

Thermal fluctuations and disorder effects in vortex lattices

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(Received 30 March 1999)

We calculate using loop expansion the effect of fluctuations on the structure function and magnetization of the vortex lattice and compare it with existing Monte Carlo results. In addition to renormalization of the height of the Bragg peaks of the structure function, there appear characteristic saddle shape “halos” around the peaks. The effect of disorder on magnetization is also calculated. All the infrared divergencies related to soft shear cancel. [S0163-1829(99)11837-X]

I. INTRODUCTION

Decoration,¹ neutron scattering,² and scanning tunneling microscopy³ have clearly demonstrated the Abrikosov flux line lattice in low- and high- T_c type-II superconductors. There are, however, important differences between the two classes of materials. The Ginzburg parameter G_i characterizing the importance of thermal fluctuations is much larger in high- T_c superconductors than in the low temperature ones. Moreover, in the presence of magnetic field the importance of fluctuations in high- T_c superconductors is further enhanced. The lattice melts and becomes a vortex liquid over large portions of the phase diagram.⁴⁻⁶ In “strongly fluctuating” superconductors, even far below the melting line, corrections to various physical quantities such as magnetization or specific heat are not negligible. The vortex lattice becomes distorted. It is quite straightforward to systematically account for the fluctuation effect on magnetization, specific heat, or conductivity perturbatively above the mean field transition line using a Ginzburg-Landau (GL) description.⁷ However, in the interesting region below this line it turned out to be extremely difficult to develop a quantitative theory.

A direct approach to the low temperature fluctuations physics is to start from the mean field solution and then take fluctuations around this inhomogeneous solution into account perturbatively. Experimentally it is reasonable since, for example, specific heat at low temperatures is a smooth function and the fluctuation contribution is quite small. For some time this was in disagreement with theoretical expectations. Eilenberger calculated the spectrum of harmonic excitations of the triangular vortex lattice⁸ and noted that the gapless mode is softer than the usual Goldstone mode expected as a result of spontaneous breaking of translational invariance. The inverse propagator for the “phase” excitations behaves as $k_z^2 + \text{const}(k_x^2 + k_y^2)$.² It was shown^{9,10} that the constant in front of $(k_x^2 + k_y^2)^2$ is directly related to the shear modulus c_{66} and is in agreement with numerous experiments. An interesting question is whether the $(k_x^2 + k_y^2)^2$ behavior disappears nonperturbatively. We point out that Monte Carlo simulation of the structure function¹¹ provides direct evidence that it is not so.

The influence of this additional “softness” goes beyond

enhancement of the contribution of fluctuations at leading order. It apparently leads to disastrous infrared divergencies at higher orders rendering the perturbation theory around the vortex state doubtful. One therefore tends to think that non-perturbative effects are so important that such a perturbation theory should be abandoned.¹² However, it was shown in Ref. 13 that a closer look at the diagrams reveals that in fact one encounters actually only logarithmic divergencies. This makes the divergencies similar to so-called “spurious” divergencies in the theory of critical phenomena with broken continuous symmetry and they exactly cancel at each order provided we are calculating a symmetric quantity. One can effectively use properly modified perturbation theory to quantitatively study various properties of the vortex liquid phase. Magnetization calculated using this perturbative approach agrees very well with the direct Monte Carlo (MC) simulation of Ref. 11. The method was then extended beyond the lowest Landau level (LLL).¹⁴

In this paper we calculate the effect of fluctuations on the magnetic field distribution and structure function of the vortex lattice and compare with existing MC results. Fluctuations cause the spread of the peaks in the diffraction pattern in a very specific way, while the height of the peaks is slightly corrected. Effects of fluctuation and disorder on magnetization and specific heat are computed. The paper is organized as follows. In Sec. II the model and the fluctuation spectrum approximation are briefly reviewed. In Sec. III the calculation of the structure function is presented. Section IV contains analysis of the result, comparison with MC simulation, and some generalizations. In Sec. V the distribution of magnetic field is calculated, while effects of weak disorder on magnetization and specific heat are treated in Sec. VI. A summary is given in Sec. VII.

II. MODEL, MEAN FIELD SOLUTION, AND THE PERTURBATION THEORY

A. Model

Our starting point is the GL free energy:

$$F = \int d^3x \frac{\hbar^2}{2m_{ab}} \left| \left(\nabla - \frac{ie^*}{\hbar c} \mathbf{A} \right) \psi \right|^2 + \frac{\hbar^2}{2m_c} |\partial_z \psi|^2 + a |\psi|^2 + \frac{b'}{2} |\psi|^4. \quad (1)$$

Here $\mathbf{A}=(By,0)$ describes a nonfluctuating constant magnetic field. For strongly type-II superconductors ($\kappa\sim 100$) far from H_{c1} (this is the range of interest in this paper) magnetic field is homogeneous to a high degree due to superposition from many vortices. For simplicity we assume $a=\alpha(1-t)T_c$, $t\equiv T/T_c$, although this dependence can be easily modified to better describe the experimental coherence length.

Throughout most of the paper will use the following units. The unit of length is $\xi=\sqrt{\hbar^2/(2m_{ab}\alpha T_c)}$ and the unit of magnetic field is H_{c2} , so that the dimensionless magnetic field is $b\equiv B/H_{c2}$. The dimensionless free energy in these units is (the order parameter field is rescaled as $\psi^2\rightarrow(2\alpha T_c/b')\psi^2$)

$$\frac{F}{T}=\frac{1}{\omega}\int d^3x\left[\frac{1}{2}|D\psi|^2+\frac{1}{2}|\partial_z\psi|^2-\frac{1-t}{2}|\psi|^2+\frac{1}{2}|\psi|^4\right]. \quad (2)$$

The dimensionless coefficient is

$$\omega=\sqrt{2\text{Gi}\pi^2t}, \quad (3)$$

where the Ginzburg number is defined by $\text{Gi}\equiv\frac{1}{2}(32\pi e^2\kappa^2\xi T_c\gamma^{1/2}/c^2h^2)^2$ and $\gamma\equiv m_c/m_{ab}$ is an anisotropy parameter. This coefficient determines the strength of fluctuations, but is irrelevant as far as mean field solutions are concerned.

The second expansion parameter is (see Refs. 9 and 14 for details)

$$a_h\equiv\frac{1-t-b}{2}. \quad (4)$$

B. Mean field solution

If a_h is sufficiently small GL equations can be solved perturbatively:

$$\psi=\Phi=(a_h)^{1/2}[\Phi_0+a_h\Phi_1+\dots]. \quad (5)$$

It is convenient to represent Φ_0, Φ_1, \dots in the basis of eigenfunctions of operator $\mathcal{H}\equiv\frac{1}{2}(-D^2-b)$, $\mathcal{H}\varphi^n=n b\varphi^n$, normalized to unit ‘‘Cooper pairs density’’ $\langle|\varphi^n|^2\rangle\equiv\int_{\text{cell}}d^2x|\varphi^n|^2/(b/2\pi)=1$, where ‘‘cell’’ is a primitive cell of the vortex lattice. Assuming hexagonal lattice symmetry one explicitly has:

$$\begin{aligned} \varphi^n &= \sqrt{\frac{2\pi}{\sqrt{\pi}2^n n! a^l}} \sum_{l=-\infty}^{\infty} H_n\left(y\sqrt{b}-\frac{2\pi}{a}l\right) \\ &\times \exp\left\{i\left[\frac{\pi l(l-1)}{2}+\frac{2\pi\sqrt{b}}{a}lx\right]-\frac{1}{2}\left(y\sqrt{b}-\frac{2\pi}{a}l\right)^2\right\}, \end{aligned} \quad (6)$$

where $a/\sqrt{b}=\sqrt{4\pi/\sqrt{3}b}$ is the lattice spacing. One finds

$$\Phi_0=\frac{1}{\sqrt{\beta_A}}\varphi. \quad (7)$$

To order a_h^i , we expand

$$\Phi_i=g_i\varphi+\sum_{n=1}^{\infty}g_i^n\varphi^n. \quad (8)$$

These coefficients can be found in Ref. 14.

C. Fluctuation spectrum

To find an excitation spectrum one expands a free energy functional around the solution. The fluctuating order parameter field ψ is divided into a nonfluctuating (mean field) part and a small fluctuation

$$\psi(x)=\Phi(x)+\chi(x). \quad (9)$$

We expand field χ in a basis of quasimomentum eigenfunctions:

$$\begin{aligned} \varphi_{\mathbf{k}}^n &= \sqrt{\frac{2\pi}{\sqrt{\pi}2^n n! a^l}} \sum_{l=-\infty}^{\infty} H_n\left(y\sqrt{b}+\frac{k_x}{\sqrt{b}}-\frac{2\pi}{a}l\right) \\ &\times \exp\left\{i\left[\frac{\pi l(l-1)}{2}+\frac{2\pi\left(\sqrt{b}x-\frac{k_y}{\sqrt{b}}\right)}{a}l-xk_x\right]\right. \\ &\left.-\frac{1}{2}\left(y\sqrt{b}+\frac{k_x}{\sqrt{b}}-\frac{2\pi}{a}l\right)^2\right\}. \end{aligned} \quad (10)$$

Then we diagonalize the quadratic term to obtain the spectrum. The details can be found in Ref. 14. Instead of complex field $\chi_{\mathbf{k}}^n$ we will use two ‘‘real’’ fields $O_{\mathbf{k}}^n$ and $A_{\mathbf{k}}^n$ satisfying $O_{\mathbf{k}}^n=O_{-\mathbf{k}}^{*n}$, $A_{\mathbf{k}}^n=A_{-\mathbf{k}}^{*n}$:

$$\chi(x)=\frac{1}{\sqrt{2}}\int_{\mathbf{k}}\frac{e^{-ik_3x_3}}{\sqrt{2\pi}}\sum_{n=0}^{\infty}\frac{d_{\mathbf{k}}^n\varphi_{\mathbf{k}}^n(x)}{(\sqrt{2\pi})^2}(O_{\mathbf{k}}^n+iA_{\mathbf{k}}^n), \quad (11)$$

$$\chi^*(x)=\frac{1}{\sqrt{2}}\int_{\mathbf{k}}\frac{e^{ik_3x_3}}{\sqrt{2\pi}}\sum_{n=0}^{\infty}\frac{d_{\mathbf{k}}^{*n}\varphi_{\mathbf{k}}^{*n}(x)}{(\sqrt{2\pi})^2}(O_{-\mathbf{k}}^n-iA_{-\mathbf{k}}^n),$$

where $d_{\mathbf{k}}=\exp[-i\theta_{\mathbf{k}}/2]$ where $\gamma_{\mathbf{k}}=|\gamma_{\mathbf{k}}|\exp[i\theta_{\mathbf{k}}]$ when $n=0$ (all definitions and notations can be found in Ref. 14). Within the LLL, at order a_h , the eigenstates are $A_{\mathbf{k}}, O_{\mathbf{k}}$, while the eigenvalues (in two dimensions; in three dimensions simply plus $k_3^2/2$) are

$$\epsilon_A=a_h\epsilon_A^1=a_h\left(-1+\frac{2}{\beta}\beta_{\mathbf{k}}-\frac{1}{\beta}|\gamma_{\mathbf{k}}|\right), \quad (12)$$

$$\epsilon_O=a_h\epsilon_O^1=a_h\left(-1+\frac{2}{\beta}\beta_{\mathbf{k}}+\frac{1}{\beta}|\gamma_{\mathbf{k}}|\right),$$

where ϵ_A, ϵ_O are dependent on two-dimensional vector \mathbf{k} and $\beta_{\mathbf{k}}, \gamma_{\mathbf{k}}$ is defined by the following equations:¹⁴

$$\beta_{\mathbf{k}}^n=\langle|\varphi|^2\varphi_{\mathbf{k}}^*\varphi_{\mathbf{k}}^{*n}\rangle,$$

$$\bar{\beta}_{\mathbf{k}}^n=\langle\varphi^*\varphi^n\varphi_{\mathbf{k}}^*\varphi_{\mathbf{k}}^n\rangle,$$

$$\gamma_{\mathbf{k}}^n=\langle(\varphi^*)^2\varphi_{-\mathbf{k}}\varphi_{\mathbf{k}}^n\rangle,$$

$$\overline{\gamma_k^n} = \langle \varphi^* \varphi^{*n} \varphi_{\bar{k}} \varphi_{-\bar{k}} \rangle, \quad (13)$$

where the bracket $\langle \rangle$ means averaging over the function inside the bracket. $\beta_k = \beta_k^n$, $\gamma_k = \gamma_k^n$ when $n=0$. In particular, when $k \rightarrow 0$,

$$\epsilon_A \approx \frac{x_{22}}{4\beta_A} a_h |k|^4 \approx 0.1 a_h |k|^4, \quad (14)$$

where $x_{22} \equiv (2\pi/a)^4 \sum_{l,m} l^2 m^2 (-)^{lm} \exp\{-(2\pi)^2/2a^2(l^2+m^2)\} \approx 0.47$. ϵ_O has a finite gap instead.

Higher order corrections and higher Landau level eigenstates and eigenvalues can be found in Ref. 14. With spectrum of excitations and expansion of solutions of GL equations in a_h , one can start the calculation of correlators to any order in ω .

III. STRUCTURE FUNCTION OF THE VORTEX LATTICE

In this section the structure function is calculated to order ω (harmonic approximation) within the LLL, namely, neglecting higher a_h corrections. We discuss these corrections in the next section. First we calculate the density correlator defined by

$$\tilde{S}(\mathbf{z}, z_3) = \langle \rho(\mathbf{x}, x_3) \rho(\mathbf{x} + \mathbf{z}, x_3 + z_3) \rangle_{\mathbf{x}} = \langle \rho(x) \rho(y) \rangle_{\mathbf{x}}, \quad (15)$$

where $\langle \rangle_{\mathbf{x}}$ indicates average over \mathbf{x} (which means here over the unit cell) and $\rho \equiv |\psi|^2$. The correlator is calculated using the Wick expansion:

$$\tilde{S} = \tilde{S}_{mf} + \omega \tilde{S}_{fluct}. \quad (16)$$

The first term is the mean field part, while the second term is the fluctuation part.

A. Mean field contribution

The mean field part is simply

$$\tilde{S}_{mf} = \langle |\Phi(x)|^2 |\Phi(y)|^2 \rangle_{\mathbf{x}}. \quad (17)$$

The structure function is the Fourier transform $S(\mathbf{q}, 0) = \int d\mathbf{z} e^{i\mathbf{q} \cdot \mathbf{z}} \tilde{S}(\mathbf{z}, z_3=0)$. Within the LLL, $\Phi(x) = (a_h/\beta_A)^{1/2} \varphi(x)$ and the mean field part of the structure function becomes

$$\begin{aligned} S_{mf}(\mathbf{q}, 0) &\equiv \int d\mathbf{z} e^{i\mathbf{q} \cdot \mathbf{z}} \langle |\Phi(x)|^2 |\Phi(y)|^2 \rangle_{\mathbf{x}} \\ &= \left(\frac{a_h}{\beta_A} \right)^2 \frac{b}{2\pi} \int_{cell} |\varphi(x)|^2 e^{-i\mathbf{q} \cdot \mathbf{x}} \int_{\mathbf{z}} |\varphi(z)|^2 e^{i\mathbf{q} \cdot \mathbf{z}} \\ &= \left(\frac{a_h}{\beta_A} \right)^2 4\pi^2 \delta_n(\mathbf{q}) \exp\left[-\frac{\mathbf{q}^2}{2b}\right], \end{aligned} \quad (18)$$

where we made use of formulas and function $\delta_n(\mathbf{q})$ defined in the Appendix. This is just the sum of δ functions of various heights at reciprocal lattice points.

B. Fluctuation contribution

The fluctuation part contains four terms (diagrams) $\tilde{S}_1, \dots, \tilde{S}_4$. The first term is

$$\tilde{S}_1(\mathbf{z}, z_3) = \frac{1}{4\pi \cdot 2\pi\omega} \left\langle \Phi(x) \Phi(y) \sum_{n=0}^{\infty} \int_{k,l} d_k^{n*} d_l^{n*} \varphi_{\mathbf{k}}^{*n}(x) \varphi_{\mathbf{l}}^{*n}(y) \right\rangle_{\mathbf{x}} \left(\langle O_k^{*n} O_l^{*n} - A_k^{*n} A_l^{*n} \rangle \right) e^{ik_3(y-x)z_3} + \text{c.c.} \quad (19)$$

$\langle O_k^n O_l^n \rangle$ and $\langle A_k^n A_l^n \rangle$ are propagators:

$$\langle O_k^n O_l^n \rangle = \frac{\omega}{\epsilon_O^n(\mathbf{k}) + \frac{k_3^2}{2}} \delta(\mathbf{k} + \mathbf{l}), \quad (20)$$

$$\langle A_k^n A_l^n \rangle = \frac{\omega}{\epsilon_A^n(\mathbf{k}) + \frac{k_3^2}{2}} \delta(\mathbf{k} + \mathbf{l}).$$

To calculate structure functions we will need only the $z_3=0$ correlator:

$$\tilde{S}_1(\mathbf{z}, 0) = \frac{1}{4(2\pi)^2} \left\langle \Phi(x) \Phi(y) \sum_{n=0}^{\infty} \int_{\mathbf{k}} (d_k^{n*})^2 \varphi_{\mathbf{k}}^{*n}(x) \varphi_{-\mathbf{k}}^{*n}(y) \right\rangle_{\mathbf{x}} \left[\sqrt{\frac{2}{\epsilon_O^n(\mathbf{k})}} - \sqrt{\frac{2}{\epsilon_A^n(\mathbf{k})}} \right] + \text{c.c.} \quad (21)$$

Within the LLL approximation it simplified to

$$\tilde{S}_1(\mathbf{z}, 0) = \frac{1}{4(2\pi)^2} \frac{a_h}{\beta_A} \left\langle \varphi(x) \varphi(y) \int_{\mathbf{k}} (d_k^*)^2 \varphi_{\mathbf{k}}^*(x) \varphi_{-\mathbf{k}}^*(y) \right\rangle_{\mathbf{x}} \left[\sqrt{\frac{2}{\epsilon_O(\mathbf{k})}} - \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right] + \text{c.c.} \quad (22)$$

The first fluctuation correction term to structure function can be evaluated as follows:

$$\begin{aligned}
S_1(\mathbf{q},0) &= \frac{1}{4(2\pi)^2} \frac{a_h}{\beta_A} \int_{\mathbf{k}} \frac{b}{2\pi} \int_{cell} \varphi(x) \varphi_{\mathbf{k}}^*(x) e^{-i\mathbf{q}\cdot\mathbf{x}} \int_{\mathbf{z}} \varphi(z) \varphi_{-\mathbf{k}}^*(z) e^{i\mathbf{q}\cdot\mathbf{z}} (d_{\mathbf{k}}^*)^2 \left[\sqrt{\frac{2}{\epsilon_O(\mathbf{k})}} - \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right] + \text{c.c.} \\
&= \frac{a_h}{2\beta_A} \cos\left(\frac{k_x k_y + \mathbf{k} \times \mathbf{Q}}{b} + \theta_k\right) \exp\left[-\frac{\mathbf{q}^2}{2b}\right] \left[\sqrt{\frac{2}{\epsilon_O(\mathbf{k})}} - \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right], \tag{23}
\end{aligned}$$

where formulas of the Appendix were used. \mathbf{Q} is the integer part of \mathbf{q} , \mathbf{k} is the fractional part of \mathbf{q} : $\mathbf{q} = \mathbf{k} + n_1 \tilde{\mathbf{d}}_1 + n_2 \tilde{\mathbf{d}}_2 = \mathbf{k} + \mathbf{Q}$ (see the Appendix for the definitions of $\tilde{\mathbf{d}}_1, \tilde{\mathbf{d}}_2$). The second fluctuation correction term is

$$\tilde{S}_2(\mathbf{z}, z_3) = \frac{1}{4\pi \cdot (2\pi)^2 \omega} \left\langle \Phi(x) \Phi^*(y) \sum_{n=0}^{\infty} \int_{k,l} d_{\mathbf{k}}^{n*} d_l^n \varphi_{\mathbf{k}}^{*n}(x) \varphi_l^n(y) \right\rangle_{\mathbf{x}} \left(\langle \langle O_{\mathbf{k}}^{*n} O_l^n + A_{\mathbf{k}}^{*n} A_l^{*n} \rangle \rangle e^{ik_3(y-x)_3} + \text{c.c.} \right) \tag{24}$$

$\tilde{S}_2(\mathbf{z}, z_3=0)$ is equal to (in the LLL approximation)

$$\tilde{S}_2(\mathbf{z},0) = \frac{1}{4(2\pi)^2} \frac{a_h}{\beta_A} \left\langle \varphi(x) \varphi^*(y) \int_{\mathbf{k}} \varphi_{\mathbf{k}}^*(x) \varphi_{\mathbf{k}}(y) \right\rangle_{\mathbf{x}} \left[\sqrt{\frac{2}{\epsilon_O(\mathbf{k})}} + \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right] + \text{c.c.} \tag{25}$$

and

$$\begin{aligned}
S_2(\mathbf{q},0) &= \frac{1}{4(2\pi)^2} \frac{a_h}{\beta_A} \int_{\mathbf{k}} \frac{b}{2\pi} \int_{cell} \varphi(x) \varphi_{\mathbf{k}}^*(x) e^{-i\mathbf{q}\cdot\mathbf{x}} \int_{\mathbf{z}} \varphi^*(z) \varphi_{\mathbf{k}}(z) e^{i\mathbf{q}\cdot\mathbf{z}} \left[\sqrt{\frac{2}{\epsilon_O(\mathbf{k})}} + \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right] + \text{c.c.} \\
&= \frac{a_h}{2\beta_A} \exp\left[-\frac{\mathbf{q}^2}{2b}\right] \left[\sqrt{\frac{2}{\epsilon_O(\mathbf{k})}} + \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right]. \tag{26}
\end{aligned}$$

The third term is

$$\tilde{S}_3(\mathbf{z}, z_3) = \frac{1}{4\pi \cdot (2\pi)^2 \omega} \left\langle |\Phi(x)|^2 \sum_{n=0}^{\infty} \int_{k,l} d_{\mathbf{k}}^n d_l^{n*} \varphi_{\mathbf{k}}^n(y) \varphi_l^{*n}(y) \right\rangle_{\mathbf{x}} \left(\langle \langle O_{\mathbf{k}}^{*n} O_l^{*n} + A_{\mathbf{k}}^{*n} A_l^{*n} \rangle \rangle \right) + \mathbf{x} \leftrightarrow \mathbf{y} \tag{27}$$

and within the LLL at $z_3=0$ is equal to

$$\tilde{S}_3(\mathbf{z},0) = \frac{1}{4(2\pi)^2} \left\langle |\Phi(x)|^2 \int_{\mathbf{k}} \varphi_{\mathbf{k}}(y) \varphi_{\mathbf{k}}^*(y) \right\rangle_{\mathbf{x}} \left[\sqrt{\frac{2}{\epsilon_O(\mathbf{k})}} + \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right] + (\mathbf{x} \leftrightarrow \mathbf{y}). \tag{28}$$

Consequently the correction to the structure function is

$$\begin{aligned}
S_3(\mathbf{q},0) &= \frac{a_h}{4\beta_A} \int_{\mathbf{k}} \frac{b}{2\pi} \int_{cell} |\varphi(x)|^2 e^{-i\mathbf{q}\cdot\mathbf{x}} \int_{\mathbf{z}} |\varphi_{\mathbf{k}}(z)|^2 e^{i\mathbf{q}\cdot\mathbf{z}} \times \left[\sqrt{\frac{2}{\epsilon_O(\mathbf{k})}} + \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right] \\
&\quad + (\mathbf{q} \rightarrow -\mathbf{q}) \\
&= \frac{a_h}{2\beta_A} \delta_n(\mathbf{q}) \exp\left[-\frac{\mathbf{q}^2}{2b}\right] \int_{\mathbf{k}} \cos\left(\frac{\mathbf{k} \times \mathbf{Q}}{b}\right) \left[\sqrt{\frac{2}{\epsilon_O(\mathbf{k})}} + \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right]. \tag{29}
\end{aligned}$$

The final term is from the vacuum renormalization contribution. The shift \mathbf{v} in $\psi(x) = v\phi(x) + \chi(x)$ is renormalized, that is, to one loop order, $v^2 = v_0^2 + \omega v_1^2$, where $v_0^2 = a_h/\beta_A$. One can find v_1^2 by minimizing the effective one loop free energy

$$\frac{L_x L_y L_z}{\omega} \left[-a_h v^2 + \frac{1}{2} \beta v^4 \right] + \frac{1}{2} \{ \text{Tr} \ln [2\epsilon_O(\mathbf{k}, v) + k_z^2] + \text{Tr} \ln [2\epsilon_A(\mathbf{k}, v) + k_z^2] \}, \tag{30}$$

where

$$\text{Tr} \ln [2\epsilon_O(\mathbf{k}, v) + k_z^2] + \text{Tr} \ln [2\epsilon_A(\mathbf{k}, v) + k_z^2] \tag{31}$$

$$\begin{aligned}
&= L_x L_y L_z \int \frac{dk^3}{(2\pi)^3} \{ \ln [2\epsilon_O(\mathbf{k}, v) + k_z^2] \\
&\quad + \ln [2\epsilon_A(\mathbf{k}, v) + k_z^2] \},
\end{aligned}$$

and

$$\epsilon_A(\mathbf{k}, v) = -a_h + 2v^2 \beta_k - v^2 |\gamma_k|, \tag{32}$$

$$\epsilon_O(\mathbf{k}, v) = -a_h + 2v^2 \beta_k + v^2 |\gamma_k|.$$

Minimizing the effective one loop free energy with respect to v , the straightforward calculation gives

$$v_1^2 = -\frac{1}{16\pi^2} \int_{\mathbf{k}} \left[\left(\frac{2\beta_k + |\gamma_k|}{\beta} \right) \sqrt{\frac{2}{\epsilon_O(\mathbf{k})}} + \left(\frac{2\beta_k - |\gamma_k|}{\beta} \right) \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right]. \quad (33)$$

The last contribution to the one loop correction to the correlator is therefore

$$\begin{aligned} S_4(\mathbf{z}, z_3) &= 2 \frac{a_h}{\beta_A} \langle |\varphi(x)|^2 |\varphi(y)|^2 \rangle_{\mathbf{x}} (v_1)^2, \\ S_4(\mathbf{q}, 0) &= \frac{2a_h}{\beta_A} \frac{b}{2\pi} \int_{cell} |\varphi(x)|^2 e^{-i\mathbf{q}\cdot\mathbf{x}} \int_{\mathbf{z}} |\varphi(z)|^2 e^{i\mathbf{q}\cdot\mathbf{z}} v_1^2 \\ &= -\frac{a_h}{2\beta_A} \delta_n(\mathbf{q}) \exp\left[-\frac{\mathbf{q}^2}{2b}\right] \int_{\mathbf{k}} \left[\left(\frac{2\beta_k + |\gamma_k|}{\beta} \right) \right. \\ &\quad \left. \times \sqrt{\frac{2}{\epsilon_O(k)}} + \left(\frac{2\beta_k - |\gamma_k|}{\beta} \right) \sqrt{\frac{2}{\epsilon_A(k)}} \right]. \quad (34) \end{aligned}$$

The sum of all the four terms can be cast in the following form:

$$\begin{aligned} S(\mathbf{q}, 0) &= \left(\frac{a_h}{\beta_A} \right)^2 4\pi^2 \delta_n(\mathbf{q}) \exp\left[-\frac{\mathbf{q}^2}{2b}\right] + \frac{\omega}{2} \frac{a_h^{1/2}}{\beta_A} \exp\left[-\frac{\mathbf{q}^2}{2b}\right] \\ &\quad \times [f_1(\mathbf{q}) + \delta_n(\mathbf{q})f_2(\mathbf{Q}) + \delta_n(\mathbf{q})f_3], \\ f_1(\mathbf{q}) &= \left[1 + \cos\left(\frac{k_x k_y + \mathbf{k} \times \mathbf{Q}}{b} + \theta_k\right) \right] \sqrt{\frac{2}{\epsilon_O^1(\mathbf{k})}} \\ &\quad + \left[1 - \cos\left(\frac{k_x k_y + \mathbf{k} \times \mathbf{Q}}{b} + \theta_k\right) \right] \sqrt{\frac{2}{\epsilon_A^1(\mathbf{k})}}, \quad (35) \\ f_2(\mathbf{Q}) &= \int_{\mathbf{k}} \left[-1 + \cos\left(\frac{\mathbf{k} \times \mathbf{Q}}{b}\right) \right] \left[\sqrt{\frac{2}{\epsilon_O^1(\mathbf{k})}} + \sqrt{\frac{2}{\epsilon_A^1(\mathbf{k})}} \right], \\ f_3 &= -\int_{\mathbf{k}} \left[\sqrt{2\epsilon_O^1(\mathbf{k})} + \sqrt{2\epsilon_A^1(\mathbf{k})} \right] = -28.5275b. \end{aligned}$$

C. Cancellation of the infrared divergency

Although all of the four terms S_1 , S_2 , S_3 , and S_4 are divergent as any of the peaks is approached, $\mathbf{k} \rightarrow \mathbf{0}$, the sums S_1, S_2 and S_3, S_4 are not. We start with the first two:

$$S_1(\mathbf{q}, 0) + S_2(\mathbf{q}, 0) = \frac{\omega}{2} \frac{a_h}{\beta_A} \exp\left[-\frac{\mathbf{q}^2}{2b}\right] f_1(\mathbf{q}), \quad (36)$$

where $f_1(\mathbf{q})$ defined in Eq. (35) contains a function $(1/b)(k_x k_y + \mathbf{k} \times \mathbf{Q}) + \theta_k$. When $\mathbf{k} \rightarrow \mathbf{0}$ it can be shown that $k_x k_y / b + \theta_k = O(\mathbf{k}^2)$; thus $(1/b)(k_x k_y + \mathbf{k} \times \mathbf{Q}) + \theta_k \rightarrow \mathbf{k} \times \mathbf{Q}$, and $1 - \cos(k_x k_y + \mathbf{k} \times \mathbf{Q}) / b + \theta_k \rightarrow (\mathbf{k} \times \mathbf{Q})^2$. Hence it will cancel the $1/k^2$ singularity coming from $\sqrt{1/\epsilon_A^1(k)}$. Thus $f_1(\mathbf{q})$ approaches $\text{const} + \text{const} \cdot (\mathbf{k} \times \mathbf{Q})^2 / k^2$ when $\mathbf{Q} \neq \mathbf{0}$, and approaches $\text{const} + \text{const} \cdot k^6$ when $\mathbf{Q} = \mathbf{0}$.

Similarly the sum of $S_4(\mathbf{q}, 0)$ and $S_3(\mathbf{q}, 0)$ is not divergent, although separately they are. Their sum is

$$S_3(\mathbf{q}, 0) + S_4(\mathbf{q}, 0) = \frac{\omega}{2} \frac{a_h^{1/2}}{\beta_A} \delta_n(\mathbf{q}) \exp\left[-\frac{\mathbf{q}^2}{2b}\right] [f_2(\mathbf{Q}) + f_3]. \quad (37)$$

IV. COMPARISON WITH MC SIMULATIONS

A. Shape of the peaks in the structure function

Now we compare our results with numerical simulation of the LLL system in Ref. 11. The general shape of the structure function in the vicinity of a peak [see Fig. 1(b)] and the data near the origin according to a MC simulation of the same system within the same LLL approximation in Ref. 11 [Fig. 1(a)] are qualitatively the same pattern. It is easier to compare using rescaled quasimomenta, $\mathbf{q} \rightarrow \mathbf{q}\sqrt{b}$, $\mathbf{k} \rightarrow \mathbf{k}\sqrt{b}$. We get

$$\begin{aligned} S(\mathbf{q}, 0) &= \left(\frac{a_h}{\beta_A} \right)^2 4\pi^2 \frac{\delta_n(\mathbf{q})}{b} \exp\left[-\frac{\mathbf{q}^2}{2}\right] + \frac{\omega}{2} \frac{a_h^{1/2}}{\beta_A} \exp\left[-\frac{\mathbf{q}^2}{2}\right] \\ &\quad \times [f_1(\mathbf{q}) + \delta_n(\mathbf{q})f_2(\mathbf{Q}) + \delta_n(\mathbf{q})f_3], \quad (38) \end{aligned}$$

where $f_1(\mathbf{q})$, $f_2(\mathbf{Q})$, and f_3 are defined in Eq. (35), but with $b=1$ (for example, $f_3 = -28.5275$) and the region of integration in the formula rescaled to the cell with $\tilde{\mathbf{d}}_1, \tilde{\mathbf{d}}_2$ being the reciprocal lattice basis vectors

$$\tilde{\mathbf{d}}_1 = \frac{2\pi}{a} \left(1, -\frac{1}{\sqrt{3}} \right); \quad \tilde{\mathbf{d}}_2 = \left(0, \frac{4\pi}{a\sqrt{3}} \right).$$

Furthermore we define $s(\mathbf{q})$ which is used also in Ref. 11:

$$\begin{aligned} S(\mathbf{q}, 0) &= \left(\frac{a_h}{\beta_A} \right)^2 \frac{4\pi^2}{b} \exp\left[-\frac{\mathbf{q}^2}{2}\right] s(\mathbf{q}), \quad (39) \\ s(\mathbf{q}) &\equiv \delta_n(\mathbf{q}) + \frac{\beta_A b \omega (a_h)^{-3/2}}{8\pi^2} \\ &\quad \times [f_1(\mathbf{q}) + \delta_n(\mathbf{q})f_2(\mathbf{Q}) + \delta_n(\mathbf{q})f_3]. \end{aligned}$$

For reciprocal lattice vectors close to origin the values of $f_2(\mathbf{Q})$ are found in Table I.

In Ref. 11, the material parameters describe YBCO: $T_c = 93$ K, $dH_{c2}(T)/dT = -1.8 \times 10^4$ Oe/K, $\gamma = 5$, and $\kappa = 52$. At $T = 82.8$ K, $H = 50$ kOe. This leads to the following dimensionless parameters $\text{Gi} = 2.04 \times 10^{-5}$, $\omega = 0.056$, $a_h = 0.039904$. However, as discussed in Ref. 14 effective expansion parameters are $a_h/6b = 0.22268$ and $b\omega(a_h)^{-3/2}/2\sqrt{2}\pi = 2.36 \times 10^{-2}$, both less than 1. $a_h/6b$ is the parameter for the expansion of the classical solution. The factor 6 comes from the fact that due to hexagonal, only 6th, 12th, etc. Landau levels appear in perturbation expansion. $b\omega(a_h)^{-3/2}/2\sqrt{2}\pi$ is the parameter for the fluctuation (loop) expansion and is much less than 1 here. It justifies the quantum correction of the formula using perturbation expansion. The numerical factor in front of the fluctuation correction in this case is

$$c_1 = \frac{\beta_A b \omega (a_h)^{-3/2}}{8\pi^2} = 3.0932 \times 10^{-3}. \quad (40)$$

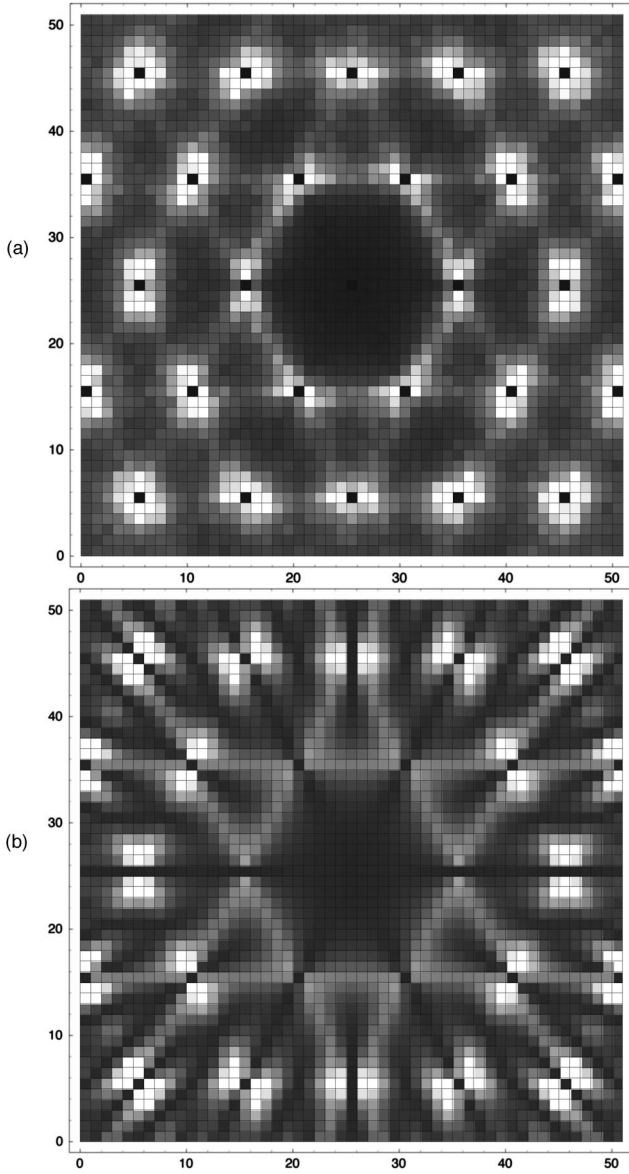


FIG. 1. (a) Structure factor from the MC simulation of Ref. 11. The peaks at reciprocal lattice points are removed. (b) Fluctuation correction to structure factor of the Abrikosov vortex lattice, Eq. (41). The peaks at reciprocal lattice points are removed.

In a finite size sample, $\delta_n(\mathbf{q})$ is equal to $L_x L_y / (2\pi)^2$ when \mathbf{q} lies on the reciprocal lattice $m_1 \tilde{\mathbf{d}}_1 + m_2 \tilde{\mathbf{d}}_2$; otherwise it is zero. Because $L_x L_y = N_\phi 2\pi$ (N_ϕ is the number of vortices of order 100 only in the MC simulation), it is equal to $N_\phi / 2\pi$. The normalized structure function $s_n(\mathbf{0}) = 1$, as it was used in Ref. 11) is

$$s_n(\mathbf{q}) = \Delta(\mathbf{q}) + \frac{1}{(1 + c_1 f_3)} [c_2 f_1(\mathbf{q}) + c_1 \Delta(\mathbf{q}) f_2(\mathbf{Q})] \quad (41)$$

TABLE I. Values of $f_2(\mathbf{Q})$ with small n_1, n_2 .

n_1, n_2	0,1	1,0	1,1	1,2	0,2	2,2	1,3
$f_2(\mathbf{Q})$	-7.35	-7.35	-7.35	-10.05	-10.242	-10.242	-11.75

and

$$c_2 = c_1 \frac{2\pi}{N_\phi} = 1.9435 \times 10^{-4},$$

$$1 + c_1 f_3 = 0.91315. \quad (42)$$

The correction to the height of the peak at \mathbf{Q} , $c_1 \Delta(\mathbf{q}) / [1 + c_1 f_3] f_2(\mathbf{Q})$, is quite small. We find the height of the peaks away from the origin found in the MC simulation¹¹ are typically smaller than ours, while around the peaks they are larger than analytical. It may be due to the finite size effect or finite samplings of the MC calculation. In the MC calculation part of the peak might “belong” to a neighboring pixel. We plot the correction to the nonpeak region in Fig. 1(b) and find that the theoretical prediction has roughly the same characteristic saddle shape “halos” around the peaks as in Ref. 11, Fig. 1(a), in which all the peaks were removed (so it is different from Fig. 2(a) in Ref. 11 in which only the central peak was removed).

We can extend our formula to higher orders which will include also the HLLs (higher Landau levels). To next order of a_h , we should include Φ_1 in Φ , $\Phi = (a_h)^{1/2} [\Phi_0 + a_h \Phi_1]$, consider $\epsilon_O(k), \epsilon_A(k)$ to next order a_h^2 , and $\epsilon_O^n(k), \epsilon_A^n(k)$ to order a_h . It is straightforward to do it.

B. Nonperturbative evidence of $\epsilon_A^1(\mathbf{k}) \rightarrow |k|^4$ for asymptotic small k_x, k_y

Conversely, the MC simulation result provides the non-perturbative evidence $\epsilon_A^1(\mathbf{k}) \rightarrow |k|^4$ for asymptotic small k_x, k_y . In Eq. (36), if $\epsilon_A^1(\mathbf{k}) \rightarrow |k|^2$, we will get a contribution from the most singular term $\text{const} + \text{const} \cdot (\mathbf{k} \times \mathbf{Q})^2 / k$. This term will become constant when $k \rightarrow 0$, and we will not get the same characteristic saddle shape “halos” around the peaks as in Ref. 11. So $\epsilon_A^1(\mathbf{k}) \rightarrow |k|^4$ for $k \rightarrow 0$ is crucial for such characteristic shape. Thus the MC simulation result provides a nonperturbative evidence that $\epsilon_A^1(\mathbf{k}) \rightarrow |k|^4$ for $k \rightarrow 0$.

V. FLUCTUATION OF MAGNETIC FIELD

Another quantity which can be measured is the magnetic field distribution. In addition to the constant magnetic field background there are $1/\kappa$ magnetization corrections due to field produced by supercurrent. To leading order in a_h it is given by $m(x) \propto \langle \rho(x) \rangle / \kappa$ (for example, see Ref. 15). $\langle \rho(x) \rangle$ can be calculated using the following equation:

$$\begin{aligned} \langle \rho(x) \rangle &= \langle |\Phi(x) + \chi(x)|^2 \rangle = \langle |\Phi(x)|^2 \rangle + \langle \Phi^*(x) \chi(x) \rangle \\ &\quad + \langle \Phi(x) \chi^*(x) \rangle + \langle \chi(x) \chi^*(x) \rangle \\ &= \frac{a_h}{\beta_A} |\phi(x)|^2 + \langle \chi(x) \chi^*(x) \rangle. \end{aligned} \quad (43)$$

Using Eq. (20) and Eq. (11), and considering only $x_3=0$, one obtains

$$\begin{aligned}\langle \chi(x)\chi^*(x) \rangle &= \frac{\omega}{16\pi^3} \int_k |\varphi_{\mathbf{k}}(x)|^2 \left[\frac{1}{\epsilon_o(\mathbf{k}) + \frac{k_3^2}{2}} + \frac{1}{\epsilon_A(\mathbf{k}) + \frac{k_3^2}{2}} \right] \\ &= \frac{\omega}{16\pi^2} \int_k |\varphi_{\mathbf{k}}(x)|^2 \left[\sqrt{\frac{2}{\epsilon_o(\mathbf{k})}} + \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right].\end{aligned}$$

However, as pointed out in Sec. III the coefficient ν in $\psi(x) = \nu\phi(x) + \chi(x)$ is renormalized to one loop order, $\nu^2 = \nu_o^2 + \omega\nu_1^2$, with ν_1 given in Eq. (33). Thus we need to add a term, $\omega\nu_1^2[\phi(x)]^2$, to Eq. (43).

$$\begin{aligned}\langle \rho(\mathbf{x}, \mathbf{0}) \rangle &= \frac{a_h}{\beta_A} |\phi(x)|^2 + \frac{\omega}{16\pi^2} \int_k |\varphi_{\mathbf{k}}(x)|^2 \\ &\quad \times \left[\sqrt{\frac{2}{\epsilon_o(\mathbf{k})}} + \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right] \\ &\quad - \frac{\omega |\phi(x)|^2}{16\pi^2} \int_k \left[\left(\frac{2\beta_k + |\gamma_k|}{\beta} \right) \sqrt{\frac{2}{\epsilon_o(\mathbf{k})}} \right. \\ &\quad \left. + \left(\frac{2\beta_k - |\gamma_k|}{\beta} \right) \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right].\end{aligned}\quad (44)$$

Its Fourier transform $\rho(\mathbf{q}) \equiv \int d\mathbf{z} e^{i\mathbf{q}\cdot\mathbf{z}} \langle \rho(\mathbf{z}, \mathbf{0}) \rangle$ can be easily calculated:

$$\begin{aligned}\rho(\mathbf{q}) &= 4\pi^2 \delta_n(\mathbf{q}) \exp \left[-\frac{\mathbf{q}^2}{4b} + \frac{iq_x q_y}{2b} + \frac{\pi i}{2} (n_1^2 - n_1) \right] \\ &\quad \times \left\{ \frac{a_h}{\beta_A} + \frac{\omega}{16\pi^2} \int_k \left[\exp \left(\frac{i\mathbf{k} \times \mathbf{q}}{b} \right) - \left(\frac{2\beta_k + |\gamma_k|}{\beta} \right) \right] \right. \\ &\quad \times \left. \sqrt{\frac{2}{\epsilon_o(\mathbf{k})}} + \left(\exp \left(\frac{i\mathbf{k} \times \mathbf{q}}{b} \right) - \left(\frac{2\beta_k - |\gamma_k|}{\beta} \right) \right) \sqrt{\frac{2}{\epsilon_A(\mathbf{k})}} \right\}.\end{aligned}\quad (45)$$

Performing integrals and rescaling the quasimomenta again, one obtains

$$\begin{aligned}\rho(\mathbf{q}) &= 4\pi^2 \frac{\delta_n(\mathbf{q})}{b} \exp \left[-\frac{\mathbf{q}^2}{4} + \frac{iq_x q_y}{2} + \frac{\pi i}{2} (n_1^2 - n_1) \right] \\ &\quad \times \left\{ \frac{a_h}{\beta_A} + \frac{\omega b a_h^{-1/2}}{16\pi^2} [-28.5275 + f_2(\mathbf{Q})] \right\}.\end{aligned}\quad (46)$$

The function $f_2(\mathbf{Q})$ appeared in Eq. (36).

VI. DISORDER EFFECT ON MAGNETIZATION AND SPECIFIC HEAT

One can introduce weak disorder by adding a quadratic term in Eq. (2),⁶

$$\Delta f \equiv \int d^3x \alpha(x) |\psi|^2. \quad (47)$$

Loosely speaking it represents a local variation of temperature. For pointlike defects one can assume that the correlation of $\alpha(x)$ is $\langle \langle \alpha(x)\alpha(y) \rangle \rangle = W\delta(\mathbf{x}-\mathbf{y})$, $\langle \langle \alpha(x) \rangle \rangle = 0$. Before the disorder average we calculate the free energy $-T \ln Z$ with

$$Z = \int \mathcal{D}\psi^* \mathcal{D}\psi \exp \left\{ -\frac{1}{\omega} \left[f[\psi^*, \psi] - \int d^3x \alpha(x) |\psi|^2 \right] \right\}. \quad (48)$$

If W is very small, we can calculate Z by perturbation theory in W . To the second order Z is given as

$$\begin{aligned}Z &= Z_0 \left[1 - \frac{1}{\omega} \int_x \alpha(x) \langle \rho(x) \rangle \right. \\ &\quad \left. + \frac{1}{2\omega^2} \int_x \int_y \langle \rho(x)\rho(y) \rangle \alpha(x)\alpha(y) \right],\end{aligned}\quad (49)$$

where Z_0 is the free energy without disorder and it had been obtained in Ref. 14. Thus the free energy with disorder is

$$\begin{aligned}F &= -T \ln Z = F_0 + \Delta F \\ &= F_0 + T \int_x \frac{\alpha(x)}{\omega} \langle \rho(x) \rangle - \frac{T}{2\omega^2} \int_x \int_y [\langle \rho(x)\rho(y) \rangle \\ &\quad - \langle \rho(x) \rangle \langle \rho(y) \rangle] \alpha(x)\alpha(y),\end{aligned}\quad (50)$$

where $F_0 = -T \ln Z_0$. Averaging free energy over disorder one obtains

$$\begin{aligned}F &= F_0 - \frac{TW}{2\omega^2} \int_x [\langle \rho(x)\rho(x) \rangle - \langle \rho(x) \rangle \langle \rho(x) \rangle] \\ &= F_0 - \frac{TWV}{2\omega^2} \omega \tilde{\mathcal{S}}_{fluct}(0).\end{aligned}\quad (51)$$

From Eq. (35), one finds that $\tilde{\mathcal{S}}_{fluct}(0) = -0.18619(a_h^{1/2}b/\beta_A)$. Hence the energy density difference due to disorder is $\mathcal{F} = \Delta F/V = -0.0931(TW a_h^{1/2}b/\omega\beta_A)$. Since $\omega = \sqrt{2Gi}\pi^2 t$, $\mathcal{F} = c a_h^{1/2} b$ with $c = -0.0931T_c W/\sqrt{2Gi}\pi^2 \beta_A$. The disorder effect on magnetization and specific heat are

$$\begin{aligned}\Delta m &= -\frac{\partial \Delta f}{\partial b} = -c \left(a_h^{1/2} - \frac{b}{4} a_h^{-1/2} \right), \\ \Delta c &= -t \frac{\partial^2}{\partial t^2} \Delta f = \frac{c}{16} t b a_h^{-3/2},\end{aligned}\quad (52)$$

respectively.

VII. CONCLUSIONS

To conclude, we have calculated the effect of fluctuations on the structure function of the vortex lattice and compared it to existing MC results. In addition to renormalization of the height of the Bragg peaks, there appear characteristic saddle

shape ‘‘halos’’ around the peaks as found in Ref. 11. The MC simulation result provides the nonperturbative evidence $\epsilon_A^1(\mathbf{k}) \rightarrow |k|^4$ for asymptotic small k . The calculated fluctuation contribution to the magnetic field can be more easily observed in low temperature strongly type-II superconductors. Finally, the predicted dependence of magnetization and specific heat on disorder via fluctuations also can be experimentally studied.

Correlations in flux lattices can be experimentally measured using neutron scattering as well as some other more exotic methods such as muon spin relaxation, electron tomography, scanning SQUID microscopy, etc.^{1-3,16,17} It would be interesting to detect the effect of fluctuations given in the present paper directly from experiments by subtracting the ‘‘background’’ of the well-known mean field correlator. The calculations show that infrared divergencies naively expected in all of the physical quantities calculated above due to ‘‘supersoft’’ shear modes in the large κ limit cancel. This strengthens the view that the loop expansion is a reliable theoretical tool to study the fluctuations effects in vortex lattice below the melting point.

ACKNOWLEDGMENTS

We are grateful to our colleagues A. Knigavko, B. Bako, and V. Yang. One of us (B.R.) is especially grateful to R. Sasik and D. Stroud for providing raw numerical data which was essential for the present comparison with the MC data. The work is part of the NCTS topical program on vortices in high T_c and was supported by NSC of Taiwan.

APPENDIX A

In this appendix, we present some basic formulas used in the calculations. The basic matrix element is

$$\begin{aligned} & \frac{b}{2\pi} \int_{cell} dx \varphi(\mathbf{x}) \varphi_{\mathbf{k}}^*(\mathbf{x}) \exp[-i\mathbf{x} \cdot \mathbf{q}] \\ & = \Delta_{\mathbf{q},\mathbf{k}} \exp \left[\frac{\pi i}{2} (n_1^2 - n_1) - \frac{\mathbf{q}^2}{4b} - \frac{i q_x q_y}{2b} + \frac{i k_x q_y}{b} \right]. \end{aligned} \quad (\text{A1})$$

The Kronecker delta is defined by

$$\Delta_{\mathbf{q},\mathbf{k}} = \Delta(\mathbf{q} - \mathbf{k}) = \begin{cases} 1, & \text{if } \mathbf{q} = \mathbf{k} + n_1 \tilde{\mathbf{d}}_1 + n_2 \tilde{\mathbf{d}}_2 \\ 0, & \text{otherwise,} \end{cases} \quad (\text{A2})$$

where integers $n_1 = (1/2\pi) \mathbf{d}_1 \cdot (\mathbf{q} - \mathbf{k})$ and

$$n_2 = (1/2\pi) \mathbf{d}_2 \cdot (\mathbf{q} - \mathbf{k}).$$

Here $\tilde{\mathbf{d}}_1, \tilde{\mathbf{d}}_2$ are the reciprocal lattice basis vectors

$$\tilde{\mathbf{d}}_1 = \frac{2\pi\sqrt{b}}{a} \left(1, -\frac{1}{\sqrt{3}} \right); \quad \tilde{\mathbf{d}}_2 = \left(0, \frac{4\pi\sqrt{b}}{a\sqrt{3}} \right), \quad (\text{A3})$$

which are dual to $\mathbf{d}_1 = (a/\sqrt{b}, 0)$, $\mathbf{d}_2 = (a/2\sqrt{b}, a\sqrt{3}/2\sqrt{b})$, and $a = \sqrt{4\pi/\sqrt{3}}$. Integrating over the sample area A , one obtains

$$\begin{aligned} & \int_A dx \varphi(\mathbf{x}) \varphi_{\mathbf{k}}^*(\mathbf{x}) \exp[-i\mathbf{x} \cdot \mathbf{q}] \\ & = 4\pi^2 \delta_n(\mathbf{q} - \mathbf{k}) \exp \left[\frac{\pi i}{2} (n_1^2 - n_1) \right] \\ & \quad \times \exp \left[-\frac{\mathbf{q}^2}{4b} - \frac{i q_x q_y}{2b} + \frac{i k_x q_y}{b} \right], \end{aligned} \quad (\text{A4})$$

where $\delta_n(\mathbf{q} - \mathbf{k})$ is defined as $\delta_n(\mathbf{q} - \mathbf{k}) = \sum_{m_1, m_2} \delta(\mathbf{q} - \mathbf{k} - m_1 \tilde{\mathbf{d}}_1 - m_2 \tilde{\mathbf{d}}_2)$.

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