Hückel theory.⁵ The idea is that free dislocations can be treated at long wavelengths by integrating, rather than summing over the Burgers vectors in Eq. (3.1).

We first evaluate the formula (3.11) for the wavevector-dependent dielectric constant $\epsilon(q)$ in this limit. The correlation function

$$[\langle \delta b_i(\vec{q}) \delta b_j(-\vec{q}) \rangle_0]_{\mathscr{P}} = [\langle b_i(\vec{q}) b_j(-\vec{q}) \rangle_0]_{\mathscr{P}} - [\langle b_i(\vec{q}) \rangle \langle b_j(-\vec{q}) \rangle_0]_{\mathscr{P}}$$

$$(4.24)$$

is conveniently evaluated by first rewriting the free energy (3.1) in Fourier space,

$$\frac{F_{\text{eff}}}{k_B T} = \frac{1}{2} \int \frac{d^2 q}{(2\pi)^2} \left| \frac{K}{q^2} \left| \delta_{jk} - \frac{q_j q_k}{q^2} \right| + \frac{2E_c a^2}{k_B T} \delta_{jk} \right| b_j(\vec{q}) b_k(-\vec{q}) + K \left[\frac{\Omega_0}{a_0} \right] \int \frac{d^2 q}{(2\pi)^2} \delta c(\vec{q}) \times \frac{\epsilon_{jk} b_j(-\vec{q})(-iq_k)}{q^2} .$$
(4.25)

The Fourier transform $\vec{b}(\vec{q})$ is well behaved provided we can regard $\vec{b}(\vec{r})$ as a continuous variable. The charge-neutrality constraint (2.25) amounts only to a restriction on $\vec{b}(\vec{q}=0)$. With the use of Eq. (4.25) it is easy to show via (4.24) that

$$[\langle \delta b_i(\vec{q}) \delta b_j(-\vec{q}) \rangle_0]_{\mathscr{P}}$$

$$= \frac{q^2}{K + 2E_c q^2 a^2 / k_B T} \left[\delta_{ij} - \frac{q_i q_j}{q^2} \right]$$

$$+ \frac{k_B T}{2E_c q^2 a^2} \frac{q_i q_j}{q^2} . \qquad (4.26)$$

The dielectric formula (3.11) becomes

$$\epsilon^{-1}(q) = \frac{2E_c q^2 a^2 / k_B T}{K + 2E_c q^2 a^2 / k_B T} , \qquad (4.27)$$

indicating that $\epsilon(q)$ exhibits metallic behavior (diverging like $1/q^2$) for small q. Equation (4.27) means that the logarithmic interaction energy between dislocations in Eq. (3.1) is replaced by screened exponential interaction at long wavelengths.

In analogy with pure systems⁵ one might expect

the dislocation instability to produce a fluid with residual bond-orientational order rather than an isotropic liquid. To take over the analysis of Ref. 5, we need to know the bond-orientation field

$$\theta^*(\vec{\mathbf{r}}) = \frac{1}{2} \left[\partial_x u_y^*(\vec{\mathbf{r}}) - \partial_y u_x^*(\vec{\mathbf{r}}) \right]$$
(4.28)

associated with the extremal strain (2.16). It is straightforward to check that the part of $\vec{u} * (\vec{r})$ due to random impurities does not contribute to (4.28), so that

$$\theta^{*}(\vec{r}) = \frac{-a_{0}}{2\pi} \sum_{\vec{r}} \frac{\vec{b}(\vec{r}') \cdot (\vec{r} - \vec{r}')}{|\vec{r} - \vec{r}'|^{2}}$$
(4.29)

just as in pure systems.⁵ If bond-orientational order persists we would expect a nonzero stiffness K_A entering an effective free energy

$$F_A \equiv \frac{1}{2} K_A \int d^2 r \mid \vec{\nabla}\theta \mid^2 . \tag{4.30}$$

An analogy to pure systems, K_A is given by⁵

$$\frac{k_B T}{K_A} = \lim_{q \to 0} q^2 [\langle |\theta^*(\vec{q})|^2 \rangle]_{\mathscr{P}}$$
(4.31)

$$=\lim_{q\to 0}\frac{a_0^2q_iq_j}{q^2}[\langle b_i(\vec{q})b_j(-\vec{q})\rangle]_{\mathscr{P}}.$$
 (4.32)

The contribution of fluctuations in the smoothly varying part of the phonon field to this quantity is negligible at long wavelengths.⁵ Using the Debye-Hückel approximation discussed above, we find that

$$[\langle b_i(\vec{q})b_j(-\vec{q})\rangle]_{\mathscr{P}} = \frac{q^2}{K + 2E_c q^2 / k_B T} \left[\delta_{ij} - \frac{q_i q_j}{q^2} \right]$$
$$+ \frac{k_B T}{2E_c q^2 a^2} \frac{q_i q_j}{q^2}$$
$$+ [\langle b_i(\vec{q})b_j(-\vec{q})\rangle]_{\mathscr{P}}.$$
(4.33)

Although the last term in Eq. (4.33) is nonzero, it is straightforward to show that it vanishes when contracted with q_iq_j/q^2 in Eq. (4.32). Our final result for K_A is the same as in pure systems,⁵

$$K_A \approx 2E_c a^2 \neq 0 . \tag{4.34}$$

By scaling out to temperatures such that Debye-Hückel theory is valid, one can show that K_A diverges near the dislocation unbinding transition,

$$K_A \sim \xi_T^2 \ . \tag{4.35}$$

A second, disclination-unbinding transition would be necessary to produce an isotropic liquid. The effective interaction between disclinations associated with (4.30) is logarithmic, rather than the $r^2 \ln r$ interaction expected in a crystalline solid.²⁶ Since such a disclination-unbinding transition is driven by entropic effects,⁷ we would not expect this instability to occur as the temperature is decreased further below $T_m^-(\sigma)$. As discussed in the Introduction, the hexatic phase shown in Fig. 3, can, in principle, persist down to T=0. As discussed in Ref. 12, one finds that orientational order decays algebraically even at T=0, due to the presence of unbound dislocations in the ground state.

ACKNOWLEDGMENTS

It is a pleasure to acknowledge stimulating discussions with B. I. Halperin, M. Rubinstein, and F. Spaepen. This research was supported by the National Science Foundation, in part, through the Harvard Materials Research Laboratory, and also through Grant No. DMR-82-07431. I would also like to acknowledge a grant from the A. P. Sloan Foundation.

APPENDIX: DISRUPTION OF TRANSLATIONAL ORDER BY HARMONIC PHONONS AND QUENCHED IMPURITIES

We wish to evaluate the translational correlation function

$$C_{\vec{G}}(\vec{r}) = [\langle \exp\{i\vec{G}\cdot[\vec{u}(\vec{r}) - \vec{u}(\vec{0})]\}]_{\mathscr{P}}, \quad (A1)$$

where \vec{G} is a reciprocal-lattice vector, $\vec{u}(\vec{r})$ is a phonon displacement, and we exclude dislocations. Using the free energy (1.1), we rewrite the thermal part of the average in Eq. (A1) as

$$\langle e^{i\vec{G}\cdot[\vec{u}(\vec{r})-\vec{u}(\vec{0})]}\rangle = \frac{\left\langle \exp\{i\vec{G}\cdot[\vec{u}(\vec{r})-\vec{u}(\vec{0})]\}\exp\left[-\frac{w}{k_BT}\int d^2r\,\delta c\,(\vec{r})(\vec{\nabla}\cdot\vec{u})\right]\right\rangle_0}{\left\langle \exp\left[-\frac{w}{k_BT}\int d^2r\,\delta c\,(\vec{r})(\vec{\nabla}\cdot\vec{u})\right]\right\rangle_0},\tag{A2}$$

where here $\langle \rangle_0$ means an average with respect to the free energy (1.1) with $w \equiv 0$. Since the averages in Eq. (A2) are over a simple Gaussian probability, we readily find that

$$\langle \exp\{i\vec{G}\cdot[\vec{u}(\vec{r})-\vec{u}(\vec{0})]\}\rangle = \frac{1}{r^{\eta_{\vec{G}}^{(1)}(T)}}e^{-iI(\vec{r},\vec{0})}, \qquad (A3)$$

where $\eta_G^{(1)}(T)$ is the exponent characterizing the algebraic decay of translational order in the absence of impurities,⁵

$$\eta_{\vec{G}}^{(1)}(T) = \frac{k_B T |\vec{G}|^2 (3\mu + \lambda)}{4\pi\mu(2\mu + \lambda)} , \qquad (A4)$$

and

$$I(\vec{r}_{1},\vec{r}_{2}) = \frac{w}{k_{B}T}G_{j}\int d^{2}r\,\delta c\,(\vec{r})\partial_{i}[C_{ij}(\vec{r}_{1}-\vec{r})-C_{ij}(\vec{r}_{2}-\vec{r})].$$
(A5)

The correlation matrix $C_{ii}(\vec{r})$ entering (A5) is the Fourier transform of

$$C_{ij}(\vec{q}) \equiv \langle u_i(\vec{q})u_j(-\vec{q})\rangle = \frac{k_B T}{\mu q^2} \left[\delta_{ij} - \frac{q_i q_j}{q^2} \right] + \frac{k_B T}{2\mu + \lambda} \frac{q_i q_j}{q^4} .$$
(A6)

To obtain $C_{\vec{G}}(\vec{r})$, we average Eq. (A3) over the Gaussian impurity distribution (1.3),

$$C_{\vec{G}}(r) = \frac{1}{r^{\eta_{\vec{G}}^{(1)}(T)}} \exp[-iI(\vec{r},0)]_{\mathscr{P}} = \frac{1}{r^{\eta_{\vec{G}}^{(1)}(T)}} \exp[-\frac{1}{2}[I^{2}(\vec{r},0)]_{\mathscr{P}}.$$
(A7)

Since

$$[\delta c(\vec{r})\delta c(\vec{r}')]_{\mathscr{P}} = \sigma \delta(\vec{r} - \vec{r}') , \qquad (A8)$$

it follows using Eq. (A5) that

$$[I^{2}(\vec{r},\vec{0})]_{\mathscr{P}} = \left[\frac{w}{k_{B}T}\right]^{2} \sigma G_{k}G_{l} \int d^{2}r' \partial_{i}' [C_{ik}(\vec{r}-\vec{r}')-C_{il}(\vec{r}')]\partial_{j}' [C_{il}(\vec{r}-\vec{r}')-C_{jl}(\vec{r}')] .$$
(A9)

Passing to a Fourier representation and using (A6), we readily find that

$$[I^{2}(\vec{r},\vec{0})]_{\mathscr{P}} = \frac{2w^{2}\sigma}{(2\mu+\lambda)^{2}} G_{k}G_{l} \int \frac{d^{2}q}{(2\pi)^{2}} \frac{q_{k}q_{l}}{q^{4}} (1-e^{i\vec{q}\cdot\vec{r}}) , \qquad (A10)$$

from which it can easily be shown that

$$[I^{2}(\vec{\mathbf{r}},0)]_{\mathscr{P}} \simeq \frac{w^{2}\sigma}{2\pi(2\mu+\lambda)^{2}} |\vec{\mathbf{G}}|^{2}\ln(r/a)$$
(A11)

for large r. Our final result for the decay of translational correlations is

$$C_{\vec{\tau}}(\vec{r}) \sim r^{-[\eta_G^{(1)}(T) + \eta_G^{(2)}(\sigma)]},$$
(A12)

where $\eta_{\vec{G}}^{(1)}(T)$ is given by (A4), and

$$\eta_{\vec{G}}^{(2)}(T) = \frac{w^2 \sigma |\vec{G}|^2}{4\pi (2\mu + \lambda)^2} .$$
(A13)

- ¹See, e.g., Proceedings of the 1978 Les Houches Summer School: Ill-Condensed Matter, edited by R. Balian, R. Maynard, and G. Toulouse (North-Holland, New York, 1979).
- ²C. Domb and M. S. Green, *Phase Transitions and Critical Phenomenae* (Academic, New York, 1976), Vol. 6.
- ³D. R. Nelson, Phys. Rev. B <u>18</u>, 2318 (1978).
- ⁴B. I. Halperin and D. R. Nelson, Phys. Rev. Lett. <u>41</u>, 121 (1978); <u>E41</u>, 519 (1978).
- ⁵D. R. Nelson and B. I. Halperin, Phys. Rev. B <u>19</u>, 2457 (1979).
- ⁶A. P. Young, Phys. Rev. B 19, 1855 (1979).
- ⁷J. M. Kosterlitz and D. J. Thouless, J. Phys. C <u>6</u>, 1181 (1973).
- ⁸F. R. Nabarro, *Theory of Dislocations* (Clarendon, New York, 1967).
- ⁹L. D. Landau and E. M. Lifshitz, *Theory of Elasticity* (Pergamon, New York, 1970).
- ¹⁰B. Jancovici, Phys. Rev. Lett. <u>19</u>, 20 (1967); see also R.
 E. Peierls, Ann. Inst. Henri Poincaré <u>5</u>, 177 (1935); L.
 D. Landau, Phys. Z. Sowjetunian II, 26 (1937).
- ¹¹This result has also been obtained by M. Rubinstein, Ph.D. thesis, Harvard University, 1983 (unpublished).
- ¹²D. R. Nelson, M. Rubinstein, and F. Spaepen, Philos. Mag. A <u>46</u>, 105 (1982). The assertion that quenched impurities cause algebraic decay of translational order at T=0 appears as a footnote on p. 121.
- ¹³A. M. Kosevich, in *Dislocations in Solids*, edited by F.
 R. N. Nabarro (North-Holland, Amsterdam, 1979),
 Vol. 1.
- ¹⁴D. S. Fisher, B. I. Halperin, and R. Morf, Phys. Rev. B

<u>20,</u> 4692 (1979); S.-T. Chui, Phys. Rev. Lett. <u>48</u>, 933 (1982).

- ¹⁵M. Rubinstein, B. Shraiman, and D. R. Nelson, Phys. Rev. B <u>27</u>, 1800 (1983).
- ¹⁶A. Houghton, R. D. Kenway, and S. C. Ying, Phys. Rev. B <u>23</u>, 298 (1981); J. Cardy and S. Ostlund, Phys. Rev. B <u>25</u>, 6899 (1982); Y. Goldschmidt and A. Houghton, Nucl. Phys. B <u>210</u>, 155 (1982).
- ¹⁷Y. Imry and S.-K. Ma, Phys. Rev. Lett. <u>35</u>, 1399 (1975).
- ¹⁸See, e.g., R. Bruinsma, B. I. Halperin, and A. Zippelius, Phys. Rev. B <u>25</u>, 579 (1982), and references therein.
- ¹⁹P. S. Pershan, J. Phys. (Paris) Colloq. <u>40</u>, C3 (1979).
- ²⁰P. Pieranski, Phys. Rev. Lett. <u>45</u>, 569 (1980).
- ²¹C. C. Grimes and G. Adams, Phys. Rev. Lett. <u>42</u>, 795 (1979).
- ²²J. P. McTague, M. Nielsen, and L. Passell, in Ordering in Strongly Fluctuating Condensed Matter Systems, edited by T. Riste (Plenum, New York, 1980).
- ²³See, for example, Sec. II of Ref. 3.
- ²⁴For an analogous discussion of screening in a nonrandom scalar Coulomb gas, see P. Minhagen and G. G. Warren, Phys. Rev. B <u>24</u>, 2526 (1981), and D. R. Nelson, in *Fundamental Problems in Statistical Mechanics V*, edited by E. G. D. Cohen (North-Holland, Amsterdam, 1979). Reference 15 discusses screening in a scalar Coulomb gas immersed in a medium of random dipoles.
- ²⁵See, e.g., V. J. Emery, Phys. Rev. B <u>11</u>, 239 (1975); G. Grinstein and A. Luther, *ibid.* <u>13</u>, 1329 (1976).
- ²⁶D. R. Nelson, Phys. Rev. B <u>26</u>, 269 (1982).