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# Calculation of the shear modulus of a two-dimensional vortex lattice

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We have calculated the temperature-dependent shear modulus $\mu(T)$ of a vortex lattice in a two-dimensional superconductor. We include fluctuations by expanding the Ginzburg-Landau free-energy functional in states from the lowest Landau level, and evaluate the shear modulus by standard Monte Carlo techniques for rectangular samples containing up to 224 vortices. At the thermodynamic melting transition, which is apparently first order as found by previous workers, the shear modulus falls from a finite value in the solid phase to zero in the liquid. Despite the first-order transition, the magnitude of the drop may be near the universal value envisioned in dislocation-unbinding theories.

Berezinskii[1] suggested that two-dimensional (2D) systems can have very unusual phase transitions. For example, the so-called 2D $XY$ or planar model has a continuous phase transition marked by the unbinding of thermally excited vortex-antivortex pairs,[2] with a characteristically diverging correlation length, and a universal jump in the spin-wave stiffness (or helicity modulus).[3] The melting of a 2D elastic solid has characteristics which are less universally agreed upon than those of the 2D $XY$ model. Kosterlitz and Thouless[4] suggested that this melting proceeds by the unbinding of dislocation pairs. Halperin and Nelson,[5] and independently Young,[6] derived renormalization-group (RG) equations for this phase transition, which they also found to be continuous, provided the fugacity of bound dislocation pairs is small. The dislocation-unbinding transition is characterized by a discontinuous jump in the coupling constant

$$K(T) = (1/k_BT)[4\mu(\mu+\lambda)/(2\mu+\lambda)]a^2, \tag{1}$$

from $16\pi$ to zero on melting. Here $\mu$ is the shear modulus, $\lambda$ is the second of Lamé elastic constants, and $a$ is the crystal lattice constant. These ideas are commonly referred to as the KTBHNY theory.[7]

A particularly convenient model system for studying 2D melting is a thin superconducting film placed in a transverse magnetic field. Such a field produces a density of vortices, which may form either a lattice or a fluidlike state. Recently, several workers[8,9] have used a simple Ginzburg-Landau (GL) model Hamiltonian in the so-called lowest Landau level (LLL) approximation[10] to provide strong numerical evidence in favor of a *first-order* phase transition in this system, in contrast to the continuous melting proposed by the KTBHNY theory (although no transition at all has been found in Ref. 11 using the same approximation in a spherical geometry). A more recent calculation[12] treats 2D flux lattice melting in the London limit (probably appropriate at lower fields than the LLL approximation) and also finds a first-order transition.

In this paper we calculate the temperature-dependent shear modulus of a 2D vortex lattice. The behavior of this quantity is of particular interest, because it seems, at first glance, difficult to reconcile the prediction of a universal jump with the reported first-order melting transition. Our basic result is that, despite the first-order transition, the shear modulus is near the suggested universal value at the extrapolated first-order melting temperature of a very large system. At the end of this paper, we speculate about some possible reasons for this behavior.

To calculate the shear modulus $\mu(T)$, we consider a vortex lattice in equilibrium with a thermal reservoir at temperature $T$, and apply an external force which generates a small shear strain in this lattice. If the force does reversible mechanical work $\delta W$ on the lattice, the free energy of the system changes by $\delta\mathcal{F} = \delta W$. The isothermal shear modulus is the second derivative of free energy per unit area with respect to the shear angle $\theta$, i.e.,

$$\mu = (1/S)(\partial^2\mathcal{F}/\partial\theta^2)_{T;\theta=0}, \tag{2}$$

where $S$ is the sample surface area. We also introduce the shear modulus per vortex $\mu_\phi = (S/N_\phi)\mu$, where $N_\phi$ is the number of vortices in the sample.

We assume that equilibrium properties of a 2D superconductor are described by the GL energy functional

$$\mathcal{H}[\psi] = L_z\int d^2r\left\{a(T)|\psi(\mathbf{r})|^2 + \frac{1}{2m^*}\times\left|\left(-i\hbar\boldsymbol{\nabla} - \frac{q\mathbf{A}}{c}\right)\psi(\mathbf{r})\right|^2 + \frac{b}{2}|\psi(\mathbf{r})|^4\right\}, \tag{3}$$

where $\psi(\mathbf{r})$ is the complex order parameter, $\mathbf{r}\equiv(x,y)$, $L_z$ is the sample thickness, $|q| = 2e$ is the charge of supercurrent carriers, and $a(T), b$ and $m^*$ are material-dependent parameters. $\mathbf{A} = -By\hat{x}$ is the vector potential of a (uniform) magnetic field perpendicular to the sample surface. This is an approximation valid in the extreme-type-II limit ($\kappa \gg 1$), where $\kappa$ is the standard GL parameter.

In order to calculate thermal averages, following Refs. 8 and 9, the order parameter is expanded in an orthogonal set of wave functions drawn from the lowest band of the Hamiltonian $(2m^*)^{-1}(-i\hbar\boldsymbol{\nabla} - q\mathbf{A}/c)^2$, known as lowest Landau levels (LLL's). These states are labeled with a continuous index $k$, and are degenerate with an eigenvalue $\hbar\omega_c/2 = \hbar eB/(m^*c)$. By making this approximation we assume that fluctuations in higher LL channels either can be neglected or have already been included in a suitably renormalized coefficient $a(T)$.[10] The LLL approximation is valid for fields $B$ near the upper critical field $H_{c2}(T)$ defined by $a(T) + \hbar\omega_c/2 = 0$. We now write

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$$\psi(\mathbf{r}) = \left( \frac{\sqrt{3}a_H^2(T)}{4b^2} \right)^{1/4} \sum_k c_k e^{ikx} \exp[-(y-kl^2)^2/2l^2], \tag{4}$$

where $a_H(T) \equiv a(T)[1 - B/H_{c2}(T)]$, and $l = (|q|B/\hbar c)^{-1/2}$ is the magnetic length. Further we will only consider the superconducting region, $a_H(T) < 0$.

With periodic boundary conditions along the $x$ axis so that $\psi(x,y) = \psi(x+L_x, y)$, $k$ assumes values $k_m = 2\pi m/L_x$, where $m$ is an integer. We adopt the concise notation $c_m \equiv c_{k_m}$. If there are $N_\phi$ independent amplitudes, the set $\{c_m\}$ with $m = 0 \ldots N_\phi - 1$ describes a state $\psi(\mathbf{r})$ with $N_\phi$ zeros (i.e., vortex cores). A quasiperiodicity along the $y$ axis of the form $|\psi(x,y)| = |\psi(x, y+L_y)|$ is achieved by allowing $m$ to span all integer values, but with the constraint $c_m = c_{m'}$ for all $m = m' \bmod N_\phi$. Evidently, $L_y = N_\phi \times 2\pi l^2/L_x$.

In the unstrained ground state,[13,14] the vortices form a triangular lattice with a nearest-neighbor distance $l_0 = (4\pi/\sqrt{3})^{1/2} l$. One way of generating the ground state is to choose $L_x/l_0 = n_x$ to be an integer. The only nonzero amplitudes then are $c_{(2p+1)n_x} = ic_{2pn_x} = i(2/\beta_A)^{1/2}$, where $p$ is an arbitrary integer and $\beta_A = 1.159595\ldots$ is the Abrikosov ratio. The ground-state energy is $\mathcal{H}^{\rm MF} = -k_B T g^2(T) N_\phi/\beta_A$.

The thermodynamics of the system is given by the free energy

$$\mathcal{F} = -k_B T \ln \int \Pi_m dc_m dc_m^* \exp(-\mathcal{H}[\{c_m\}]/k_B T),$$

where

$$-\frac{\mathcal{H}[\{c_m\}]}{k_B T} = -g^2(T)\left\{ -n_x \sum_m |c_m|^2 + n_x 3^{1/4} 2^{-5/2} \sum_{\substack{m \\ n,n'}} c_m c_{m+n}^* c_{m+n'}^* c_{m+n+n'} \exp\left( -\frac{\sqrt{3}\pi}{2} \frac{n^2+n'^2}{n_x^2} \right) \right\}. \tag{5}$$

This form makes clear that the system is described by a single intensive variable[10] $g(T) = a_H(\pi l^2 L_z/bk_B T)^{1/2}$. In Eq. (5), $1/g^2$ appears as the dimensionless temperature and is the natural variable of the problem: $1/g^2$=0 corresponds to $T = 0$ K, and $1/g^2 = +\infty$ marks the mean-field transition at $T_c(B)$.

Within this representation, we turn now to an explicit expression for the shear modulus. First, Eq. (2) can be written as

$$\mu_\phi = \frac{1}{N_\phi} \left[ \left\langle \frac{\partial^2 \mathcal{H}}{\partial \theta^2} \right\rangle - \frac{1}{k_B T} \left\langle \left( \frac{\partial \mathcal{H}}{\partial \theta} \right)^2 \right\rangle \right]_{\theta=0}, \tag{6}$$

where the brackets denote thermal averaging in the canonical ensemble. Thus, it remains to determine the dependence of $\mathcal{H}$ on the shear angle $\theta$.

A uniform shear such that $|\psi(x,y)| = |\psi(x+\theta L_y, y+L_y)|$ (see Fig. 1) is generated by imposing the condition $c_m \to c_m \exp[-i\sqrt{3}\pi m^2\theta/(2n_x^2)]$. Direct differentiation of $\mathcal{H}$ in this state and taking the limit $\theta \to 0$ leads to

$$\mu_\phi = \frac{k_B T g^2(T)}{N_\phi} \left\{ \left\langle -3^{5/4} 2^{-5/2} \pi^2 n_x \sum_{\substack{m \\ n,n'}} \mathrm{Re}\{c_m c_{m+n}^* c_{m+n'}^* c_{m+n+n'}\} \left( \frac{nn'}{n_x^2} \right)^2 \exp\left( -\frac{\sqrt{3}\pi}{2} \frac{n^2+n'^2}{n_x^2} \right) \right\rangle \right.$$
$$\left. -g^2(T) \left\langle 3^{3/2} 2^{-5} \pi^2 \left[ n_x \sum_{\substack{m \\ n,n'}} \mathrm{Im}\{c_m c_{m+n}^* c_{m+n'}^* c_{m+n+n'}\} \left( \frac{nn'}{n_x^2} \right) \exp\left( -\frac{\sqrt{3}\pi}{2} \frac{n^2+n'^2}{n_x^2} \right) \right]^2 \right\rangle \right\}. \tag{7}$$

Since the vortex lattice in the LLL approximation is incompressible, $\lambda \to +\infty$ and the KTBHNY theory predicts a universal jump for the shear modulus $\mu$ alone.

The mean-field value of the shear modulus, $\mu_\phi^{\rm MF}(T) = 0.354 k_B T g^2(T)$, obtained by evaluating (7) in the ground state, can be equivalently written as

$$\mu^{\rm MF}(T) = 0.477\{[H_{c2}(T) - B]^2/[8\pi(2\kappa^2)\beta_A^2]\} L_z. \tag{8}$$

This result is almost identical to that of Labusch[15] and Brandt,[16] with two small differences. First, these authors obtain $(2\kappa^2 - 1)$ in the denominator instead of just $(2\kappa^2)$ as we do. This difference occurs because they deal with a 3D system of straight flux lines where the screening magnetic field can be included. It is algebraically prohibitive to do so in our case, where the order parameter is limited to a thin layer in the $z$ direction, while the magnetic field is not. In any case, the two expressions merge together in the extreme type-II limit $\kappa \to \infty$, which is the case studied here. Second, they obtain a numerical factor, 0.475, which differs slightly from ours. We believe that the difference is real and is caused by a slightly different definition of the shear deformation. Labusch and Brandt assume that the lattice under shear can actually change dimensions, although the surface area $L_x \times L_y$ remains constant. For example, at the largest allowed shear angle, Labusch and Brandt obtain a square flux lattice, whereas the procedure used here generates a vortex lattice with a rectangular unit cell still having an aspect ratio $1{:}\sqrt{3}/2$. Our definition seems more relevant to an experiment, in which the vortex lattice in the $y$ direction is limited by the edges of the sample. In either case, the difference is very small.

We have evaluated the shear modulus $\mu(T)$ for this model, using standard Monte Carlo (MC) techniques within the Metropolis algorithm, and initializing the system in its ground state before each run. Since the modulus is a second derivative calculated in the absence of shear, the calculation can be conveniently done using periodic boundary conditions. In these circumstances, we obtain evidence suggestive of a first-order phase transi-

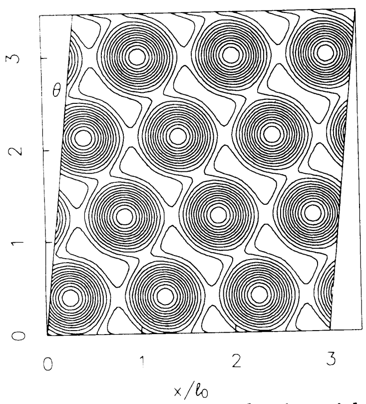


FIG. 1. Ground state of the vortex lattice with $N_\phi = 3\times 4$, subjected to a uniform shear with angle $\theta$ ($\tan\theta = 0.1$). The lines are loci of constant $|\psi(\mathbf{r})|^2$.

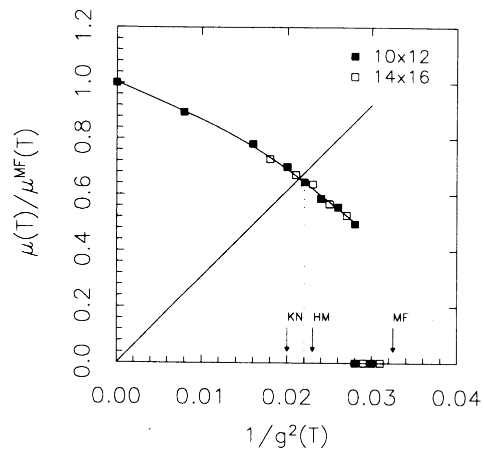


FIG. 2. Calculated temperature dependence of the shear modulus $\mu(T)$, in units of the mean-field shear modulus $\mu^{\rm MF}(T)$ for two lattice sizes, $N_\phi = 120$ and 224. Estimated errors are comparable to symbol sizes. The straight line with a slope $2\sqrt{3}\pi/0.354$ represents the Kosterlitz-Thouless instability criterion. Arrow labeled "MF" denotes the mean-field instability temperature; arrows labeled "KN" and "HM" denote the thermodynamic melting temperature at infinite size as estimated by Kato and Nagaosa (Ref. 8) and by Hu and MacDonald (Ref. 9). For $N_\phi = 120$, in the temperature range bounded by dotted lines, $0.022< 1/g^2(T) < 0.028$, both liquid and solid phases can coexist.

tion in the MC calculation, just as found previously.[8,9] In particular, there is a range of temperatures between a lower ("supercooling") limit $T_{\rm sc}$ and an upper ("superheating") limit $T_{\rm sh}$, where the system jumps back and forth between a solidlike and a liquidlike state. These limits seem to be numerically quite well defined, but depend on sample size. The jumps occur typically about once every $10^4$–$10^5$ passes through the entire lattice, for the sample sizes $N_\phi = 120$ and 224.

Figure 2 shows the shear modulus $\mu(T)$ plotted in units of the mean-field shear modulus $\mu^{\rm MF}(T)$. The sample cell has dimensions $L_x \times L_y = 10l_0 \times 12(\sqrt{3}/2)l_0$ for the smaller system of $N_\phi = 120$ vortices and $L_x \times L_y = 14l_0 \times 16(\sqrt{3}/2)l_0$ for the larger system of 224 vortices. Between $T_{\rm sc}$ and $T_{\rm sh}$, $\mu$ is, of course, evaluated by averaging only over the solidlike configurations. These are easily distinguished from the liquid configurations, since the energy among the latter fluctuates around a value $\sim 2\%$ above that of the solid. Among the liquid configurations $\mu$ averages to zero, as expected. For $N_\phi = 120$, $T_{\rm sc}$ and $T_{\rm sh}$ correspond to the values $1/g^2_{\rm sc} \approx 0.022$, $1/g^2_{\rm sh} \approx 0.028$. The exact thermodynamic melting transition is not easily determined by this procedure, however. The values of Fig. 2 represent averages over about $10^4$–$10^5$ passes through the sample. They show very little dependence on sample size.

In order to compare our results with the predictions of the KTBHNY theory, we rewrite the stability criterion $\lim_{T\to T_c^-} K(T) \equiv \lim_{T\to T_c^-} 4\mu(T)l_0^2/k_BT = 16\pi$ as

$$\lim_{T\to T_c^-} \frac{\mu_\phi(T)}{\mu_\phi^{\rm MF}(T)} = \frac{2\sqrt{3}\pi}{0.354}\frac{1}{g^2(T_c)}, \tag{9}$$

shown as a straight line in Fig. 2. Substitution of the mean-field value $\mu_\phi^{\rm MF}(T)$ for $\mu_\phi(T)$ into Eq. (9) leads to a mean-field estimate for the KTBHNY critical value, $g^{\rm MF}(T_c) = -5.54$. This point is marked with an arrow in Fig. 2, and clearly lies above the superheating limit, as might be expected from a mean-field theory. On the other hand, for $N_\phi = 120$, the KTBHNY prediction appears to coincide roughly with the *supercooling* limit, which is the point where a liquid can first be locally stable.

The critical temperature, determined as a point at which the energy distribution has 2 equal-height maxima,[17] suffers from large finite-size effects due to the large correlation length in the vortex liquid.[8,9] Kato and Nagaosa[8] have suggested an extrapolation of the thermodynamic melting temperature for $N_\phi \to \infty$, $g(T_c) = -7.15 \pm 0.10$ or $1/g^2(T_c) = 0.020$. This value does lie very near the temperature at which the instability criterion of Kosterlitz and Thouless is satisfied. Thus, our results for the shear modulus at melting could be consistent with the instability criterion. However, the exact value of $T_c$ at infinite size is still a matter of controversy. This is indicated in Fig. 2, where the infinite-size extrapolation of $T_c$ by Kato and Nagaosa,[8] and an alternative extrapolation by Hu and MacDonald,[9] are denoted by arrows.

According to the RG calculations of Halperin, Nelson, and Young, the shear modulus should have a power-law cusp as $T \to T_c^-$, $K(T) \sim 16\pi/(1 - c|1 - T/T_c|^\nu)$, where $c$ is a nonuniversal positive constant and $\nu = 0.3696\ldots$. There is no evidence of such behavior seen in our data, which is further evidence against the continuous transition.

In order to gain further insight into the two coexisting phases, we have examined the structure factor in each one. The instantaneous structure function $S(\mathbf{q}) \equiv S(q_x, q_y)$ is defined by

$$S(\mathbf{q}) = \int d^2\mathbf{r}\, d^2\mathbf{r}' |\psi(\mathbf{r})|^2 |\psi(\mathbf{r}')|^2 e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}, \tag{10}$$

evaluated in a randomly chosen representative of the MC ensemble. The instantaneous structure factor $I(\mathbf{q})$ is defined as the structure function for a given configuration reduced by the "atomic" structure factor, $I(\mathbf{q}) = S(\mathbf{q})/\exp(-q^2l^2/4)$. Figure 3 shows $I(\mathbf{q})$ for

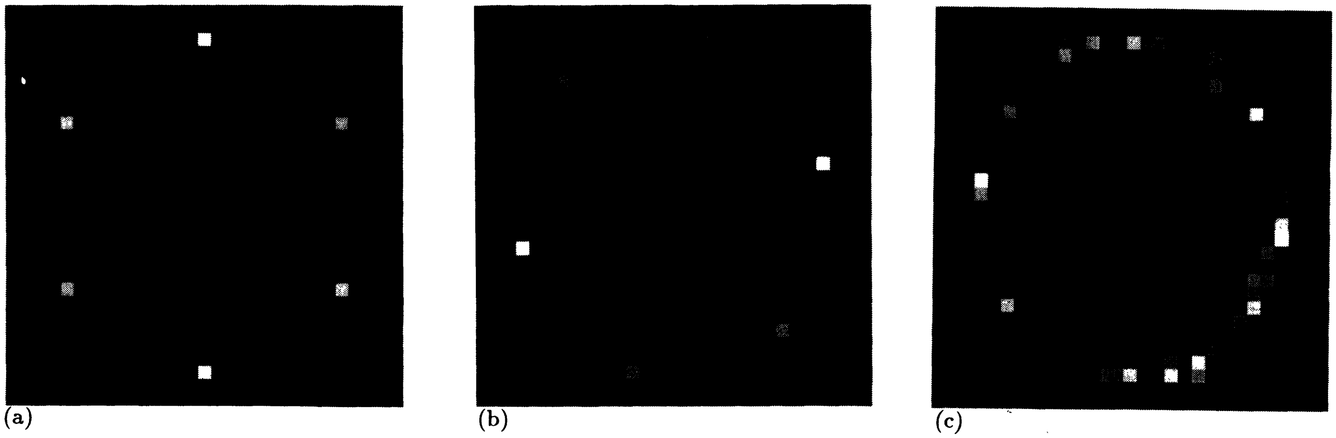

FIG. 3. Instantaneous structure factor $I(\mathbf{q})$ for a vortex lattice with $N_\phi = 120$ in a state drawn from (a) the solid phase at $1/g^2(T) = 0.020$; (b) the superheated solid at $1/g^2(T) = 0.026$; and (c) the liquid at $1/g^2(T) = 0.030$. Central maxima at $\mathbf{q} = 0$ have been eliminated in these plots.

$N_\phi$=120 and three different cases: (a) the solid phase at $1/g^2(T) = 0.020$; (b) the superheated solid at $1/g^2(T) = 0.026$; and (c) the liquid at $1/g^2(T) = 0.030$. These figures clearly confirm the structural identification of the two phases as solid and liquid, and in conjunction with Fig. 2 further show that the structural solid is the phase with the nonzero shear modulus. Note also the superheated solid in Fig. 3(b), which shows that the solid structure may be formed at various angles with respect to the coordinate axes. This suggests that the absence of full rotational invariance in this representation, with these boundary conditions, may not prevent the accurate calculation of physical properties.

The present results suggest that the shear modulus in a 2D vortex lattice does have a jump from 0 to a finite value at the thermodynamic freezing temperature $T_c$, and that the magnitude of the jump is near the postulated universal value. It is difficult to make a more precise statement because $T_c$ is significantly size dependent, while $\mu(T)$ (cf. Fig. 2) is not. At our largest size ($N_\phi = 224$), $\mu(T_c)$ is still slightly smaller than the universal value, but at the value of $T_c$ extrapolated to infinite lattice size, it may be equal to this value, or even slightly larger.

If $\mu[T_c(N_\phi \to \infty)]$ is, in fact, larger than the universal value, this would suggest that the first-order melting may intervene before the continuous melting transition can occur, as in the melting of the 2D Lennard-Jones solid studied by Abraham.[18] Our simulations may also be consistent with an alternative to the KTBHNY scenario, namely, the simultaneous unbinding of dislocations and disclinations at a first-order transition, as proposed by Kleinert.[19] The occurrence of a first-order melting transition presumably also explains the absence of a cusplike behavior in $\mu(T)$ just below $T_c$ in our calculations. On the other hand, since $\mu$ has a jump close to the universal value, it is clear that this first-order transition is quite weak, and could possibly be made continuous with only a slight change in the Hamiltonian.

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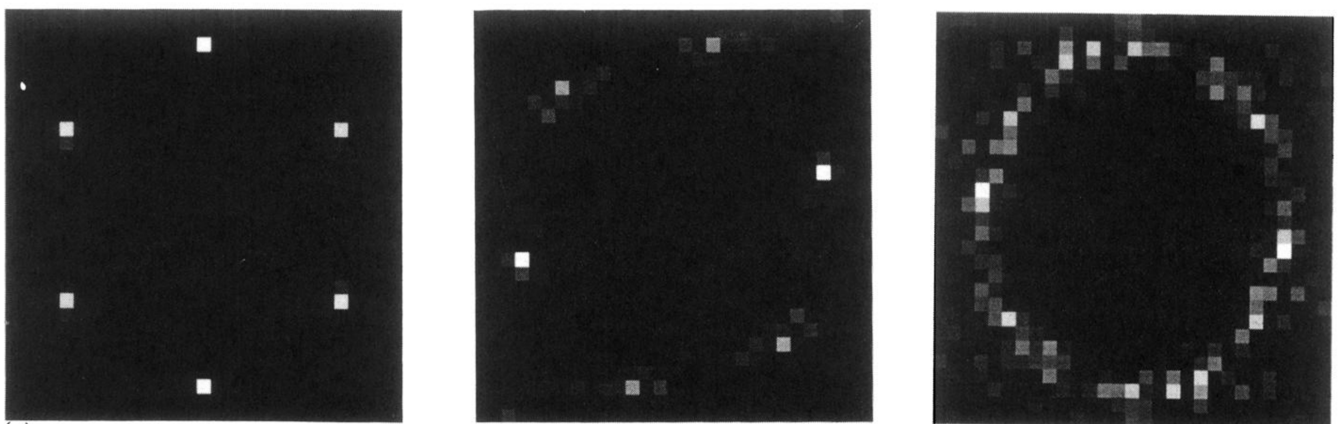

(a) (b) (c)

FIG. 3. Instantaneous structure factor $I(\mathbf{q})$ for a vortex lattice with $N_\phi = 120$ in a state drawn from (a) the solid phase at $1/g^2(T) = 0.020$; (b) the superheated solid at $1/g^2(T) = 0.026$; and (c) the liquid at $1/g^2(T) = 0.030$. Central maxima at $\mathbf{q} = 0$ have been eliminated in these plots.