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Variational theory of flux line liquids

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We formulate a variational (Hartree like) description of flux line liquids which improves on the theory developed in an earlier paper [A.M. Ettouhami, Phys. Rev. B **65**, 134504 (2002)]. We show, in particular, that the massive term confining the fluctuations of flux lines is strongly reduced by thermal fluctuations. This results in an anomalous temperature dependence of the mean square projected area of a single flux line $\langle u^2\rangle \sim T^{3/2}$ which is a signature of the weakly entangled state introduced previously, and which should be measurable in numerical simulations.

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I. INTRODUCTION

The study of the properties of flux line solids and liquids in high-temperature superconductors (HTSC's) has been, during the past few years, one of the most active areas of research in the field of superconductivity. One theoretical approach that has had a rather strong impact on our present understanding of flux liquids in HTSC's is the boson mapping,[1–5] which is based on the observation[6] that there is a formal mapping between the partition function of a three-dimensional system of interacting flux lines, and the imaginary-time partition function of quantum bosons in two-dimensions). One of the main results of this approach, which has in fact been reproduced using other methods,[7] is that the structure factor

$$S(\mathbf{r},z)=\langle \hat\rho(\mathbf{r},z)\hat\rho(\mathbf{0},0)\rangle \tag{1.1}$$

of a liquid of flux lines described by the trajectories $\mathbf{R}_i(z)=[\mathbf{r}_i(z),z]$ as they traverse the superconducting sample (here $\hat\rho(\mathbf{r},z)=\Sigma_{i=1}^{N}\delta[\mathbf{r}-\mathbf{r}_i(z)]$ is the density operator in the $\mathbf{r}=(x,y)$ plane at height z, N being the total number of vortices in the sample), is such that the partial Fourier transform $S(\mathbf{q},z)=\langle \hat\rho(\mathbf{q},z)\hat\rho(-\mathbf{q},0)\rangle$ is given by

$$S(\mathbf{q},z)=S(\mathbf{q},z=0)e^{-\varepsilon(q)|z|/T}, \tag{1.2}$$

where $\varepsilon(q)$ is the excitation spectrum of the equivalent boson superfluid (whose precise form will be given below), and T is temperature (throughout this paper, we use units such that Boltzmann's constant $k_B=1$). Although the boson mapping (and other similar approaches[7] which use the density as the basic dynamical variable[8]) does not make any explicit predictions for the correlations of conformational variables of flux lines, the exponential decay (1.2) of density correlations along the direction of the lines is generally *interpreted* as an indication that the flux line liquid is in a heavily entangled or "superfluid" state characterized by correlations of the form

$$\langle |\mathbf{r}(z)-\mathbf{r}(0)|^2\rangle = 2D|z|, \tag{1.3}$$

with a "diffusion" constant D of order (here κ is the tilt modulus of the flux lines)

$$D\approx \frac{T}{\kappa} \tag{1.4}$$

and by a mean projected area of the flux lines

$$\langle u^2\rangle \approx DL, \quad \mathbf{u}(z)=\mathbf{r}(z)-\langle \mathbf{r}(z)\rangle \tag{1.5}$$

which *diverges* with the superconducting sample thickness L.

Since its inception by Nelson and Seung,[2] the boson mapping has had a widespread acceptance and a rather strong impact on our understanding of flux line liquids. It has been applied, in particular, to disorder-free vortex liquids,[5] as well as to vortex liquids in presence of point[3] and correlated[9] disorder. In all these studies, the boson mapping gave seemingly reasonable results, except at one occurrence where it was noticed by Täuber and Nelson[4] that the boson mapping gives nonsensical results in the presence of splayed columnar disorder.[10]

In a recent paper,[11] henceforth referred to as paper I, I proposed an approach to study three-dimensional flux line liquids in type-II superconductors. This approach, which makes contact with the standard theory of classical fluids, is based on the separation of the flux lines' conformal variables into center of mass (c.m.) and internal modes, and on the observation that the interactions between flux lines may lead, under certain conditions, to the confinement of the internal modes whose fluctuations are now bounded and no-longer diverge with the sample thickness L as in Eq. (1.5). While, as mentioned above, the Boson mapping does not deal with the conformation variables of flux lines themselves, the theory developed in paper I predicted that the effective Hamiltonian of the *internal modes* of interacting flux lines in a vortex liquid has the form (i here labels flux lines, and N is the total number of vortices in the sample)

$$H_{\rm eff}[\mathbf{u}_i]=\sum_{i=1}^{N}\int_0^L dz\left[\frac{1}{2}\kappa\left(\frac{d\mathbf{u}_i}{dz}\right)^2+\frac{1}{2}\mu_0 u_i^2(z)\right], \tag{1.6}$$

where the mass μ_0 is given by

$$\mu_0=\frac{\rho}{2}\int d^2\mathbf{r}\nabla^2 V(\mathbf{r})g_0(\mathbf{r}). \tag{1.7}$$

In the above equation, V is the interaction potential between vortices [see below, Eq. (2.1)] and g_0 is the pair distribution function of the two-dimensional liquid formed by the centers of mass of the flux lines. Because in paper I we only used a simple Taylor expansion of the total Hamiltonian of flux lines in terms of the $\mathbf{u}_i$'s, the "mass" term μ_0 of Eq. (1.7) above does not capture the effect of thermal fluctuations, and varies with temperature only through the (weak) variation of g_0. In particular, Eq. (1.7) shows that the value of the "mass" term μ_0 remains almost unchanged as temperature $T \to \infty$, which, of course, is unrealistic, since we expect the vortex liquid to behave as an ideal gas of freely fluctuating flux lines in this limit.

In the present paper, we generalize the method proposed in paper I, and construct a variational theory of interacting flux lines in the vortex liquid state. This variational method, which in fact turns out to be nothing but a self-consistent Hartree approximation, captures the effect of thermal fluctuations and leads to a "renormalized" mass term $\mu(T)$ which vanishes at high enough temperatures, as suggested by physical intuition.

Our method of approach will be as follows. In Sec. II we construct our variational approach and derive the expression of the renormalized $\mu(T)$. In Sec. III, we compare the method developed in paper I and in the present paper with the approaches of Refs. 1–5,7, and discuss in particular the interacting structure factor $S(\mathbf{r},z)$ derived using both methods. Section IV contains our conclusions.

II. VARIATIONAL THEORY OF FLUX LINE LIQUIDS

We thus consider a liquid of interacting flux lines in a $d=(d_\perp+1)$-dimensional superconducting sample of thickness L. We here will use the following Hamiltonian:[2,9]

$$H=\sum_{i=1}^{N}\int_0^L dz\left\{\frac{1}{2}\kappa\left(\frac{d\mathbf{r}_i}{dz}\right)^2+\frac{1}{2}\sum_{j(\neq i)}V[\mathbf{r}_i(z)-\mathbf{r}_j(z)]\right\}, \tag{2.1}$$

where κ is the tilt modulus per unit length of the flux lines and $V(\mathbf{r})$ is the interaction potential between flux line elements at equal height z. For a uniaxial HTSC, with both the average vortex direction and the unit vector $\hat{\mathbf{z}}$ aligned with the $\hat{\mathbf{c}}$ axis, $\kappa\simeq\varepsilon^2\varepsilon_0$ and $V(r)=2\varepsilon_0 K_0(r/\lambda_{ab})$, where the energy scale ε_0 is given by $\varepsilon_0=(\phi_0/4\pi\lambda_{ab})^2$, $\varepsilon=\lambda_{ab}/\lambda_c$ is the ratio of the London penetration depths in the (ab) planes and in the direction of the $\hat{\mathbf{c}}$ axis, respectively; $\phi_0=hc/2e$ is the flux quantum, and K_0 is a modified Bessel function.[12] In the developments that will follow, we will find it useful to work in Fourier space, and to write down the following decomposition of the flux line trajectories $\mathbf{r}_i(z,t)$ into Rouse[13] modes

$$\mathbf{r}_i(z)=\sum_{n=-\infty}^{\infty}\mathbf{r}_i(q_n)e^{iq_nz}, \tag{2.2}$$

where $q_n=2\pi n/L$, and where the Fourier coefficients $\mathbf{r}_i(q_n)$ are given by

$$\mathbf{r}_i(q_n)=\frac{1}{L}\int_0^L dz\,\mathbf{r}_i(z)e^{-iq_nz}. \tag{2.3}$$

It will also be convenient to write $\mathbf{r}_i(z)$ as the sum

$$\mathbf{r}_i(z)=\mathbf{r}_{0i}(t)+\mathbf{u}_i(z,t), \tag{2.4}$$

where $\mathbf{r}_{0i}(t)=\mathbf{r}_i(q_n=0,t)$ is the c.m. position and $\mathbf{u}_i(z)$ the flux line displacement with respect to the center of mass position at height z.

The statistical mechanics of the flux line system, Eq. (2.1), is described by the partition function

$$\mathcal{Z}=\int\prod_{i=1}^{N}[d\mathbf{r}_i(z)]e^{-\beta H} \tag{2.5}$$

$$=\int\prod_{i=1}^{N}d\mathbf{r}_{0i}\int\prod_{i=1}^{N}[d\mathbf{u}_i(z)]e^{-\beta H}, \tag{2.6}$$

where $\beta=1/T$ is the inverse temperature, and where in going from the first to the second line we separated the path integral over every flux line trajectory into a path integral over all internal modes and an ordinary integral over the c.m. coordinates. The integration measure $[d\mathbf{u}_i(z)]$ is given by

$$[d\mathbf{u}_i(z)]=\prod_{n=1}^{\infty}d\mathbf{u}_{re}(q_n)d\mathbf{u}_{im}(q_n) \tag{2.7}$$

with $\mathbf{u}_{re}(q_n)$ and $\mathbf{u}_{im}(q_n)$ the real and imaginary parts of $\mathbf{u}(q_n)$, respectively. Now, if we were able to perform the functional integrations over the internal modes, such an integration would give us an expression of the form

$$\mathcal{Z}=\int\prod_{i=1}^{N}d\mathbf{r}_{0i}e^{-\beta H_{\text{eff}}[\{\mathbf{r}_{0i}\}]}, \tag{2.8}$$

with an effective Hamiltonian H_{eff} which depends only on the c.m. coordinates $\{\mathbf{r}_{0i}\}$. The above expression of $\mathcal{Z}$ looks similar to the partition function of a system of N ordinary classical particles with spatial coordinates $\{\mathbf{r}_{0i}\}$, interacting through the Hamiltonian $H_{\text{eff}}[\{\mathbf{r}_{0i}\}]$, whose thermodynamics can be studied by standard methods of statistical mechanics. Unfortunately, since the internal modes $\{\mathbf{u}_i(z)\}$ appear explicitly in the argument of the interaction potential V in Eq. (2.1), it is not possible, in general, to perform the functional integrations over these variables in closed form. In paper I, we used a simple Taylor expansion of the interaction potential $V[\mathbf{r}_i(z)-\mathbf{r}_j(z)]=V[\mathbf{r}_{0i}-\mathbf{r}_{0j}+\mathbf{u}_i(z)-\mathbf{u}_j(z)]$ in terms of the $\mathbf{u}_i$'s to be able to perform the integrations in Eq. (2.6) and make predictions for physical observables of our flux liquid. Here, and in order to better capture the effect of thermal fluctuations, we want to improve on the above Taylor expansion and use a variational approach to derive the statistical mechanics of our model system.

In general, variational approaches to classical statistics are based on the Jensen-Peirels inequality[14]

$$\mathcal{Z}\geqslant Z_v=Z_1e^{-\beta\langle H-H_1\rangle_1}, \tag{2.9}$$

where H_1 is *any* Hamiltonian and the average $\langle\cdots\rangle_1$ is performed with the statistical weight $\exp(-\beta H_1)/Z_1$, with $Z_1=Tr(e^{-\beta H_1})$. While an arbitrary choice of H_1 will not necessarily lead to good results, a judicious choice of the variational Hamiltonian H_1 (that is simple enough so that thermal averages can be calculated and at the same time general enough to capture the physics of the full Hamiltonian) will lead to a variational free energy

$$F_v = -T \ln Z_v = -T \ln Z_1 + \langle H - H_1 \rangle_1 \qquad (2.10)$$

which is a very good approximation of the true free energy of the system, and to an accurate description of the overall behavior of the original model.

We now have to choose a variational Hamiltonian to approximate the Hamiltonian H of Eq. (2.1). In what follows, we shall assume that we can write for our variational Hamiltonian H_1 a decomposition of the form

$$H_1[\{\mathbf{r}_{0i}\},\{\mathbf{u}_i(z)\}] = H_0[\{\mathbf{r}_{0i}\}] + H_u[\{\mathbf{u}_i(z)\}]. \qquad (2.11)$$

In the above decomposition, $H_0[\{\mathbf{r}_{0i}\}] = H_0(\mathbf{r}_{01}, \ldots, \mathbf{r}_{0N})$ is an effective variational Hamiltonian describing the interactions of the c.m. modes, while $H_u[\{\mathbf{u}_i(z)\}]$ describes the elasticity and mutual interactions of the internal modes of flux lines. For $H_u[\{\mathbf{u}_i(z)\}]$, we shall use the following Gaussian approximation

$$H_u = \frac{1}{2L^2} \sum_{i,j} \int dz \int dz' [G^{-1}(z-z')]_{ij} \mathbf{u}_i(z) \cdot \mathbf{u}_j(z'). \qquad (2.12)$$

Throughout the rest of the paper, it will be understood that integrals over the z and z' variables run from 0 to L. The above expression can be rewritten in Fourier space in the form

$$H_u = \frac{1}{2} \sum_{i,j} \sum_{n \neq 0} [G^{-1}(q_n)]_{ij} \mathbf{u}_i(q_n) \cdot \mathbf{u}_j(-q_n). \qquad (2.13)$$

In Eqs. (2.12), (2.13), $[G^{-1}(q_n)]_{ij}$ is an $N \times N$ matrix of variational parameters describing the interactions of the internal modes of flux lines.[15] In the boson language, the decomposition (2.11) of the total Hamiltonian into c.m. and internal modes pieces can be seen as the generalization of the Feynman-Kleinert variational method[16] for single quantum particles in imaginary time to an assembly of interacting quantum particles. Both quantities H_0 and $[G^{-1}(q_n)]_{ij}$ will be determined variationally, and one can in fact show, following Ref. 17, that the Gaussian approximation (2.13), with the optimal choice for the propagator $[G^{-1}(q_n)]_{ij}$ to be determined below, becomes *exact* in the limit of a large number of components of the displacement field $\{\mathbf{u}_i(z)\}$ (i.e., in the limit $d_\perp \to \infty$).

Using the Hamiltonian H_1 above, Eqs. (2.11)–(2.13), to evaluate the variational free energy in Eq. (2.10), we find [we use the shorthand notation $\int_{\mathbf{q}} = \int d\mathbf{q}/(2\pi)^{d_\perp}$]

$$\begin{aligned} F_v = {} & -T \ln Z_1 + \frac{1}{Z_1} \int \prod_{i=1}^{N} d\mathbf{r}_{0i} \Phi(\mathcal{G}) \\ & \times e^{-\beta H_0} \Bigg[\frac{1}{2} \sum_{i,j} \sum_{n \neq 0} d_\perp T L \{ [G_0^{-1}(q_n)]_{ij} \\ & - [G^{-1}(q_n)]_{ij} \} G_{ij}(q_n) \\ & + \frac{1}{2} L \sum_{i,j} \int_{\mathbf{q}} V(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{r}_{0i}-\mathbf{r}_{0j})} e^{-(1/2)q^2 C_{ij}} - H_0[\{\mathbf{r}_{0i}\}] \Bigg], \end{aligned} \qquad (2.14)$$

where

$$\begin{aligned} Z_1 = {} & \int \prod_{i=1}^{N} d\mathbf{r}_{0i} \int [d\mathbf{u}_i(z)] e^{-\beta H_0} \\ & \times \exp\left(-\frac{\beta}{2} \sum_{i,j} \sum_{n \neq 0} [G^{-1}(q_n)]_{ij} \mathbf{u}_i(q_n) \cdot \mathbf{u}_j(-q_n) \right) \\ = {} & \int \prod_{i=1}^{N} d\mathbf{r}_{0i} \Phi(\mathcal{G}) e^{-\beta H_0} \end{aligned} \qquad (2.15)$$

and

$$\Phi(\mathcal{G}) = \prod_{n=1}^{\infty} \left(\frac{2\pi}{\det[T\mathcal{G}(q_n)]} \right)^{d_\perp}, \qquad (2.16)$$

and where $\mathcal{G}(q_n)$ denotes the $N \times N$ matrix $G_{ij}(q_n)$. The correlation function C_{ij} is on the other hand given by

$$C_{ij} = \frac{1}{d_\perp} \langle [\mathbf{u}_i(z) - \mathbf{u}_j(z)]^2 \rangle. \qquad (2.17)$$

Variation of the above expression with respect to the c.m. Hamiltonian H_0 shows that F_v is minimal for the particular choice

$$\begin{aligned} \tilde{H}_0 = {} & \frac{1}{2} \sum_{i,j} \sum_{n \neq 0} d_\perp T L \{ [G_0^{-1}(q_n)]_{ij} - [G^{-1}(q_n)]_{ij} \} G_{ij}(q_n) \\ & + \frac{1}{2} L \sum_{i,j} \int_{\mathbf{q}} V(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{r}_{0i}-\mathbf{r}_{0j})} e^{-(1/2)q^2 C_{ij}}. \end{aligned} \qquad (2.18)$$

The trial free energy F_v of Eq. (2.14) thus reduces to

$$F_v = -T \ln Z_1, \qquad (2.19)$$

where now in the expression of Z_1, Eq. (2.15), the expression (2.18) of $\tilde{H}_0$ should be used for H_0.

Further minimization of F_v with respect to $G_{ij}(q_n)$ leads to the following results (Appendix A):

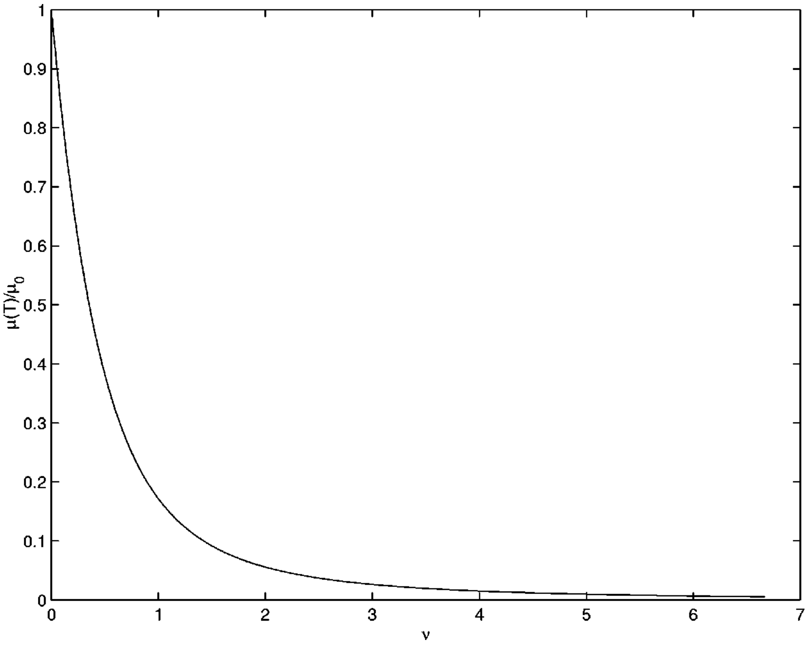

FIG. 1. Plot of $\mu(T)/\mu_0$ versus $\nu = \alpha T/a^2\sqrt{\kappa\mu_0}$.

$$[\tilde{G}^{-1}(q_n)]_{ij}$$

$$=\kappa q_n^2 - \frac{\rho}{d_\perp}\int_{\mathbf{q}} q^2 V(\mathbf{q}) g_0(\mathbf{q}) e^{-q^2\langle u^2\rangle/d_\perp} \quad \text{for } i=j \tag{2.20a}$$

$$=\frac{\rho}{d_\perp(N-1)}\int_{\mathbf{q}} q^2 V(\mathbf{q}) g_0(\mathbf{q}) e^{-q^2\langle u^2\rangle/d_\perp} \quad \text{for } i\neq j, \tag{2.20b}$$

where the tilde indicates that the inverse propagator $\tilde{G}^{-1}(q_n)$ has been averaged over all possible configurations of the c.m. positions $\{\mathbf{r}_{0i}\}$ compatible with a liquid structure.

As the integral on the right-hand side of Eq. (2.20b) is finite and independent of the total number of vortices N, we see that the off-diagonal elements $[\tilde{G}^{-1}(q_n)]_{i\neq j}$ vanish in the thermodynamic $N\to\infty$ limit, in which case the internal modes elastic propagator is diagonal and given by

$$[\tilde{G}^{-1}(q_n)]_{ij} = L(\kappa q_n^2 + \mu)\delta_{ij} \tag{2.21}$$

with δ_{ij} the Kronecker delta symbol and where μ is given by

$$\mu = -\frac{\rho}{d_\perp}\int_{\mathbf{q}} q^2 V(\mathbf{q}) g_0(\mathbf{q}) e^{-q^2\langle u^2\rangle/d_\perp}. \tag{2.22}$$

In the above equation, the mean square width of a flux line [here $\tilde{G}(q_n)$ is the diagonal element $\tilde{G}_{ii}(q_n)$]

$$\langle u^2\rangle = d_\perp T\sum_{n\neq 0}\tilde{G}(q_n) = \frac{d_\perp T}{2\sqrt{\kappa\mu}} \tag{2.23}$$

depends on μ. Thus we see that Eq. (2.22) is in fact a self-consistent equation for the "mass" coefficient μ. From Eq. (2.22), we also see that μ depends on the density ρ of flux lines, not only through the prefactor in front of the integral, but also through the pair distribution function $g_0(\mathbf{r})$. Through this last quantity, μ also depends on temperature and on higher, nontrivial correlations between the positions of flux lines in the vortex liquid. The strongest dependence of μ on temperature, however, occurs through the "Debye-Waller" factor $e^{-q^2\langle u^2\rangle/d_\perp}$ which was missing in our more elementary Taylor expansion in paper I, and which describes the effect of internal fluctuations of flux lines.

From Eq. (2.22), it is not possible to derive a general expression of the coefficient μ without making assumptions about the analytic form of the pair correlation function $g_0(\mathbf{r})$. Here, we shall place ourselves in the case of a dilute flux liquid and use the analytical ansatz we proposed in paper I for the pair correlation function $g_0(\mathbf{r})$, namely,

$$g_0(\mathbf{r}) = 1 - \eta\exp(-\alpha r^2/a^2), \tag{2.24}$$

where α is a constant of order unity, $a = 1/\sqrt{\rho}$ is the average vortex separation, and $0<\eta<1$. The numerical constant η quantifies the correlations between c.m. positions of flux lines. It is close to unity when flux lines are strongly anticorrelated due to the repulsive interactions between their surrounding supercurrents, and close to zero in situations where there is considerable cutting and crossing of flux lines. Using the above ansatz for $g_0(r)$, we obtain the following expression for the "mass" μ of the internal modes as a function of T:

$$\mu(T) = \mu_0\left[\sqrt{1+\left(\frac{\alpha T}{a^2\sqrt{\kappa\mu_0}}\right)^2} - \left(\frac{\alpha T}{a^2\sqrt{\kappa\mu_0}}\right)\right]^2, \tag{2.25}$$

where $\mu_0 = \mu(T=0) = 4\eta\pi\rho\varepsilon_0/d_\perp$. Figure 1 shows a plot of $\mu(T)/\mu_0$ as a function of the variable $\nu = \alpha T/(a^2\sqrt{\kappa\mu_0})$.

From Eq. (2.25), it is not difficult to see that the above expression has the limiting value $\mu(T)\to\mu_0$ when $T \ll a^2\sqrt{\kappa\mu_0}$, while at higher temperatures $T\gg a^2\sqrt{\kappa\mu_0}$, $\mu(T)\simeq\mu_0(a^2\sqrt{\kappa\mu_0}/\alpha T)$ and goes to zero as $1/T$. We thus see that $\langle u^2\rangle$ in Eq. (2.23) will vary with temperature like $T^{3/2}$. More generally, any realistic form of the pair distribution function $g_0(r)$ (other than the trivial choice $g_0(r)=1$) in Eqs. (2.20a), (2.20b) will result in a nontrivial temperature dependence of $\mu(T)$ and hence of the mean projected area of a flux line $\langle u^2\rangle$. This temperature variation of $\langle u^2\rangle$ can be measured in numerical simulations and is actually a good way to test the predictions of the present paper. Note also that as T becomes very large, $\mu(T)$ vanishes and we recover a liquid of freely fluctuating flux lines with $\langle u^2\rangle$ diverging with the sample thickness L.

III. THE INTERACTING STRUCTURE FACTOR OF FLUX LINE LIQUIDS

We now turn our attention to a comparison and a discussion of the results obtained by the approach developed in paper I and the present paper, and the Boson-mapping type of approach. Since this last type of approach only makes predictions for correlations of coarse-grained variables, such as the density, and makes no predictions for microscopic conformation variables of the flux lines, we here shall focus on comparing the interacting structure factor $S(\mathbf{r},z)$ obtained with both methods.

Let us first start by deriving the structure factor of a liquid of flux lines from our variational approach. This can be done in a straightforward way, with the result (Appendix B)

$$S(\mathbf{q},z)=\rho^2 g_0(\mathbf{q})e^{-q^2\langle u^2\rangle/d_\perp}+\rho e^{-(1/2d_\perp)q^2\phi(z)}. \tag{3.1}$$

Let us insist that this result is actually very general, and only requires that an approximate decomposition of the form (2.11) can be written for the Hamiltonian in terms of the conformational degrees of freedom of flux lines, and that the internal modes of flux lines obey a Gaussian distribution such as the one implied by Eq. (2.13). With these assumptions, the mean square relative displacement in Eq. (3.1), for an arbitrary form of the propagator $G_{ij}(q_n)$ in Eq. (2.13), is given by [here again $\tilde{G}(q_n)=\tilde{G}_{ii}(q_n)$]

$$\phi(z)=\langle[\mathbf{u}_i(z)-\mathbf{u}_i(0)]^2\rangle=2d_\perp T\sum_{n\neq 0}\tilde{G}(q_n)[1-\cos(q_n z)] \tag{3.2}$$

while the mean projected area of a given flux line is given by

$$\langle u^2\rangle=d_\perp T\sum_{n\neq 0}\tilde{G}(q_n). \tag{3.3}$$

Having derived the structure factor through our approach, Eq. (3.1), we want to compare it to the corresponding quantity derived through the Boson mapping and similar approaches. It has been shown in Ref. 2 using the boson mapping that this last quantity, in Fourier space, is given by

$$S(\mathbf{q},q_z)=\frac{\rho T q^2/\kappa}{q_z^2+\varepsilon^2(\mathbf{q})/T^2}, \tag{3.4}$$

where the excitation spectrum of the equivalent bosons has the usual form

$$\frac{\varepsilon(\mathbf{q})}{T}=\left[\left(\frac{Tq^2}{2\kappa}\right)^2+\frac{\rho q^2 V(\mathbf{q})}{\kappa}\right]^{1/2}. \tag{3.5}$$

From Eq. (3.4), it is not difficult to obtain the partial Fourier transform $S(\mathbf{q},z)$:

$$S(\mathbf{q},z)=\int_{-\infty}^{\infty}\frac{dq_z}{2\pi}S(\mathbf{q},q_z)e^{iq_z z}=\frac{\rho e^{-\varepsilon(\mathbf{q})|z|/T}}{\sqrt{1+4\rho V(q)\kappa/(Tq)^2}}. \tag{3.6}$$

We first note that the above analytic form of the structure factor, (3.1) and the hydrodynamic result (3.6) cannot be brought to agreement. In other words, *no* Gaussian approximation of the form (2.13) can produce a structure factor of the form (3.6).

As we already mentioned in the Introduction, it has already been noticed[4,10] that the boson mapping gives nonsensical results when applied to flux liquids in the presence of splayed columnar disorder. In Appendix B, we comment on the definition of the chemical potential of flux lines in the boson mapping, which appears to us a little problematic. While this may be considered to be a rather ‘‘cosmetic’’ issue, in what follows we show that the boson mapping yields other unphysical results (in addition to those already noticed in Ref. 4) even in the simplest case of pure, disorder free vortex liquids. To this end, let us make the following two observations regarding the analytic form of $S(\mathbf{q},z)$ in the boson scheme.

(i) By taking the limit $\kappa\to\infty$ in Eq. (3.4), one should be able to obtain the structure factor of a liquid of rigid flux lines, which we expect to be independent of z. Taking the above limit in Eq. (3.6), we see that the z dependence does indeed cancel out, since $\varepsilon(\mathbf{q})\to 0$ as $\kappa\to\infty$. However, the prefactor

$$S(\mathbf{q},z=0)=\frac{\rho T q^2/\kappa}{2[\varepsilon(\mathbf{q})/T]}=\frac{\rho}{\sqrt{1+4\rho V(q)\kappa/(Tq)^2}}$$

also goes to zero in the limit $\kappa\to\infty$, which means that the whole structure factor $S(\mathbf{q},z=0)$ will vanish as κ gets very large, which is not exactly what we would expect for a liquid of rigid flux lines. In contrast to this behavior, the structure factor derived within our variational perturbation theory is well behaved in the limit $\kappa\to\infty$, and it is not difficult to see from Eqs. (3.1)–(3.3) that we obtain, for the two possible choices of $[G^{-1}(q_n)]_{ii}=L(\kappa q_n^2+\mu)$, with either $\mu=0$ or a nonzero μ, in the above limit:

$$S(\mathbf{q},z)=\rho[1+\rho g_0(\mathbf{q})] \tag{3.7}$$

which is the correct result for a liquid of rigid hard rods.

(ii) For an ‘‘ideal gas’’ of noninteracting flux lines, the mean projected area $\langle u^2\rangle$ of a given flux line is given by

$$\langle u^2\rangle=\frac{d_\perp TL}{12\kappa} \tag{3.8}$$

and the mean square displacement $\phi(z)$ is given by (in the rest of this section we use $d_\perp=2$)

$$\phi(z)=\frac{2T}{\kappa}|z|. \tag{3.9}$$

Using these expressions in Eq. (3.1) above, one finds, for noninteracting flux lines in the thermodynamic ($L\rightarrow\infty$) limit

$$S_{id}(\mathbf{q},z)=\rho \exp\left(-\frac{Tq^2}{2\kappa}|z|\right). \tag{3.10}$$

Comparing this expression to the expression (3.6) of the structure factor of an interacting flux liquid in the boson mapping and given the expression (3.5) of the Boguliubov spectrum, we see that, at any given value of $\mathbf{q}$, $S(\mathbf{q},z)$ decays more rapidly as a function of z than its free counterpart $S_{id}(\mathbf{q},z)$. This result is very surprising, to say the least, as it is very difficult to imagine a flux line assembly where the density decorrelates on shorter length scales and vortices fluctuate more strongly than in an ‘‘ideal gas’’ of freely fluctuating flux lines. Indeed, the effect of the repulsive interactions between flux lines is to reduce the fluctuations of vortices, as is evidenced at the freezing transition: in the absence of interactions, a liquid of vortices would never freeze into a vortex solid and would continue to have large fluctuations, Eqs. (3.8), (3.9), down to $T=0$. Going back to Eq. (3.1), it is not difficult to verify that our result for the structure factor does *not* exhibit the above behavior. With the particular choice (2.24) for the pair distribution function $g_0(r)$, we obtain[11]

$$\begin{aligned}S(\mathbf{q},z)=&\rho^2 g_0(\mathbf{q})e^{-q^2T/2\sqrt{\kappa\mu(T)}}\\&+\rho \exp\left(-\frac{Tq^2}{2\sqrt{\kappa\mu(T)}}\left(1-e^{-\sqrt{\mu(T)/\kappa}|z|}\right)\right)\end{aligned} \tag{3.11}$$

which has the following, nonvanishing limit as $z\rightarrow\infty$:

$$S(\mathbf{q},z\rightarrow\infty)=\rho \exp\left(\frac{-Tq^2}{2\sqrt{\kappa\mu(T)}}\right)[1+\rho g_0(\mathbf{q})] \tag{3.12}$$

indicating that the flux line densities $\rho(\mathbf{q},z)=\langle\hat{\rho}(\mathbf{q},z)\rangle$ at both sides $z=0$ and $z=L$ of a superconducting sample are not very much decorrelated, in agreement with the experimental findings of Ref. 18. In this reference, the authors have performed a two-sided decoration experiment on both sides of a superconducting sample, and observed the same pattern of vortices in each case. If the structure factor obeyed the boson mapping result (3.6), the densities $\rho(\mathbf{q},0)$ and $\rho(\mathbf{q},L)$ would have been completely decorrelated and very different from one another. The fact that both density patterns in the experiments of Ref. 18 look exactly the same might be evidence of the fact that there is a strong correlation between $\rho(\mathbf{q},0)$ and $\rho(\mathbf{q},L)$, and that $S(\mathbf{q},z)$ is finite in the limit $z\rightarrow\infty$.

In fact, one can even attempt a slightly more quantitative comparison of our results, Eqs. (3.11), (3.12), and the experimental findings of Ref. 18. From Eqs. (3.11), (3.12), it is not difficult to see that the ratio $S(\mathbf{q},z=0)/S(\mathbf{q},z=L)$ is of order unity for $\mathbf{q}$ not too close to 0, and is such that

$$\frac{S(\mathbf{q},z=0)}{S(\mathbf{q},z=L)}\rightarrow 1 \quad \text{as} \quad \mathbf{q}\rightarrow 0. \tag{3.13}$$

in agreement with the decoration experiments of Yoon *et al.* It would be interesting to do a more detailed analysis of the experimental results in light of the present model (taking into account nonlocal elasticity[19]), as such an analysis may lead to values of the elastic constants of the flux line system (in particular, of the tilt modulus κ) which are closer to the conventional values of these quantities (recall that the analysis of the experiments of Ref. 18 using the boson mapping yields elastic constants which are three to four orders of magnitude below what is expected from the standard theory of elasticity of vortices in uniaxial type-II superconductors[19–21]).

IV. CONCLUSION

In summary, in this paper we have extended the approach developed in paper I to better take into account the effect of thermal fluctuations of flux lines in vortex liquids. Using a variational Hartree approximation, we have shown that thermal fluctuations strongly reduce the ‘‘mass’’ term which confines the fluctuations of the internal modes of flux lines. We have also argued that our approach, which is based on the use of the conformation variables $\{\mathbf{r}_n(z)\}$ as the *true* dynamical variables in terms of which all (Gaussian) averages are taken, yields physically more reasonable results than the boson mapping[2–4] or other hydrodynamic approaches[7] which, in contrast, use the density $\hat{\rho}(\mathbf{r},z)$ as the basic dynamical variable of the system. With that said, it is worth noting, as has been discussed at length in paper I, that the presence of the confining term $\mu(T)$ in the Hamiltonian of interacting flux lines, does not necessarily imply that the flux liquid is in a disentangled state: depending on the value of $\mu(T)$, the present approach can describe a disentangled flux line liquid ($\mu\approx\mu_0$) as well as a heavily entangled vortex liquid as predicted by Nelson *et al.*[1,2] when $\mu(T)\rightarrow 0$.

In paper I, we have argued that a careful numerical measurement of the pair distribution function for the c.m. mode $g_0(r)$ could shed more light on the confining mass term μ_0 in a vortex liquid. Here, we have shown that a numerical measurement of the temperature dependence of the mean square projected area of flux lines can also be used to test the predictions of the present approach. In particular, a nonlinear temperature dependence of $\langle u^2\rangle$ could be the signature of a weakly entangled state, where vortex fluctuations, as measured by $\langle u^2\rangle$, do *not* diverge with the sample thickness L.

It is worth noting that the considerations of paper I and of the present work can be easily extended to the dynamics of flux liquids. This will be the subject of a future contribution.[22]

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APPENDIX A: MINIMIZATION OF THE VARIATIONAL FREE ENERGY

In this Appendix, we present a few details of the minimization of the free energy of Eq. (2.19) with respect to the propagator of internal fluctuations $G_{kl}(q_m)$. Taking the derivative of Eq. (2.19) with respect to this last quantity amounts to computing the following expression:

$$\frac{\partial F_v}{\partial G_{kl}(q_m)}=\frac{1}{Z_1}\int\prod_{i=1}^{N}d\mathbf{r}_{0i}\frac{\partial H_{\mathrm{eff}}}{\partial G_{kl}(q_n)}e^{-\beta H_{\mathrm{eff}}[\{\mathbf{r}_{0i}\}]}\tag{A1}$$

with the effective Hamiltonian of the c.m. modes

$$H_{\mathrm{eff}}=\widetilde{H}_0-T\ln\Phi(\mathcal{G})\tag{A2}$$

and the partition function

$$Z_1=\int\prod_{i=1}^{N}d\mathbf{r}_{0i}e^{-\beta H_{\mathrm{eff}}[\{\mathbf{r}_{0i}\}]}.\tag{A3}$$

The derivative of the first term in H_{eff} can be found in a straightforward way, and gives (here and in the following, we sum over repeated indices unless otherwise indicated):

$$\frac{\partial\widetilde{H}_0}{\partial G_{kl}(q_m)}=LTd_\perp\kappa q_m^2\delta_{kl}-\frac{1}{2}TL\sum_{i,j}\int_{\mathbf{q}}q^2V(\mathbf{q})e^{i\mathbf{q}\cdot[\mathbf{r}_{0i}-\mathbf{r}_{0j}]}\times e^{-(1/2)k^2C_{ij}}[(\delta_{ik}+\delta_{jk})\delta_{kl}-2\delta_{ik}\delta_{jl}].\tag{A4}$$

On the other hand, the derivative of the second term in Eq. (A2) can be taken in a standard way, with the result

$$\frac{\partial}{\partial G_{kl}(q_m)}\ln\Phi(\mathcal{G})=Ld_\perp[G^{-1}(q_m)]_{kl}.\tag{A5}$$

With hindsight from the results of paper I, we can expect $\langle\mathbf{u}_i(z)\cdot\mathbf{u}_j(z)\rangle\simeq0$, so that

$$C_{ij}=\langle[\mathbf{u}_i(z)-\mathbf{u}_j(z)]^2\rangle/d_\perp\simeq2\langle u^2\rangle/d_\perp.$$

Using this last approximation into Eq. (A4), and averaging over the c.m. positions in Eq. (A1), using the fact that

$$\begin{aligned}\frac{1}{Z_1}\int\prod_{i=1}^{N}d\mathbf{r}_{0i}e^{i\mathbf{q}\cdot(\mathbf{r}_{0i}-\mathbf{r}_{0j})}e^{-\beta H_{\mathrm{eff}}[\{\mathbf{r}_{0i}\}]}&=\frac{\rho^2}{N(N-1)}\int d\mathbf{r}_{0i}d\mathbf{r}_{0j}g_0(\mathbf{r}_{0i}-\mathbf{r}_{0j})e^{i\mathbf{q}\cdot(\mathbf{r}_{0i}-\mathbf{r}_{0j})}\\&=\frac{\rho}{N-1}g_0(\mathbf{q})\end{aligned}\tag{A6}$$

we immediately arrive at Eqs. (2.20a), (2.20b) of the text.

APPENDIX B: STRUCTURE FACTOR OF THE FLUX LIQUID

In this appendix, we show some details of the derivation of the structure factor

$$S(\mathbf{r},z;\mathbf{r}',z')=\langle\hat{\rho}(\mathbf{r},z)\hat{\rho}(\mathbf{r}',z')\rangle,\tag{B1}$$

where the statistical average $\langle\cdots\rangle$ is taken with the statistical weight $\exp(-\beta H)/\mathcal{Z}$, with H the Hamiltonian defined in Eq. (2.11) and $\mathcal{Z}=Z_0Z_u$, with $Z_0=\mathrm{Tr}(e^{-\beta\widetilde{H_0}})$ and $Z_u=\mathrm{Tr}(e^{-\beta H_u})$. We expect flux liquids at equilibrium to be translationally invariant, and the structure factor to depend only on the relative coordinates $(\mathbf{r}-\mathbf{r}')$ and $(z-z')$, i.e., $S(\mathbf{r},z;\mathbf{r}',z')=S(\mathbf{r}-\mathbf{r}',z-z')$. As a consequence, we have for the Fourier transform of the density-density correlation function

$$\langle\hat{\rho}(\mathbf{q},q_z)\hat{\rho}(\mathbf{q}',q_z')\rangle=(2\pi)^d\delta(\mathbf{q}+\mathbf{q}')\delta(q_z+q_z')S(\mathbf{q},q_z).\tag{B2}$$

In the following, we shall be interested in the quantity

$$S(\mathbf{q},q_z)=\frac{1}{LL_\perp^{d_\perp}}\langle\hat{\rho}(\mathbf{q},q_z)\hat{\rho}(-\mathbf{q},-q_z)\rangle,\tag{B3}$$

where we used Eq. (B2) above and the fact that $(2\pi)^d\delta(\mathbf{q}=\mathbf{0})\delta(q_z=0)\equiv LL_\perp^{d_\perp}$ in the limit $L,L_\perp\to\infty$. We have

$$\begin{aligned}\langle\hat{\rho}(\mathbf{q},q_z)\hat{\rho}(-\mathbf{q},-q_z)\rangle&=\int d\mathbf{r}dz\int d\mathbf{r}'dz'\langle\hat{\rho}(\mathbf{r},z)\hat{\rho}(\mathbf{r}',z')\rangle e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}e^{-iq_z(z-z')}\\&=\sum_{i=1}^{N}\sum_{j=1}^{N}\int d\mathbf{r}dz\int d\mathbf{r}'dz'\langle\delta[\mathbf{r}-\mathbf{r}_i(z)]\delta[\mathbf{r}'-\mathbf{r}_j(z')]\rangle e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}e^{-iq_z(z-z')}\\&=\sum_{i=1}^{N}\sum_{j\neq i}\int dz\int dz'\langle e^{-i\mathbf{q}\cdot(\mathbf{r}_{0i}-\mathbf{r}_{0j})}\rangle_0\langle e^{-i\mathbf{q}\cdot[\mathbf{u}_i(z)-\mathbf{u}_j(z')]}\rangle_u e^{-iq_z(z-z')}\\&\quad+\sum_{i=1}^{N}\int dz\int dz'\langle e^{-i\mathbf{q}\cdot[\mathbf{u}_i(z)-\mathbf{u}_j(z')]}\rangle_u e^{-iq_z(z-z')}\\&=\sum_{i=1}^{N}\sum_{j\neq i}\int dz\int dz'\langle e^{-i\mathbf{q}\cdot(\mathbf{r}_{0i}-\mathbf{r}_{0j})}\rangle_0 e^{-(1/2)q_\alpha q_\beta\langle[u_{i,\alpha}(z)-u_{j,\alpha}(z')][u_{i,\beta}(z)-u_{j,\beta}(z')]\rangle_u}\\&\quad\times e^{-iq_z(z-z')}+\sum_{i=1}^{N}\int dz\int dz'e^{-(1/2)q_\alpha q_\beta\langle[u_{i,\alpha}(z)-u_{i,\alpha}(z')][u_{i,\beta}(z)-u_{i,\beta}(z')]\rangle_u}e^{-iq_z(z-z')}.\end{aligned}\tag{B4}$$

In the above equations, $\langle\cdots\rangle_0$ and $\langle\cdots\rangle_u$ denote averages over the c.m. and internal modes, with statistical weights $\exp(-\beta H_0)$ and $\exp(-\beta H_u)$, respectively [H_0 and H_u are the Hamiltonians given in Eqs. (2.18) and (2.13) of the text]. In our variational model, we find that the internal degrees of freedom $\mathbf{u}_i(z)$ and $\mathbf{u}_j(z)$ belonging to two different lines $i \neq j$ are decoupled. We therefore can write for $i\neq j$

$$\begin{aligned}\langle[u_{i,\alpha}(z)-u_{j,\alpha}(z')][u_{i,\beta}(z)-u_{j,\beta}(z')]\rangle_u\\ =\langle u_{i,\alpha}(z)u_{i,\beta}(z)+u_{j,\alpha}(z')u_{j,\beta}(z')\rangle_u=\frac{2\delta_{\alpha\beta}}{d_\perp}\langle u^2\rangle,\end{aligned} \tag{B5}$$

where, in going from the first to the second line, we used the fact that $\langle u_{i,\alpha}u_{i,\beta}\rangle_u=\delta_{\alpha,\beta}\langle u_{i,\alpha}^2\rangle$. Equation (B4) becomes

$$\begin{aligned}&\langle\hat{\rho}(\mathbf{q},q_z)\hat{\rho}(-\mathbf{q},-q_z)\rangle\\ &\quad=\sum_{i=1}^{N}\sum_{j\neq i}\int dz\int dz'\langle e^{-i\mathbf{q}\cdot(\mathbf{r}_{0i}-\mathbf{r}_{0j})}\rangle_0\\ &\qquad\times e^{-(1/d_\perp)q^2\langle u^2\rangle}e^{-iq_z(z-z')}+\sum_{i=1}^{N}\int dz\int dz'\\ &\qquad\times e^{-(1/2)q_\alpha q_\beta\langle[u_{i,\alpha}(z)-u_{i,\alpha}(z')][u_{i,\beta}(z)-u_{i,\beta}(z')]\rangle_u}\\ &\qquad\times e^{-iq_z(z-z')}.\end{aligned} \tag{B6}$$

Using the fact that $\int dz\int dz' e^{-iq_z(z-z')}=L^2\delta_{q_z,0}$, and noticing that

$$\sum_{i=1}^{N}\sum_{j\neq i}\langle e^{-i\mathbf{q}\cdot\mathbf{r}_{0i}}e^{-i\mathbf{q}'\cdot\mathbf{r}_{0j}}\rangle_0=(2\pi)^{d_\perp}\delta(\mathbf{q}+\mathbf{q}')\rho^2 g_0(\mathbf{q}) \tag{B7}$$

which gives us here (with $\mathbf{q}'=-\mathbf{q}$)

$$\begin{aligned}\sum_{i=1}^{N}\sum_{j\neq i}\langle e^{-i\mathbf{q}\cdot\mathbf{r}_{0i}}e^{i\mathbf{q}\cdot\mathbf{r}_{0j}}\rangle_0&=(2\pi)^{d_\perp}\delta(\mathbf{q}=0)\rho^2 g_0(\mathbf{q})\\ &=L_\perp^{d_\perp}\rho^2 g_0(\mathbf{q})\end{aligned} \tag{B8}$$

we finally obtain

$$\begin{aligned}&\langle\hat{\rho}(\mathbf{q},q_z)\hat{\rho}(-\mathbf{q},-q_z)\rangle\\ &\quad=L^2\delta_{q_z,0}L_\perp^{d_\perp}\rho^2 g_0(\mathbf{q})e^{-(1/d_\perp)q^2\langle u^2\rangle}+\sum_{i=1}^{N}\int dz\int dz'\\ &\qquad\times e^{-(1/2d_\perp)q^2\langle[\mathbf{u}_i(z)-\mathbf{u}_i(z')]^2\rangle_u}e^{-iq_z(z-z')},\end{aligned} \tag{B9}$$

where we used the fact that $\langle[u_{i,\alpha}(z)-u_{i,\alpha}(z')][u_{i,\beta}(z)-u_{i,\beta}(z')]\rangle_u=(\delta_{\alpha,\beta}/d_\perp)\langle[\mathbf{u}_i(z)-\mathbf{u}_i(z')]^2\rangle_u$. The partial Fourier transform of this last expression with respect to q_z leads directly to expression (3.1).

APPENDIX C: CHEMICAL POTENTIAL OF A FLUX LINE LIQUID

In this appendix, we briefly comment on the "chemical potential" of a flux line liquid adopted in Refs. 2,3,9,4, which seems to us to be a little unconventional. In what follows, we shall be considering, in the notation of the text, a flux line liquid in a superconducting sample of thickness L along the $\hat{\mathbf{z}}$ axis. We will call Ω the area of the sample in the (x,y) plane. The self-energy per unit length of a single flux line will be denoted by ε_1, and is given by $\varepsilon_1=\varepsilon_0\ln(\lambda_{ab}/\xi_{ab})$, where λ_{ab} and ξ_{ab} are the London penetration depth and the coherence length in the basal (ab) plane. The magnitude of the magnetic induction inside the sample will be denoted by B, and it is related to the flux line density $\rho=N/\Omega$ by $B=\rho\phi_0$.

To start with, we make the observation that the chemical potential per unit length of a system of N flux lines can be easily obtained using the thermodynamic identity (in this Appendix, μ denotes the chemical potential and should not be confused with the mass of the internal modes of flux lines)

$$\mu=\frac{1}{L}\frac{\partial F}{\partial N}, \tag{C1}$$

where F is the Helmholtz free energy of the flux line system. Using the fact that the free energy per unit volume $f=F/(\Omega L)$ satisfies the following thermodynamic equality:

$$\frac{\partial f}{\partial B}=\frac{H}{4\pi} \tag{C2}$$

and remembering that $B=n\phi_0=N\phi_0/\Omega$, we readily obtain

$$\mu=\frac{H\phi_0}{4\pi}. \tag{C3}$$

Instead of the Helmholtz free energy F, Nelson and Seung[2] consider the Gibbs free energy $G=F-V(BH/4\pi)$, which for a system of flux lines is given by

$$\begin{aligned}G=&\sum_{i=1}^{N}\varepsilon_1\int dz[1+(d\mathbf{r}_i/dz)^2]^{1/2}\\ &+\frac{1}{2}\sum_{i\neq j}\int dz V[\mathbf{r}_i(z)-\mathbf{r}_j(z)]-V\frac{BH}{4\pi},\end{aligned} \tag{C4}$$

where $V(\mathbf{r})=2\varepsilon_0 K_0(r/\lambda_{ab})$ is the interaction potential between flux line elements at height z. Upon expanding the square root on the right-hand side of this last equation, and readjusting the tilt modulus $\varepsilon_1\to\kappa=\varepsilon^2\varepsilon_1$ to take anisotropy into account (and using the fact that the volume $V=\Omega L$ and $B=N\phi_0/\Omega$) they obtain

$$\begin{aligned}G=&\left(\varepsilon_1-\frac{H\phi_0}{4\pi}\right)NL+\frac{1}{2}\kappa\sum_{i=1}^{N}\int dz(d\mathbf{r}_i/dz)^2\\ &+\frac{1}{2}\sum_{i\neq j}\int dz V[\mathbf{r}_i(z)-\mathbf{r}_j(z)].\end{aligned} \tag{C5}$$

TABLE I. Summary of correspondence between vortex and classical fluids quantities.

Flux lines	Classical fluids
Helmholtz free energy	Helmholtz free energy
$F=-T\ln Z$	$F=-T\ln Z$
Gibbs free energy	Grand canonical potential
$G=F-L(\phi_0 H/4\pi)N$	$\mathcal{Q}_{\mathrm{gr}}=F-\mu N$
$(\partial G/\partial B)=0$	$(\partial \mathcal{Q}_{\mathrm{gr}}/\partial \rho)=0$
chemical potential per unit length	chemical potential
$\mu=(\partial f/\partial \rho)/L$	$\mu=(\partial f/\partial \rho)$
$=(\phi_0 H/4\pi)$	

They then identify the term proportional to N in this last expression, i.e., $(\varepsilon_1-H\phi_0/4\pi)NL$ with the "usual" chemical potential term $-\mu N$ and obtain in this way the chemical potential per unit length as

$$\mu=(H\phi_0/4\pi)-\varepsilon_1 \tag{C6}$$

which does not coincide with expression (C.3).

At the origin of this disagreement is a confusion in terminology that is worth clarifying. When we use terms such as "chemical potential" in vortex physics, we are borrowing a terminology whose most natural realm is the theory of gases and liquids. There, one defines the Helmholtz free energy F by $F_{\mathrm{liq}}=-T\ln Z$, where Z is the canonical partition function of the system (we use the subscript "liq" to distinguish quantities pertaining to liquid state theory from quantities in vortex physics bearing the same name). F_{liq} contains information about the interactions among the particles in the system and possibly, as is the case for vortices, about their self-energies. One also defines a Gibbs free energy G_{liq} by $G_{\mathrm{liq}}=\mu N$, where $\mu=(\partial F_{\mathrm{liq}}/\partial N)$ is the chemical potential. In the grand-canonical ensemble, the grand canonical potential $\mathcal{Q}_{\mathrm{gr}}=-T\ln \mathcal{Z}_{\mathrm{gr}}$ can be written in terms of F_{liq} and G_{liq} as $\mathcal{Q}_{\mathrm{gr}}=F_{\mathrm{liq}}-G_{\mathrm{liq}}=F_{\mathrm{liq}}-\mu N$. For homogeneous systems, the equilibrium density of particles ρ is obtained by minimizing the quantity $(\mathcal{Q}_{\mathrm{gr}}/V)=f-\mu\rho$, using the equation

$$\frac{\partial \mathcal{Q}_{\mathrm{gr}}}{\partial \rho}=0 \tag{C7}$$

or if a one body external potential is present, using a functional derivative

$$\frac{\delta \mathcal{Q}_{\mathrm{gr}}}{\delta \rho(\mathbf{r})}=0. \tag{C8}$$

This last equality is in fact the expression of the second Hohenberg-Kohn-Mermin theorem[23,24] which is the basis of density functional theories of classical liquids.

In the case of flux line systems, what we call Gibbs free energy $G=F-V(BH/4\pi)$ corresponds to the grand canonical potential $\mathcal{Q}_{\mathrm{gr}}$ of liquid state theory, as can easily be seen by comparing the definition of G for vortices, $G=F-L(\phi_0 H/4\pi)N$, to $\mathcal{Q}_{\mathrm{gr}}=F-\mu N$, and remembering that the equilibrium density of flux lines $\rho=B/\phi_0$ is obtained in a way reminiscent of Eq. (C7), i.e.,

$$\frac{\partial G}{\partial \rho}=\frac{\partial G}{\partial B}=0. \tag{C9}$$

The fact that G for magnetic systems corresponds to the grand canonical potential was recognized a long time ago by de Gennes,[25] who obtained the pressure in the flux line system as $P=-(\partial G/\partial \Omega)$, which is reminiscent of the thermodynamic relation $\mathcal{Q}_{gc}=-PV$ (with V the volume of the system). In view of the fact that the Helmholtz free energy F has the same meaning in liquid state theory and for magnetic systems, one is led to identify $V(BH/4\pi)$ with the Gibbs free energy μN of liquid state theory, and this identification leads to the result (C.3) for the chemical potential per unit length of the flux line system (see also Table I, where the correspondence between flux line and liquid quantities is summarized).

We now can understand the problem with the derivation of the chemical potential μ in Ref. 2. The problem with this derivation is that the term $\varepsilon_1 NL$ belongs to the Helmholtz free energy F while the true chemical potential should be identified only form the G_{liq} part of the grand canonical potential, i.e., from $V(BH/4\pi)=L(\phi_0 H/4\pi)N$. This improper identification of the chemical potential μ is, as far as the results of Refs. 2–4 are concerned, only a minor, "cosmetic" point. However, in order to obtain meaningful results in a grand-canonical formulation (using an approach similar to ours in paper I and in the present work), it is very important that the correct expression of μ, Eq. (C3), is properly identified.

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[1] D.R. Nelson, Phys. Rev. Lett. **60**, 1973 (1988).

[2] D.R. Nelson and H.S. Seung, Phys. Rev. B **39**, 9153 (1989).

[3] D.R. Nelson and P. Le Doussal, Phys. Rev. B **42**, 10 113 (1990).

[4] U. Täuber and D.R. Nelson, Phys. Rep. **289**, 157 (1997).

[5] P. Benetatos and M.C. Marchetti, Phys. Rev. B **59**, 6499 (1999).

[6] M.P.A. Fisher and D.H. Lee, Phys. Rev. B **39**, 2756 (1989).

[7] L. Radzihovsky and E. Frey, Phys. Rev. B **48**, 10 357 (1993).

[8] Note here that in the rest of the paper, we will use the term "boson mapping" somewhat to refer not only to model Hamiltonian (2.1) to be defined below, but also to the approximation used by Nelson and co-workers (Refs. 1–4), and which consists

in taking the density as a dynamical variable in functional integration measures ($[d\rho(\mathbf{r},z)]$, etc.) when calculating the partition function and statistical averages of physical observables in the above model.

[9] D.R. Nelson and V.M. Vinokur, Phys. Rev. B **48**, 13 060 (1993).

[10] For further discussion, see the introduction of the paper by R.A. Lehrer and D.R. Nelson, Physica C **331**, 317 (2000).

[11] A.M. Ettouhami, Phys. Rev. B **65**, 134504 (2002).

[12] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I.A. Stegun (Dover, 1965).

[13] M. Doi and S.F. Edwards, *The Theory of Polymer Dynamics* (Oxford University Press, Oxford, 1986).

[14] R.P. Feynman, *Statistical Mechanics* (Reading, 1972).

[15] Note that, had we chosen to use the most general form of the Hamiltonian of interacting flux lines in anisotropic superconductors (Refs. 16,20,21), we would have had to use an effective Hamiltonian for the internal modes $H_u = \frac{1}{2}\Sigma_{i,j}\Sigma_{n\neq 0}[G^{-1}(q_n)]_{ij}^{\alpha\beta}u_{i\alpha}(q_n)u_{j\beta}(-q_n)$ with an elastic propagator $[G^{-1}(q_n)]_{ij}^{\alpha\beta}$ which is nondiagonal in the spatial indices α,β.

[16] R.P. Feynman and H. Kleinert, Phys. Rev. A **34**, 5080 (1986).

[17] M. Mézard and G. Parisi, J. Phys. I **1**, 809 (1991).

[18] S. Yoon, Z. Yao, H. Dai, and C.M. Lieber, Science **270**, 270 (1995).

[19] E.H. Brandt, J. Low Temp. Phys. **26**, 735 (1977); Physica C **165&166**, 1129 (1990); Int. J. Mod. Phys. B **5**, 751 (1991); Physica C **195**, 1 (1992); Rep. Prog. Phys. **58**, 1465 (1995).

[20] E. Sardella, Phys. Rev. B **45**, 3141 (1992).

[21] G. Blatter, M.V. Feigel'man, V.B. Geshkenbein, A.I. Larkin, and V.M. Vinokur, Rev. Mod. Phys. **66**, 1125 (1994).

[22] A.M. Ettouhami (unpublished).

[23] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).

[24] D. Mermin, Phys. Rev. **137**, A1441 (1965).

[25] P.G. de Gennes, *Superconductivity of Metals and Alloys* (Addison-Wesley, New York, 1966).