Simple analytical model of vortex-lattice melting in two-dimensional superconductors

V. Zhuravlev

Department of Chemistry, Technion-Israel Institute of Technology, Haifa 32000, Israel

T. Maniv

Department of Chemistry, Technion-Israel Institute of Technology, Haifa 32000, Israel

and Grenoble High Magnetic Field Laboratory, Max-Planck-Institute fur Festkorperforschung and CNRS, Grenoble, France

(Received 8 February 1999)

The melting of the Abrikosov vortex lattice in a two-dimensional (2D) type-II superconductor at high magnetic fields is studied analytically within the framework of the phenomenological Ginzburg-Landau theory. It is shown that local phase fluctuations in the superconducting order parameter, associated with low-energies sliding motions of Bragg chains along the principal crystallographic axes of the vortex lattice, lead to a weak first-order "melting" transition at a certain temperature T_m , well below the mean-field T_c , where the shear modulus drops abruptly to a nonzero value. The residual shear modulus above T_m decreases asymptotically to zero with increasing temperature. Despite the large phase fluctuations, the average positions of Bragg chains at finite temperature correspond to a regular vortex lattice, slightly distorted with respect to the triangular Abrikosov lattice. It is also shown that a genuine long-range phase coherence exists only at zero temperature; however, below the melting point the vortex state is very close to the triangular Abrikosov lattice. A study of the size dependence of the structure factor at finite temperature indicates the existence of quasi-long-range order with $S(\vec{G}) \sim N^{\sigma}$, and $1/2 < \sigma < 1$, where superconducting crystallites of correlated Bragg chains grow only around pinning chains. This finding may suggest a very efficient way of generating pinning defects in quasi-2D superconductors. Our results for the melting temperature and for the entropy jump agree with the state-of-the-art Monte Carlo simulations. [S0163-1829(99)08129-1]

I. INTRODUCTION

Many potentially important superconductors, such as some of the high- T_c cuprates or the organic charge-transfer salts κ -(BEDT-TTF)₂X,¹ are highly anisotropic compounds with nearly two-dimensional electronic structure. These compounds are extremely type-II superconductors with very small in-plane coherence length. Consequently, the Ginzburg critical region is relatively large and so one expects drastic deviations from the predictions of the mean-field theory for these materials, due to strong thermal fluctuations in the superconducting order parameter.

In the mixed state at very low temperatures amplitude fluctuations are suppressed, but phase fluctuations can lead to the melting of the vortex lattice at a certain magnetic field $H_m(T)$, $H_{c1} < H_m < H_{c2}$.^{2,3} A soft shear Goldstone mode, which can be described by long-wavelength phase fluctuations⁴ is responsible for this remarkable melting phenomenon. Unfortunately, rigorous analytical approaches to this problem have encountered fundamental difficulties: large order high-temperature perturbation expansion with Borel-Pade approximants to the low-temperature behavior, $5,6$ has no indication of an ordered vortex lattice even at zero temperature. The existing nonperturbative approaches have not completely clarified the situation: Renormalization-group studies, $7,8$ as well as Monte Carlo simulation,⁹ have predicted no crystal vortex state in a pure two-dimensional $(2D)$ super $conductor (SC)$ at finite temperature, while the functional integral formalism suggested in Refs. 10 and 11, has led to some kind of a vortex liquid freezing transition without breaking the *U*(1) symmetry. Several Monte Carlo simulations have recently shown^{12–15} that in a 2D SC a true vortexlattice melting phase transition takes place at finite temperature and that the transition is of the first order.¹⁶

In this paper we present a simple model of the vortexlattice melting in 2D extremely type-II superconductors. Our model is based on the observation that at low temperature the main correction to the mean-field free energy arises from ''Bragg-chain fluctuations,'' namely, fluctuations which preserve long-range periodic order along a principal crystallographic axis in the vortex lattice. This simplification reduces our 2D problem to a 1D one, which can then be solved exactly.

Our calculations show that the Abrikosov triangular lattice is subject to strong phase fluctuations. As a result of these fluctuations the sharp mean-field transition into the Abrikosov lattice state becomes a smooth crossover. Since the strength of the phase dependent terms in the SC free energy is relatively small (\sim 2% of the SC condensation energy) the scale of the crossover temperature T_{cm} is well below the mean-field T_c . At temperatures higher than T_{cm} the vortex lattice transforms to an ensemble of strongly uncorrelated vortices, fluctuating independently around equilibrium lattice positions. It is found that because of a discontinuous (rotational) symmetry change in the mean positions of vortices there is a weak first-order transition, superimposed on the smooth solid-liquid crossover, which is reflected in a small jump of the vortex system entropy at a certain melting temperature $T_m \approx T_{cm}$. Calculation of the structure factor shows that exact long-range translational order exists only at zero temperature, in agreement with previous results.^{8,17,18} However, below the melting temperature

 T_m , the vortex state is very close to the triangular Abrikosov lattice. Our results for various thermodynamic parameters agree well with numerical calculations in Ref. 12.

II. THE SLIDING BRAGG-CHAINS MODEL

Our starting point is the Ginzburg-Landau (GL) freeenergy functional

$$
F_{GL} = \int d^2r \bigg[-\alpha |\psi(\vec{r})|^2 + \frac{1}{2} \beta |\psi(\vec{r})|^4 \bigg] \tag{1}
$$

with the order parameter $\psi(\vec{r})$, defined on the subspace of the lowest Landau level (LLL) .¹⁹ This approximation is valid at sufficiently low temperatures or high magnetic fields (i.e., for $k_B T \ll \hbar \omega_c$, when thermal excitations to higher Landau levels in the condensate of Cooper pairs can be neglected. All possible configurations of the order parameter in this subspace can be taken into account by considering the free energy

$$
F = -k_B T \ln Z \tag{2}
$$

with the partition function *Z* defined by the functional integral

$$
Z = \int D\psi D\psi^* \exp[-F_{GL}/k_B T]. \tag{3}
$$

In Eq. (1) $\alpha = \alpha'(H_{c2} - H)$ and β are phenomenological constants. The integral in Eq. (3) is performed over all nonequivalent states.

An arbitrary wave function (in the symmetric gauge) from the LLL subspace can be written as a one-dimensional integral:

$$
\psi(x,y) = e^{ixy} \int dq c(q) \phi_q(x,y), \tag{4}
$$

where $\phi_q(x,y) = \exp[iqx - (y + q/2)^2]$ is a Landau function with an orbital center located at $-q/2$ along the *y* axis. Note that all spatial lengths are measured in the units of the magnetic length $a_H = (c\hbar/eH)^{1/2}$. A system of *N* vortices, with size $L_x = a_x \sqrt{N}$ along the *x* direction, where a_x is an arbitrary constant, is described by *N* coefficients $c_i \equiv c(q_i)$, q_i $= (2\pi/L_{x})i$ with $i=-N/2+1,...,N/2$.

It is well known that the minimal value of the GL freeenergy functional is obtained when only \sqrt{N} coefficients from the whole set of *N* coefficients are different from zero (i.e., $c_{n,\overline{N}} \neq 0$, for $n = -\sqrt{N}/2 + 1, \ldots, \sqrt{N}/2$). At sufficiently low temperatures, when amplitude fluctuations are suppressed (see below), this minimum corresponds to the minimum of the Abrikosov parameter:

$$
\beta_a = \left(\frac{1}{V} \int d^2 r |\psi|^4\right) / \left(\frac{1}{V} \int d^2 r |\psi|^2\right)^2, \tag{5}
$$

where *V* is the volume of the superconductor. From the definition of β_a it is seen that the absolute minimum $\beta_a=1$ is obtained for a spatially uniform order parameter. Any deviation from $|\psi|$ = const leads to an increase in β_a . Under the constraint of the LLL subspace, however, $|\psi| \neq 0$ cannot be a constant (since $|\psi|=0$ at the vortex cores), and the minimum $\beta_a = \beta_A \approx 1.159$ is obtained for the triangular Abrikosov lattice, which is the closest configuration to the homogeneous

FIG. 1. The two families of Bragg chains in the triangular lattice along the principal axes *x* and *x'*. The parameters a_x and a_{x} are the periods of the order parameter modulus along these axes, respectively, while π/a_x and $\pi/a_{x'}$ are the respective distances between chains.

one. Other periodic lattices yield small positive deviations from β_A , while any departure of ψ from the quasiuniform distribution of the vortex lattice towards a localized structure leads to a drastic increase of the free energy.20

Thus we conclude that the main correction to mean-field order parameter arises from fluctuations of c_n and a_x , and take

$$
c(q) = \sum_{n=-\sqrt{N}/2+1}^{\sqrt{N}/2} c_n \delta\left(q - \frac{2\pi n}{a_x}\right).
$$
 (6)

Note that regardless of the choice of c_n , $e^{-ixy}\psi(x, y)$ is a periodic function of x with a period a_x . Therefore the used representation of $c(q)$ allows the order parameter to fluctuate only along the *y* direction. Each coefficient, $c_n = |c_n|e^{i\varphi_n}$, describes a set of \sqrt{N} Landau orbital centers, periodically arranged within a certain chain along the x axis $(Bragg)$ chain). These Bragg chains $(Fig. 1)$ are allowed to slide independently along their common axis, where the phase φ_n determines the relative position $x_n = -\varphi_n/q_n$ of the *n*th chain. The ideal lattice states are obtained by selecting $c_n^{(L)}$ $= c_0 \exp(i\gamma n^2)$, $0 \le \gamma \le \pi/2$.²¹ Then for an arbitrary rhombic lattice the lattice constant a_x in units of magnetic length and the angle $\Theta/2$ between the principal crystallographic axes are expressed through γ as $a_x^2 = \pi/\sqrt{1-(\gamma/\pi)^2}$, cos $\Theta = \gamma/\pi$.

The partition function (3) can be therefore approximated by the multiple functional integral

$$
Z \approx \int \prod_n dc_n dc_n^* \exp(-f_{GL}), \qquad (7)
$$

where

$$
f_{GL} = \frac{F_{GL}}{k_B T \sqrt{N}} = -\bar{\alpha} \sum_n |c_n|^2
$$

$$
+ \frac{\bar{\beta}}{2} \sum_{n,s,t} \lambda^{s^2 + t^2} c_n^* c_{n+s+t}^* c_{n+s} c_{n+t}
$$
 (8)

with $\bar{\alpha} = \alpha a_x / \sqrt{2\pi} k_B T$, $\bar{\beta} = \beta a_x / \sqrt{4\pi} k_B T$, $\lambda = \exp(-\pi^2/2)$ a_x^2). The inclusion of the factor $\sqrt{\overline{N}}$ in the denominator takes into account the fact that each term in the GL free-energy functional, Eq. (1) [written in the discrete representation (6)], corresponding to a certain Bragg chain in the vortex lattice, is degenerate \sqrt{N} times. This degeneracy reflects the freezing of all \sqrt{N} internal degrees of freedom within a chain. As discussed above, by relaxing these degrees of freedom the free-energy functional develops very large, highly improbable fluctuations. Therefore by dividing F_{GL} with \sqrt{N} we are left with a single nondegenerate term, which represents the dominant degree of freedom for each chain.

Note that the functional Eq. (8) is invariant under an arbitrary linear shift of the phases φ_n :

$$
\varphi_n' = \varphi_n + an + b. \tag{9}
$$

This symmetry follows from the symmetry of the GL freeenergy Eq. (1) under the magnetic translation group.²²

The functional (8) has a set of local minima with a single amplitude for the entire set of lattice configurations:

$$
|c_n|^2 = \frac{\overline{\alpha}}{\overline{\beta}\overline{\beta}_a}, \ \varphi_n = \gamma n^2, \ f_s = -\frac{\overline{\alpha}^2}{2\overline{\beta}\overline{\beta}_a},
$$

where

$$
\bar{\beta}_a = \sum_{sp} \exp[-z(s^2 + p^2)]\cos(2\gamma sp)
$$

is a reduced Abrikosov parameter, and $z = \pi^2/a_x^2$. These minima can be immediately obtained if we use the symmetry of the functional f_{GL} under the translation $n \rightarrow n+1$. The Abrikosov parameter β_a , defined by Eq. (5), is proportional to $\overline{\beta}_a$: $\beta_a = \sqrt{\pi} \overline{\beta}_a / a_x$. The triangular lattice, with β_a $= \beta_A^2$,²³ corresponds to $\gamma = \pi/2$, $a_x^2 = 2\pi/\sqrt{3}$. The meanfield condensation energy per unit vortex is F_{GL}/N $=-\pi\alpha^2/2\beta\beta_A$.

Our main approximation at this point is based on the small value of the parameter $\lambda \approx e^{-\pi}$, which enables us to neglect in Eq. (8) all terms of the order higher than λ^2 , i.e., to retain, in addition to the first-order terms in λ , only the leading-order terms in the phase (φ_n) dependent part of the free energy. Thus up to this order in λ

$$
f_{GL} = -\overline{\alpha} \sum_{n} |c_{n}|^{2} + \frac{\overline{\beta}}{2} \sum_{n} [|c_{n}|^{4} + 4\lambda |c_{n}|^{2} |c_{n+1}|^{2}
$$

$$
+ 4\lambda^{2} |c_{n-1}| |c_{n+1}| |c_{n}|^{2} \cos \chi_{n}].
$$
 (10)

The angles χ_n are linear combinations of the phases φ_n ,

$$
\chi_n = -2\,\varphi_n + \varphi_{n-1} + \varphi_{n+1},\tag{11}
$$

which are clearly invariant under the transformation (9) .

III. SHEAR MOTIONS: THE MELTING MECHANISM

The model presented in the previous section is based on our observation that the low-lying excitations of the Abrikosov vortex lattice are associated with the sliding motions of the lattice Bragg chains along the principal crystallographic axes. These excitations are closely related to the soft shear modes discussed by Moore⁴ in connection with the vortex lattice melting.

Let us consider this analogy in a greater detail. Following Ref. 4 we first invoke a perturbative approach with respect to the Abrikosov vortex-lattice solution $c_n^{(L)}$, by defining the displacements b_n through $c_n = c_n^{(L)}(1 + b_n)$, and their normal

mode (phonon) coordinates $u_k^{\pm} = (\frac{1}{N})^{1/4} \sum_n (b_n \pm b_n^{\star}) e^{ikn}$, with $k = (2\pi/\sqrt{N})l$, $l = -\sqrt{N/2}\cdots\sqrt{N/2}$, and then expanding the free-energy functional (10) to second order in these coordinates. Omitting the details of calculations our result can be written as

$$
\delta f_{GL} = \frac{2\,\bar{\alpha}^2}{\bar{\beta}\bar{\beta}_a} \sum_{k \ge 0} [P_k|u_k^+|^2 + Q_k|u_k^-|^2],\tag{12}
$$

where in the long-wavelength limit $k \rightarrow 0$, $P_k \rightarrow 2$, and Q_k $\rightarrow -\lambda^2 k^4 \cos 2\gamma$. Thus it can be readily shown that the relative variance of the order parameter diverges, i.e., $({\langle \psi^2 \rangle})$ $-\langle \psi \rangle^2$ / $\langle \psi \rangle^2$ \sim $\int (dk/k^4)$. Therefore we can conclude that although the lattice states with $\pi/4 < \gamma < \pi/2$ are thermodynamically stable ($\delta f_{GL} > 0$), the soft modes Q_k , $k \rightarrow 0$, are responsible for infinite fluctuations of the order parameter. This result is similar to that obtained by Moore⁴ for a 2D system of fluctuations. The divergence, which arises because of the perturbative nature of the above calculation, is stronger in our 1D model. However, within the nonperturbative method developed below this divergence is removed.

It should be noted that the soft mode described above is associated with the long wavelength component of the phase fluctuations in Eq. (10) ; this can be seen by neglecting amplitude fluctuations, defining fluctuating phases:

$$
\varphi_f(n) \equiv \varphi_n - \varphi_n^{(L)} = \varphi_n - \frac{1}{2} \pi n^2
$$

and taking the continuous limit [see Eq. (11)], i.e., $\chi_n \rightarrow \pi$ $+\partial^2 \varphi_f / \partial y^2$, so that the relevant part in the free-energy functional (10) can be written as

$$
\delta f_{ph} = K_A \int \cos(\pi + \partial^2 \varphi_f / \partial y^2) dy
$$

$$
\approx \frac{1}{2} K_A \int (\partial^2 \varphi_f / \partial y^2)^2 dy,
$$
(13)

where $K_A \approx \lambda^2(\bar{\alpha}^2/2\bar{\beta})$. It is instructive to compare this expression with that derived in Ref. 4 for the effective Hamiltonian associated with a smoothly varying phase $\theta(x, y)$, namely, $H_{ph} = \frac{1}{2} c_{66} \int d^2 r (\nabla^2 \theta)^2$, where c_{66} is an isotropic shear modulus of the vortex lattice, which is given approximately by $\frac{1}{2}(\vec{\alpha}^2/\vec{\beta})$.

The agreement between the two approaches is, however, incomplete, not only because of the one-dimensional nature of our model (in contrast to the 2D analysis of Ref. 4), but also because of the significant difference in the ''stiffness'' parameters K_A and c_{66} , namely, $K_A/c_{66} \approx \lambda^2 \sim 10^{-2}$. The reason for the disagreement can be understood within our approach by considering shear motions along families of Bragg chains with Miller indices higher than of the principal ones. For these families the values of a_x are relatively large, and the corresponding values of λ^2 are not small compared to unity. In the limit of very large Miller indices, $a_x \rightarrow \infty$ and $\lambda^2 \rightarrow 1$, so that the corresponding stiffness parameter approaches c_{66} , and becomes independent of the chain orientation, as in Moore's theory.

Thus in contrast to the isotropic shear model used in Ref. 4, the appearance of the small parameter λ^2 in front of the leading phase dependent terms of the free-energy functional (10) implies that the shear motions along the two principal crystallographic axes cost a small fraction of the condensation energy, and so lead to significant distortions of the vortex lattice along these particular directions at very low temperatures (i.e., with respect to the mean-field T_c).

Considering this low-temperatures regime, the calculation of the partition function *Z* can be simplified considerably since amplitude fluctuations can be neglected. The functional integrals in Eq. (3) over the order parameter $\{\psi, \psi^{\star}\}$ should be replaced by integrals over the new variables $\{c_n, c_n^{\star}\}\$ $\equiv \{|c_n|, \varphi_n\}.$

For an arbitrarily large system due to the invariance of free energy under the magnetic translation group, the transformation Eq. (11) is degenerate, and the inverse transformation, $\varphi_n = \varphi_n(\{\chi_m\})$, is not unique. It is determined up to a linear function of *n*. To determine the phases φ_n uniquely, we have to impose additional conditions, determining the arbitrary constant a and b in Eq. (9) . These conditions are equivalent to boundary conditions of Eq. (11) . Linear boundary conditions lead to linear dependence of *a* and *b* on χ_m . Since the determinant of any such transformation does not depend on the variables, the partition functions for various *a* and *b* differ by a constant factor. Therefore instead of $\{\varphi_n\}$ one can integrate over $\{\chi_n\}$ with the same free-energy functional. The GL free energy has different values when the phases $\{\chi_n\}$ lie within the interval $[0,\pi]$. To satisfy this condition and to exclude double counting of fluctuation we integrate over interval $\chi_n \in [0,\pi]$ and allow the phases φ_n in Eq. (11) to have arbitrary values.

Omitting unimportant constant factor we obtain after integration over angle variables that the partition function can be written as

$$
Z = Z_v^{\sqrt{N}} \propto \int_0^\infty \prod_n |c_n| d|c_n| e^{-f_s}, \tag{14}
$$

where

$$
f_s = \sum_{n} \left\{ -\overline{\alpha} |c_n|^2 + \frac{\overline{\beta}}{2} (|c_n|^4 + 4\lambda |c_n|^2 |c_{n+1}|^2) - \frac{1}{\pi} \ln I_0(2\overline{\beta}\lambda^2 \pi |c_{n-1}||c_{n+1}||c_n|^2) \right\}
$$
(15)

and $I_k(x)$ is the modified Bessel function of the order *k*.

Neglecting amplitude fluctuations, the integrals in Eq. (14) can be performed by the stationary phase approximation. Since the last term in Eq. (15) is of the order λ^2 or smaller, the approximate solution to the stationary point equations, $\partial f_s / \partial |c_n| = 0$, can be simply obtained by using the translational symmetry of the free-energy functional f_s . It is similar to the mean-field solution $|c_n|^2 = \overline{\alpha}/\overline{\beta} \overline{\beta}_{fl}$ with the generalized Abrikosov parameter

$$
\bar{\beta}_{fl} \approx 1 + 4\lambda - 4\lambda^2 \frac{I_1(\tau)}{I_0(\tau)},\tag{16}
$$

FIG. 2. Dependence of the Abrikosov parameter β_a on *z* $=(\pi/a_x)^2$. The two minima at $z_1 = \pi/2\sqrt{3}$ and $z_2 = \sqrt{3}\pi/2$ correspond to the triangular Abrikosov lattice, $\beta_a = \beta_A$, with different choice of the Bragg chains direction. The maximum at $z = \pi/2$ corresponds to the square lattice.

$$
\tau = \frac{4\lambda^2}{\left(1+4\lambda\right)^2} \frac{\pi \bar{\alpha}^2}{2\bar{\beta}} \equiv \frac{T_{cm}}{T}.
$$

The temperature $T_{cm}(a_x)$ determines a smooth crossover from the mean-field lattice state with $\gamma = \pi/2$, $\bar{\beta}_{fl} = \bar{\beta}_l = 1$ $+4\lambda-4\lambda^2$, to a new state corresponding to $\overline{\beta}_{fl} = \overline{\beta}_m = 1$ $+4\lambda$, where the phase dependent terms in the free energy are completely destroyed by fluctuations. Note that the energy difference between these states is of the order of the small parameter λ^2 .

In the zero temperature limit $T \ll T_{cm}(a_x)$ the parameter $\beta_{fl} \approx (\sqrt{\pi}/a_x)(1+4\lambda-4\lambda^2)$ has minimal values at a_x^2 $=2\pi/\sqrt{3}$, and $a_x^2 = 2\sqrt{3}\pi$ (Fig. 2), depending on the choice of the Bragg chains family²⁴ (i.e., along the *x* or *x'* axis in Fig. 1). Both of the minima describe a triangular Abrikosov lattice with $\beta_{fl} = \beta_A \approx 1.1596$. Both directions can be selected in three equivalent ways in the Abrikosov lattice. All equivalent configurations can be obtained from the invariance of the mean-field Abrikosov parameter $\beta_a = \sqrt{z/\pi} \sum_{sp} exp[-z(s^2+p^2)]cos(2\gamma sp)$, where $z = \pi^2/a_x^2$, under the transformations $z' = \pi^2 z/(z^2 + \gamma^2)$, $\gamma' = \pi^2 \gamma'$ $(z^2 + \gamma^2)$, and $z' = z$, $\gamma' = -\gamma$, or $\gamma' = \gamma + \pi n$ with an arbitrary integer *n*.

The doubly degenerate equilibrium state at $T=0$, just described, is stabilized by the competition between two types of interactions among parallel chains: the repulsive interaction between any two neighboring chains, which is linear in the coupling parameter λ , and the attractive three-body phase dependent interaction (i.e., involving any three neighboring chains), which is quadratic in λ [see Eq. (10)]. At finite, low temperatures, i.e., when $T \sim T_{cm}$, the shear fluctuations destroy the phase coherence among parallel Bragg chains, thus diminishing the small attractive interaction, and raising the total free energy. The relatively large, repulsive interaction is affected only at higher temperatures.

The interchain coupling parameter λ , depends on the lattice parameter a_x , through $\lambda = e^{-\pi^2/a_x^2}$. Since $a_x > a_x$ (Fig. 1), the chains along $x³$ are closer to each other than those

FIG. 3. Free energy of fluctuating Bragg chains (normalized by the mean-field free energy), $-\beta_A/\beta_{fl}$, as a function of the parameter t (see text). Solid and dashed lines correspond to Bragg chains along the x and $x³$ directions, respectively. The intersection point at $t = t_m \approx -16.5$ determines the phase transition.

along *x*, and so $\lambda(a_{x}) > \lambda(a_x)$. Consequently, at low temperatures, $T \leq T_{cm}(a_x)$, when the attractive three-body interaction diminishes with increasing temperature, the first state (a_x) is more stable than the second one (a_x) , since its free energy increases more slowly with increasing temperature than that of the second one $(Fig. 3)$. At higher temperatures $T \geq T_{cm}(a_{x})$, when the repulsive interchain couplings determine the temperature dependence, the tendency is reversed and the free energy of the first state (a_x) increases faster with increasing temperature than that of the second one (a_x) . Thus there is an intersection point $T_{cm}(a_x) \le T_m \le T_{cm}(a_{x}),$ at which the free energies of the these states are equal, but the corresponding entropies are a little different. Therefore we conclude that at $T=T_m$, there is a weak first-order transition characterized by a small jump of the lattice entropy. Defining the parameter $t = -\alpha \sqrt{2\pi/\beta k_B T}$,¹² the position of the crossing point corresponds to $t = t_m \approx -16.5$, and the jump in the entropy $[S = -T(\partial F/\partial T)]$ is $\Delta S \approx 7.5$ $\times 10^{-3}F_{MF}/T$. The values of t_m and ΔS agree fairly well with the Monte Carlo simulations.¹²

The physical nature of this transition can be illuminated by considering the shear modulus μ . The vanishing of the shear modulus in atomic crystals is usually regarded as a definition of the crystal melting point. In our case μ can be calculated by transforming $c'_n = e^{i\eta n^2}c_n$ (Ref. 15) and taking the limit

$$
\mu = \left(\frac{\partial^2 F_{GL}}{\partial \eta^2}\right)_{\eta \to 0}.
$$

Note that the considered transformation shifts the phases χ_n by -2η . Therefore the shear modulus is proportional to the phase factor in the free energy, i.e., $\mu \propto \langle \cos \chi_n \rangle$. Normalized by the mean-field value μ_{MF} , where cos $\chi_n = -1$, it is reduced to

$$
\frac{\mu}{\mu_{MF}} = \frac{I_1(\tau)}{I_0(\tau)}.
$$
\n(17)

FIG. 4. Dependence of the shear modulus μ on the reduced temperature *t*. The jump of μ at $t = t_m$ reflects the melting transition.

The dependence of the shear modulus on the parameter *t* is plotted in Fig. 4. At the transition point $t = t_m$ the value of the parameter a_x , corresponding to the minimum free energy, changes abruptly and the shear modulus jumps from μ_1 to μ_2 . It should be stressed that $\mu_2 \neq 0$. The residual shear energy on the high-temperature side of the transition point reflects an incomplete melting at $t = t_m$. The "liquid" state on this side of the transition point retains some degree of phase coherence between different chains, which continues to decrease gradually to zero with increasing temperature, reaching the complete liquid state only asymptotically. This behavior seems to be due to the persistence of long-range periodic order along the chains axis in our model at any temperature.

Interesting structural information on the ''quasiliquid'' states described above can be obtained from the calculation of the average values

$$
\langle \chi_n^k \rangle = \frac{1}{\pi I_0(\tau)} \int_0^{\pi} d\chi_n \chi_n^k \exp(-\tau \cos \chi_n)
$$

with $k=1,2$. In the low- and high-temperature limits,

$$
\langle \chi_n \rangle = \pi - \sqrt{\frac{2}{\pi \tau}}, \ \langle \chi_n^2 \rangle = \pi^2 - \left(\frac{8\,\pi}{\tau}\right)^{1/2} + \frac{1}{\tau} \text{ for } \tau \gg 1
$$
\n(18)

$$
\langle \chi_n \rangle = \pi/2 + 2\tau/\pi
$$
, $\langle \chi_n^2 \rangle = \pi^2/3 + 2\tau$ for $\tau \ll 1$.

The square root of the relative variance σ $=\sqrt{\langle \chi_n^2 \rangle - \langle \chi_n \rangle^2}/\langle \chi_n \rangle$, is found to be $\sigma \approx (\pi - 2)/\pi \tau \ll 1$ in the low-temperatures regime and $\sigma \approx 1/\sqrt{3}$ in the hightemperatures one. These results show that with the temperature increase the fluctuations destroy the phase correlation between chains so that the SC state transforms from a frozen Abrikosov lattice at zero temperature to a new, ''liquid'' state with strong vortex fluctuations. However, in contrast to the usual liquid state, here we find that the average vortex positions form a regular lattice with $\gamma = \pi/4$ and π^2/a_x^2 \approx 2.97, where a_x corresponds to the minimum free energy. For this lattice the angle $\Theta/2$ between the principal crystallographic axes corresponds to $\Theta \approx 75^{\circ}$.

The first-order "melting" point at $t = t_m$ thus corresponds to a discontinuous (rotational) symmetry breaking in this lattice of average vortex positions, from $\Theta \approx 60^{\circ}$ (Abrikosov lattice) on the low-temperature side, to $\Theta \approx 75^{\circ}$ on the hightemperature one.

IV. BRAGG-CHAINS PINNING AND THE ABSENCE OF LONG-RANGE ORDER

An intriguing issue in the theory of the vortex-lattice melting concerns the existence or the absence of long-range phase coherence in the SC mixed state. In this section we address the problem of long-range order (LRO) and the related topic of vortex lines pinning, as they appear in our model.

As discussed in Sec. III, the fluctuating phases φ_n cannot be uniquely determined from χ_n ; they depend on the choice of the boundary conditions for Eq. (11) . Since the general solution of the homogeneous equation $(\chi_n=0)$ is a linear function of n [Eq. (9], two constants (a and b) are required to uniquely determine φ_n . A possible choice is to take *a* $=$ b=0, which corresponds to the selection φ_0 =0, and $\varphi_{-1} = \varphi_1$. The physical meaning of the first condition is that the chain, labeled $n=0$ (i.e., located vertically at $y=0$), is pinned to a fixed "horizontal" (i.e., along the *x* axis) position. The second condition has a clear physical meaning in the long-wavelength limit, namely that the horizontal displacement $u_x = (\partial \theta / \partial y)$ of the vortex lines vanishes at the pinning site $y=0$.

The solution of Eq. (11) which satisfies this particular pinning condition is (for $n > 0$)

$$
\varphi_{\pm n} = \sum_{l=0}^{n} (n-l)\chi_{\pm l} + \frac{n}{2}\chi_0.
$$
 (19)

This transformation enables us to calculate any correlation function of phase factors; in particular, the pair correlation function

$$
\langle e^{i(\varphi_n/\varphi_n)} \rangle = \Pi_{\nu} \int_0^{\pi} d\chi_{\nu} e^{-\tau \cos \chi_{\nu}} e^{i(\varphi_n/\varphi_n)} / \Pi_{\nu}
$$

$$
\times \int_0^{\pi} d\chi_{\nu} e^{-\tau \cos \chi_{\nu}}
$$

can be readily evaluated by using Eq. (19) to yield

$$
\langle e^{i(\varphi_n - \varphi_n)} \rangle = \frac{\Pi_{\nu}^n I_v(-\tau)}{I_0(-\tau)^{n+1}},
$$
\n(20)

where the function $v \equiv v(v;n,n') = v(v;n',n')$ is defined (for $n > n'$) by $\frac{1}{2} |n - n'|$ at $\nu = 0$, $|n - n'|$ for $0 < \nu \le n'$, $|n|$ $|-\nu|$ for $n' < \nu \leq n$, and 0 for $\nu > n$.

In the high-temperature limit $\tau \ll 1$, far above the melting point, the small argument expansion of the modified Bessel function $I_v(-\tau)$ yields

$$
\langle e^{i(\varphi_{n'}-\varphi_n)}\rangle \propto \tau^{\ln^2 - n'^2/2} \to \delta_{n,n'}
$$
 (21)

meaning no phase correlation at all.

In the low-temperature limit $\tau \geq 1$, the asymptotic expansion of I_v ($-\tau$) leads (for any $n' \ge n \ge 1$) to the expression

$$
\langle e^{i(\varphi_n - \varphi_n)} \rangle \approx e^{i\pi (n'-n^2)/2} \exp \bigg[-\frac{\bar{n}}{2\tau} (\Delta n)^2 \bigg], \qquad (22)
$$

where $\Delta n = n' - n$ and $\bar{n} = n'/3 + 2n/3 - 1/2$. Equation (22) is identical to a second-order cumulant expansion with $\langle \varphi_n \rangle = \frac{1}{2} \langle \chi_n \rangle n^2 \approx \frac{1}{2} \pi n^2$.

This result shows that a genuine long-range phase correlation exists only at zero temperature; it also shows that a cluster of highly correlated chains can grow only around a pinned chain, since the phase fluctuations diverge with the distance from the pinning chain [see Eq. (19)]. Note that the position of such a chain is arbitrary since there is no energy cost to pinning in the GL theory used. In real samples the translational symmetry is broken by impurities, crystal defects, and the termination of the lattice at the sample surface, which can pin chains of orbital centers to fixed positions. A single pinning center located near a given chain may pin the entire chain due to the chain rigidity. To maximize the pinning strength, however, additional pinning centers should be distributed uniaxially along the same chain, rather than randomly.

Let us now study the range of SC order existing in the vortex state at finite temperature. This can be done by considering the size dependence of the structure factor: 12

$$
S(\vec{G}) = \frac{1}{N} \langle |I(\vec{G})|^2 \rangle,
$$

where

$$
I(\vec{G}) = \int d^2r |\psi(\vec{r})|^2 e^{i(\vec{G}\cdot\vec{r})}
$$

and \tilde{G} is a reciprocal-lattice vector of the Abrikosov lattice with $G_x = 2\pi \nu/a_x$, $G_y = (2\pi m/b_y) - 2\nu b_x$; $b_y = \pi/a_x$, b_x $= \langle \chi_n \rangle a_x/2\pi$, and v, *m* integers. At zero temperature the long-range order is reflected by the Bragg peaks with $S(G)$ \propto *N*. At finite temperature,

$$
S(\vec{q}) = \frac{\pi a_x^2}{2} e^{-q^2/4} \sum_{n,n',\nu} \delta_{q_x,2\pi\nu/a_x}
$$

× C₄(n' + ν ,n,n',n + ν)e^{-i(\pi/a_x)(n-n')q_y}, (23)

where at $\tau \geq 1$

$$
C_4(n_1, n_2, n_3, n_4) \equiv \langle e^{i[\varphi_f(n_1) + \varphi_f(n_2) - \varphi_f(n_3) - \varphi_f(n_4)]} \rangle
$$

=
$$
\exp\left[-\frac{s^2(p - s/3 + 1/3)}{2\tau}\right]
$$

+
$$
i\langle \chi_n \rangle \nu(n - n')\right] \quad \nu \ge 0
$$
 (24)

with $s = min(v, |n'-n|), p = max(v, |n'-n|), n_1 = n' + v, n_2$ $=n, n_3=n', n_4=n+\nu$. Note that C_4 is the four-chain phase correlation function appearing in the quartic term of the GL free energy.

Now, since $\langle \chi_n \rangle = \overline{\chi}$ is independent of *n*, the sum over *n* yields a factor \sqrt{N} , and Eq. (23) can be rewritten as

$$
S(\vec{G}) = \sqrt{N} \frac{\pi a_x^2}{2} e^{-G^2/4} \times \left\{ \sum_{|l| \leq \nu} \exp\left[i l (\nu \overline{\chi} - b_y G_y) - |l|^2 \left(\nu - \frac{1}{3} |l|\right) / 2\tau\right] + \sum_{|l| > \nu} \exp\left[i l (\nu \overline{\chi} - b_y G_y) - \nu^2 \left(|l| - \frac{1}{3} \nu\right) / 2\tau\right] \right\}.
$$
 (25)

This expression reflects the extreme anisotropy characterizing our Bragg chains model: Along the reciprocal-lattice axis $G_x=0$ [i.e., for $\nu=0$ in Eq. (25)] one finds perfect LRO, since $S(G_x=0, G_y) \sim N$. For any $G_x \neq 0$, however, the corresponding Bragg peaks reflect only the 1D LRO within the real lattice chains, i.e., $S(G_x \neq 0, G_y) \sim N^{1/2}$. This feature is due to the finite range of the off-diagonal phase correlation function (i.e., to the absence of off-diagonal LRO) at finite temperature.

It should be stressed here that in the triangular Abrikosov lattice there are three equivalent ways to select the principal axes. Since the reciprocal-lattice points with $G_x=0$ depend on our concrete choice of the coordinate system one may expect that by averaging over all three equivalent orientations, the size dependence of the structure factor will be isotropic, satisfying $S \sim N^{\sigma}$ with $1/2 < \sigma < 1$.

This result is consistent with the quasi-LRO obtained by Kato and Nagaosa, 12 which is reminiscent of the Kosterlitz-Thouless-Halperin-Nelson-Young²⁵ theory of 2D melting, according to which $S \sim N^{\sigma}$ with $\sigma \le 5/6$.

V. CONCLUSION

In this paper we have studied the melting of the SC vortex lattice in 2D at high magnetic fields and low temperatures (i.e., in the LLL approximation) by using an approximate analytical approach. Our results basically agree with the state-of-the-art Monte Carlo simulations. The simple analytical approach used enables us to draw a clear picture of the melting process: The skeleton of this picture consists of the principal crystallographic axes in the triangular Abrikosov lattice, along which families of almost rigid Bragg chains slide nearly freely at low temperatures due to thermal fluctuations. Similar motions along crystal axes with higher Miller indices cost significantly more energy and are therefore quenched at low temperatures.

The melting of the lattice occurs essentially when these fluctuations overcome the weak attractive interaction between chains. This interaction is not the same for the two principal axes; it is stronger for the more closely packed family of chains.

Thus the fluctuations destroy the order within the more loosely packed family of chains at lower temperature. Consequently the configuration based on the more closely packed family is the more stable one at low temperatures (i.e., below T_m). However, at higher temperatures (i.e., above T_m) when the order in the closely packed family is also destroyed, the configuration based on the loosely packed family of chains becomes the more stable one, since the remaining interaction between chains at these temperatures is repulsive and weaker for the loosely packed family.

The first-order transition at T_m is therefore a discontinuous transformation between two different average configurations of chains. The low-temperature configuration is an ideal Abrikosov triangular lattice with small fluctuations about the mean positions of vortices. In the high-temperature configuration the phase fluctuations are significantly larger than in the low-temperature one, whereas the mean positions of the vortices are still forming an exactly regular lattice, but now with $\Theta \approx 75^{\circ}$.

A correlated cluster of chains nucleates only around a pinned chain. Since according to our model, the pinning force of a whole chain can be strengthened dramatically by distributing pinning centers uniaxially along this chain, it may suggest a very efficient way of generating pinning defects in quasi-2D SC. This pinning mechanism may be tested experimentally by producing columnar defects²⁶ along the conducting planes in quasi-2D SC.

The neighboring-chains appoximation used in the derivation of our Eq. (10) is similar to that employed by Balents and Radzihovsky, 27 in studying freezing transition in a 3D Ginzburg-Landau model of layered superconductors. In that work the authors considered vortices confined by an external 1D periodic potential, which partially removes the LLL degeneracy, a procedure which enabled them to show how the neighboring SC layers continuously freeze into a triangular vortex lattice. We stress, however, that in our work, we study 2D SC, where the two principal crystallographic axes of the vortex lattice determine the propagation directions of the soft modes, without any need for a confining external potential. The existence of two inequivalent principal directions for sliding chains in our approach, in contrast to the single direction dictated by the 1D external potential in Ref. 27 approach, is responsible for the discontinuous, first-order transition appearing in our work, which is absent in Ref. 27.

We would like to thank I. D. Vagner and P. Wyder for stimulating discussions and Z. Tesanovic for helpful comments. This research was supported by The Israel Science Foundation founded by The Academy of Sciences and Humanities, and by the Fund for the Promotion of Research at the Technion.

- ¹ For a review, see *The Physics and Chemistry of Organic Superconductors*, edited by G. Saito and S. Kagoshima, Springer Proceedings in Physics Vol. 51 (Springer, Berlin, 1990).
- 2S. Friemel, C. Pasquier, Y. Loirat, and D. Jerome, Physica C **259**, 181 (1996).
- ³T. Sasaki, W. Biberacher, K. Neumaier, W. Hehn, K. Andres, and T. Fukase, Phys. Rev. B 57, 10 889 (1998).
- ⁴ M.A. Moore, Phys. Rev. B **39**, 136 (1989).
- 5 G.J. Ruggeri and D.J. Thouless, J. Phys. F 6, 2063 (1976).
- 6E. Brezin, A. Fujita, and S. Hikami, Phys. Rev. Lett. **65**, 1949 $(1990).$
- 7 L. Radzihovsky, Phys. Rev. Lett. **74**, 4722 (1995).
- 8 M.A. Moore and D.J. Newman, Phys. Rev. Lett. **75**, 533 (1995); D.J. Newman and M.A. Moore, Phys. Rev. B 54, 6661 (1996).
- 9 J.A. O'Neil and M.A. Moore, Phys. Rev. Lett. 69 , 2582 (1992).
- 10 Z. Tesanovic and A.V. Andreev, Phys. Rev. B 49, 4064 (1994).
- 11 I.F. Herbut and Z. Tesanovic, Phys. Rev. Lett. **73**, 484 (1994); Physica C 255, 324 (1995).
- ¹² Yusuke Kato and Naoto Nagaosa, Phys. Rev. B 48, 7383 (1993).
- 13 Jun Hu and A.H. MacDonald, Phys. Rev. Lett. 71 , 432 (1993).
- 14S. Hikami, A. Fujita, and A.I. Larkin, Phys. Rev. B **44**, 10 400 $(1991).$
- ¹⁵ R. Sasik and D. Stroud, Phys. Rev. B **49**, 16 074 (1994).
- ¹⁶Earlier Monte Carlo simulations carried out by L. Xing and Z. Tesanovic, Phys. Rev. Lett. 67, 2729 (1991), and Physica C 196, 241 (1992), found a melting phase transition, but the nature of this transition was not completely clear.
- ¹⁷ A.V. Nikulov, Phys. Rev. B **52**, 10 429 (1995).
- 18R. Sasik, D. Stroud, and Z. Tesanovic, Phys. Rev. B **51**, 3042 $(1995).$
- ¹⁹G. Eilenberger, Phys. Rev. **164**, 628 (1967).
- ²⁰ For example, by adding N_0 degrees of freedom to each unit cell, corresponding to the wave numbers $q_{n,m} = (2\pi/L_x)(\sqrt{N}n)$ $+m)$ ($m=-N_0/2+1,...,N_0/2$), and taking the coefficients $c_{n,m}$ with equal amplitudes, the superfluid density can be shown to be localized along the *x* direction with size $\sim L_x/N_0$. For such a state we find $\beta_a \sim N_0$, and the corresponding SC condensation energy is by the factor $1/N_0$ smaller than the mean-field conden-

sation energy. Also, by allowing the positions of c_n to deviate from the equilibrium periodic array $q_n=2\pi n/a_x$, the mean values of $|c_n|^2$ are no longer independent of *n*, and the corresponding fluctuations cause variations in the free-energy functional of lower orders than λ^2 . Consequently, this type of fluctuation is also significantly more energetic than the phase fluctuations considered in the present paper.

- 21T. Maniv, A.I. Rom, I. Vagner, and P. Wyder, Phys. Rev. B **46**, 8360 (1992); V.N. Zhuravlev, T. Maniv, I. Vagner, and P. Wyder, *ibid.* **56**, 14 693 (1997).
- 22 E. Brown, Solid State Phys. **22**, 312 (1968).
- 23W.H. Kleiner, L.M. Roth, and S.H. Autler, Phys. Rev. **133**, A1226 (1964).
- ²⁴ We neglect families of Bragg chains with Miller indices higher than of the principal ones as a result of larger values of stiffness parameter along these chains. The quantitative treatment of such chains is rather difficult because of necessity to go beyond the nearest-neighbor approximation.
- ²⁵ J.M. Kosterlitz and D.J. Thouless, J. Phys. C **6**, 1181 (1973); B.I. Halperin and D. Nelson, Phys. Rev. Lett. **41**, 121 (1978); A.P. Young, Phys. Rev. B 19, 1855 (1979).
- 26L. Klein, E.R. Yacoby, Y. Yeshurun, M. Konczykowski, and K. Kishio, Phys. Rev. B 48, 3523 (1993).
- 27 L. Balents and L. Radzihovsky, Phys. Rev. Lett. **76**, 3416 (1996).