Thermodynamic scaling functions in the critical region of type-II superconductors

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A recently proposed nonperturbative method for evaluation of the thermodynamic scaling functions in the nominal critical region of quasi-two-dimensional type-II superconductors is generalized and extended to arbitrary type-II systems. It is found that, in general, layered superconductors do not exhibit single-parameter scaling except in two opposite limits corresponding to two-dimensional (2D) and (an)isotropic 3D systems. Explicit, closed-form expressions for the scaling functions are constructed in these two limits. The results are found to be in good agreement with experiments and Monte Carlo simulations. The limits on the applicability of the Landau level description of fluctuations are also discussed.

Fluctuating behavior near $H_{c2}(T)$ in type-II superconductors has recently been the subject of an intense experimental[1–7] and theoretical[8,9] interest. In this region the problem of fluctuations can be investigated within a framework of the Ginzburg-Landau (GL) free-energy functional, with the order parameter confined to the lowest Landau level (LLL) for Cooper pairs. This GL-LLL theory exhibits characteristic dimensional reduction[10] and associated scaling properties, leading to expressions for various thermodynamic quantities, such as magnetization and heat capacity, which are functions only of a particular combination of temperature T and magnetic field H.[11,12] Such single-parameter scaling depends only on the effective dimensionality of fluctuations and its two- and three-dimensional versions have been observed in numerous experiments.[3,5–7]

In this regard, the basic theoretical task is to determine the thermodynamic scaling functions, in particular the free energy $f(x)$, where x is the scaling variable ($x = \text{const}[T - T_c(H)]/(TH)^{1/2}$ in 2D while $x = \text{const}[T - T_c(H)]/(TH)^{2/3}$ in 3D). $f(x)$ has been evaluated in the past by a large order perturbative expansion, valid far above $H_{c2}(T)$ ($x \gg 1$). The Padé and Borel-Padé approximants are then employed to reconstruct the low-temperature behavior of $f(x)$, far below $H_{c2}(T)$ ($x \ll -1$).[13] This procedure is often augmented by the condition requiring that the Abrikosov's mean-field result for $f(x)$ be obtained in the $T \to 0$ limit.

Recently, a rather different approach to the problem has been proposed by Tešanović *et al.*[14] The gist of their nonperturbative method is as follows: The physics of the GL-LLL theory naturally splits into two very different energy scales. The first of these is the familiar BCS condensation energy, associated with the overall growth of the square of the order parameter. The second energy scale is associated with the motion of vortices $\{z_i\}$ in the plane perpendicular to **H**. Different configurations of $\{z_i\}$ are weighted by the generalized Abrikosov parameter $\beta_A(\{z_i\})$, evaluated for *arbitrary* positions of vortices. This configuration interaction among $\{z_i\}$ is rather weak, an example being the well-known small difference between β_A for a triangular and a square lattice. Therefore, the second energy scale is only a few percent of the first one, their respective contribution to $f(x)$ approximately divided 2–98% of the total. This 98–2% rule is then exploited by Tešanović *et al.* to construct an analytic, closed-form, parameter free expression for $f(x)$ in quasi-two-dimensional (2D) superconductors. They have shown that (i) $f(x)$ can be represented entirely in terms of the thermal averages of the square of the order parameter and the lateral interaction $\beta_A(\{z_i\})$; (ii) the explicit x dependence arising from the former can be found *exactly*, in effect solving 98% of the problem. Such a physically transparent result appears more attractive for various practical applications, where better accuracy is rarely needed or possible, than the impenetrable numerics of high-order perturbation expansion. On the other hand, one could argue that, as a matter of principle, by going to higher and higher orders in perturbation theory one can ultimately attain accuracy better than 2%. As suggested recently, however, the low-T behavior of the GL-LLL theory cannot be reached by the perturbative expansion.[15] An implication is that this 2% "barrier," associated with lateral correlations, cannot be broken by *any* perturbative procedure, as is discussed in some detail below. In light of this ceiling on the accuracy of standard resummation procedures,[13] devising a simple but comprehensive description of the free energy, which can interpolate with reasonable accuracy between the perturbative limit and the mean-field results below $H_{c2}(T)$, gains additional significance.[16]

In this paper we generalize the nonperturbative method of Ref. 14 to an arbitrary type-II system. To this end, we consider the case of layered superconductors with a variable interlayer coupling. We construct the thermodynamic functions for this case and show that in general there is no single-parameter scaling. Only in two opposite limits, the strong and the weak interlayer coupling, is there such a scaling, corresponding to (an)isotropic 3D and quasi-2D systems, respectively. In these two limits,

closed-form expressions for thermodynamic scaling functions can be obtained. We find the criterion which determines the effective dimensionality of scaling functions. We then compare our results for a 3D system with experimental data of Welp *et al.*[3] and find good agreement. Finally, we discuss the general limits on the applicability of the GL-LLL description of the critical behavior in type-II superconductors.

In strongly type-II superconductors ($\kappa \gg 1$) one can neglect the fluctuations in the magnetic field and the partition function of a general layered system can be written as

$$Z = \prod_n \int_{\mathcal{H}_0} \mathcal{D}\Psi_n(\mathbf{r}) \exp\left[-\frac{d}{T}\sum_n \int d\mathbf{r}\{\tilde{\alpha}|\Psi_n(\mathbf{r})|^2 + \eta|\Psi_{n+1}(\mathbf{r}) - \Psi_n(\mathbf{r})|^2 + \tfrac{1}{2}\beta|\Psi_n(\mathbf{r})|^4\}\right], \quad (1)$$

where n is the layer index; d is of the order of the interlayer separation; $\tilde{\alpha} = \alpha(T)[1 - H/H_{c2}(T)]$; $\alpha(T)$, η, and β are the GL coefficients; $\alpha(T) = \alpha'(T - T_{c0})$; and the functional integral is to be taken over the subspace $\mathcal{H}_0$ spanned by the LLL. The field is perpendicular to the xy plane defined by the layers.

We choose to work in the symmetric gauge, where there is a simple connection between the linear and the nonlinear representations for $\Psi_n(\mathbf{r})$, namely $\Psi_n(\mathbf{r}) = \sum_{m_n=0}^{N} b_{m_n}\varphi_{m_n}(\mathbf{r}) = \Phi_n \prod_{i_n}^{N}(z - z_{i_n})\exp(-|z|^2/4)$,[17] where $\varphi_{m_n}(\mathbf{r})$ are the LLL eigenfunctions in the symmetric gauge, N is the area of the system in units of $2\pi\ell^2$, $z = (x + iy)/\ell$ is a complex coordinate in the xy plane, and ℓ is the magnetic length corresponding to charge $2e$: $\ell \equiv \sqrt{c/2eH}$.[18] The free-energy functional in (1) can be rewritten as follows:

$$F[\Psi_n(\mathbf{r})] = 2\pi\ell^2 N d \sum_n \left[\tilde{\alpha}\overline{|\Psi_n|^2} + \eta\overline{|\Psi_{n+1} - \Psi_n|^2} + \frac{\beta}{2}\overline{|\Psi_n|^4}\right]. \quad (2)$$

The bar denotes a spatial average in the xy plane. The quartic term can now be expressed as $\overline{|\Psi_n|^4} \equiv |\Phi_n|^4\overline{f_n^4} = |\Phi_n|^4\beta_A(\{z_{i_n}\})\left(\overline{f_n^2}\right)^2 = \beta_A(\{z_{i_n}\})\overline{|\Psi_n|^2}^2$ where $\beta_A(\{z_{i_n}\}) \equiv \overline{f_n^4}/\left(\overline{f_n^2}\right)^2$ is the generalized Abrikosov parameter for the nth layer and $\overline{f_n^p}(\{z_{i_n}\}) \equiv \int(dzdz^*/2\pi N)\exp(-p|z|^2/4)\prod_{i_n}|z - z_{i_n}|^p$. The correlations among $\{z_{i_n}\}$ in the nth layer enter only through β_A since the quadratic terms exhibit the exact macroscopic degeneracy of the LLL. As argued above, these correlations are weak with only collapsed or exploded $\{z_{i_n}\}$ leading to significant changes in β_A. A reflection of the presence of $\beta_A(\{z_{i_n}\})$ in (2) will be the dependence of the free energy on the thermodynamic average $\langle\beta_A\rangle$. It is the variation of this average value through the critical region which will be treated approximately in the present approach. $\langle\beta_A\rangle$ must be chosen to interpolate smoothly between its high-T [far above $H_{c2}(T)$] limit, $\langle\beta_A\rangle = 2$, and the low-$T$ [far below $H_{c2}(T)$] value for the Abrikosov lattice, $\beta_A = 1.159$. This is necessary in order to properly join the perturbation theory results in the high-T limit with the low-T mean-field behavior. The variation of $\langle\beta_A\rangle$ between these two limits is slow (actually, the relevant variation is that of $U \equiv 1/\sqrt{\langle\beta_A\rangle}$, which is even slower) and can be accounted for in a relatively straightforward manner as long as one is content with the 98% level of accuracy. Consequently, our most important task can be defined as expressing the thermodynamic functions in the critical region as accurately and completely as possible in terms of this slowly varying function $U(H,T)$, namely expressing the free energy in the form $F(H,T) = F[H,T,U(H,T)]$. If this is done, it effectively means that we have solved the rapidly changing part of the thermodynamics contained in the explicit T and H dependence, all our ignorance now residing in the several percent fraction of slowly varying $U(H,T)$. As we will show below, this can be accomplished virtually exactly in quasi-2D systems and to a very good approximation in 3D.

We will proceed toward this goal in the following way: By employing the nonlinear representation of $\Psi(\mathbf{r})$ introduced above we will use the $1/N$ expansion, where N is the total number of states in the LLL manifold, to perform the integral over the overall amplitude of the order parameter in the partition function.[17] In this way we recover the crossover to the low-T saddle point which controls the thermodynamics in the critical region and which is beyond reach of perturbative expansions. This step leads to the desired expression for the free energy in which the rapid (H,T) dependence is accounted for. We will then suggest an interpolation formula for $\langle\beta_A\rangle$ to approximate the slow part of the (H,T) dependence. We should reflect here on an important aspect of the physics described by (1) which makes the 98–2 % procedure meaningful. Let us generalize our discussion to a layered system in $2 + D_{\|}$ dimensions, by adding weak Josephson coupling between the layers in $D_{\|}$ directions "along" the field. For $D_{\|} > 2$ this model has a phase transition to a superconducting state generated entirely by the longitudinal (along the field) correlations. The rapid variation of various thermodynamic quantities through the nominal critical region in 2D and 3D ($D_{\|} = 0, 1$) arises therefore as a remnant of this true superconducting transition present for $D_{\|} > 2$. This is the part of the problem which we solve exactly. The remaining 2% arises from the effect of lateral correlations. When such correlations are treated exactly they will now produce a phase transition in 2D and 3D, but only far below the nominal critical region, once the thermodynamic functions have saturated to their low-T values.[17] The study of this transition is beyond the scope of this paper since we are here interested only in the "smooth" part of the thermodynamic and clearly cannot deal with any nonanalytic behavior. We should mention here that this transition arises solely through those weak lateral correlations contained in the "2%" part of $\beta_A(\{z_i\})$. The transition is commonly referred to in the literature as the "vortex melting" phase transition separating the "vortex liquid" from the "vortex solid" phase. Actually, the low-temperature phase of the GL-LLL theory is really better

described as a form of a charge density wave, in which the density of Cooper pairs becomes spatially modulated.[15] This description is more in line with reality: Slightly below the transition $\{z_i\}$ still move all over the xy plane and have infinite root-mean-square displacements. It is only the density of zeros and consequently $\langle|\Psi(\mathbf{r})|^2\rangle$ that is weakly modulated.

Our philosophy explained, there is now one question remaining to be addressed before we proceed with explicit calculations: How well does the 98–2 % method actually work in practice? One way of finding out is to compare thermodynamic functions derived by using this rule to the experimentally determined ones. At least in the case of quasi-2D systems the results obtained appear to be in very good agreement with experimentally observed magnetization and specific heat scaling functions.[14,6,7] Furthermore, there are now several Monte Carlo studies of the 2D case available[19–22] which enable direct comparison of the 98–2 % results with the numerically exact solution of the GL-LLL theory (1). Since such comparison does not involve uncertainties inherent to experiments it is particularly valuable in assessing the usefulness of the 98–2 % procedure. We now continue along the lines discussed in Ref. 14 and derive the exact expression for the free energy of the 2D GL-LLL theory having the required form $F[H,T,U(H,T)]$. In a 2D system η is set to zero and we drop the layer index. Using the nonlinear representation of $\Psi(\mathbf{r})$, the GL-LLL partition function (1) can be expressed as[17]

$$Z=\prod_i\int\frac{dz_i dz_i^*}{2\pi N!}\int d\Phi d\Phi^*\prod_{i<j}|z_i-z_j|^2[\Phi\Phi^*]^N \times\exp\left[-\frac{2\pi\ell^2 Nd}{T}\left(\tilde{\alpha}|\Phi|^2\overline{f^2}+\frac{\beta}{2}|\Phi|^4\overline{f^4}\right)\right]. \quad (3)$$

It is useful here to rescale $|\Phi|^2\to|\Phi|^2/\sqrt{\overline{f^4}}$ and to introduce a new variable, U, by inserting an additional integral, $1\equiv\int dU\delta(\frac{\overline{f^2}}{(\overline{f^4})^{1/2}}-U)$, in the partition function (3). In this way we obtain

$$Z=\int d\Phi d\Phi^*[\Phi\Phi^*]^N\int dU \times\exp\left[-\frac{2\pi\ell^2 Nd}{T}\left(\tilde{\alpha}|\Phi|^2U+\frac{\beta}{2}|\Phi|^4\right)\right] \times\prod_i^N\int\frac{dz_i dz_i^*}{2\pi N!}(\overline{f^4})^{-N/2}\prod_{i<j}^N|z_i-z_j|^2 \times\delta\left(\frac{\overline{f^2}}{(\overline{f^4})^{1/2}}-U\right). \quad (4)$$

If we now (formally) perform the integration over $\{z_i\}$ in Eq. (4) the partition function will be expressed entirely as an integral over the complex variable Φ and the real variable U. In the thermodynamic limit, which is equivalent to the limit $N\to\infty$, the integration over Φ and U can be done following the method of steepest descents. A careful reader will recognize here some resemblance to the familiar vector $1/N$ expansion. After all, the quadratic terms in the GL-LLL theory are exactly degenerate. There are, however, at least two very important differences: First, the quartic term is not degenerate on the LLL manifold, as evidenced by the presence of the additional variable, U, in the partition function. Second, we are not using the $1/N$ expansion in an ordinary sense, to systematically evaluate corrections to the leading, saddle-point, results. Actually, we are only interested in the leading order results, since that is all that matters in the thermodynamic limit. Therefore, the integration over Φ and U can be performed by picking up the saddle-point contribution, i.e., by retaining only the values of Φ and U which maximize the integrand. These values then determine the thermodynamic averages of Φ and U, as well as the free energy and in turn all other thermodynamic functions. The key feature for our purposes is that this saddle-point integration over Φ can be performed exactly and therefore the free energy can be expressed in terms of U only, plus the explicit T and H dependence. [This point also follows directly from the "dense vortex plasma" (DVP) representation of the partition function (1) for an individual layer introduced in Ref. 17.] The free energy is then written in the scaling form $F(T,H)=d\phi_0 THf(At)$, where $t=[T-T_c(H)]/(TH)^{\frac{1}{2}}$ is the conventional scaling variable, ϕ_0 is the superconducting flux quantum, and A is a constant specified below. The scaling function for the free energy is

$$f(g,U)=-\frac{1}{2}g^2U^2+\frac{1}{2}gU\sqrt{g^2U^2+2} +\sinh^{-1}(gU/\sqrt{2})-s(U), \quad (5)$$

where $g=\tilde{\alpha}\sqrt{2\pi\ell^2 d/2\beta T}\equiv At$, $A=\alpha'(\phi_0 d/2\beta)^{1/2}$, and $s(U)$ is defined as

$$\exp[Ns(U)]\equiv\prod_i^N\int\frac{dz_i dz_i^*}{2\pi N!}(\overline{f^4})^{-N/2}\prod_{i<j}^N|z_i-z_j|^2 \times\delta\left(\frac{\overline{f^2}}{(\overline{f^4})^{1/2}}-U\right) \quad (6)$$

apart from unimportant prefactors. The important effects of lateral correlations are contained in $s(U)$. $f(g)$ depends on g both explicitly and implicitly, through U (remember that $U=1/\sqrt{\langle\beta_A\rangle}$, where $\langle\cdots\rangle$ denotes the thermodynamic average). Thus, we have succeeded in deriving the desired form for the free energy. The explicit dependence on g is the rapidly changing part of the thermodynamics which we have extracted exactly by performing the integral over Φ. The change in U through the critical region is far slower and represents a convenient place to hide our ignorance, as discussed earlier. U as a function of g is determined from the condition that the free energy be at its minimum: $\partial f/\partial U=0$. From (5) all other thermodynamic scaling functions can be evaluated by taking appropriate derivatives. The two most important ones are magnetization and specific heat:

$$\frac{M(H,T)}{\sqrt{HT}}\frac{d\phi_0 H'_{c2}}{A}=gU^2-U\sqrt{g^2U^2+2}, \quad (7)$$

$$C(H,T)\frac{d\phi_0}{2TA^2} = \frac{1}{2}\left(1 - \frac{gU}{\sqrt{g^2U^2+2}}\right) \times \left[U^2 + (\sqrt{g^2U^2+2} - gU)\left|\frac{dU}{dg}\right|\right], \tag{8}$$

where $H'_{c2} = |dH_{c2}/dT|$ at $T = T_{c0}$. These expressions are the same as the ones obtained in Ref. 14 except for the last term in (8) containing $|dU/dg|$ which was neglected as a small correction. Note that $|dU/dg|$ was eliminated from the expression for $M(H,T)$ by using the condition that the free energy be at its minimum. We should further observe that the expression for $M(H,T)$ is exact while the one for $C(H,T)$ displays only the most relevant contributions [the full expression is easily obtained directly from $f(g)$].

In the above equations $s(U)$ (6) is unknown and thus we cannot determine $U(g)$ which is needed in expressions for $M(H,T)$ and $C(H,T)$. This comes as no surprise since finding $s(U)$ is equivalent to solving the thermodynamics of the DVP many-body problem exactly. But, it is here that we can turn the problem around. As proposed by Tešanović *et al.*, while we do not know $s(U)$, we know enough about $U(g)$ to solve the 98% part of the problem. First, in the perturbative regime ($g \gg \sqrt{2}$) $U \to 1/\sqrt{2} = 0.707$. In the opposite, non-perturbative limit ($g \ll -\sqrt{2}$), U, by definition (6), must approach its value for a triangular lattice, i.e., $U \to 1/\sqrt{1.159} = 0.928$. Thus, U changes relatively little between these two limits. This change should be monotonic and most of it should take place over the interval $g \in [-\sqrt{2}, \sqrt{2}]$ characterizing the nominal width of the critical region. Furthermore, the interactions in the DVP start growing for $g < -\sqrt{2}$, forcing U toward 0.928. (Discussion of different regimes of the DVP can be found in Ref. 17.) This suggests the following simple interpolation formula:

$$U(g) \cong 0.818 - 0.110 \times \tanh\left(\frac{g+\sqrt{2}}{2\sqrt{2}}\right). \tag{9}$$

The above expression should be a good approximation to the "smooth" part of U. It also, indirectly, provides an approximate form of $s(U)$, which can now be reconstructed by starting from Eq. (9) and working backwards from the $\partial f/\partial U = 0$ condition. When (9) is combined with Eqs. (5)–(8), it gives an analytic, closed-form, parameter-free description of the thermodynamic scaling functions for quasi-2D systems.[23]

It was already demonstrated in Ref. 14 that Eq. (7) agrees well with the measured magnetization of $Bi_2Sr_2Ca_2Cu_3O_{10}$. In particular, Eq. (7) provides a theoretical explanation for the experimentally observed crossing point, i.e., the temperature T^* at which magnetization is effectively independent of the field. Here we make use of some recent Monte Carlo numerical simulations to test the 98–2% expression for the specific heat (8). Specific heat, being the second derivative of the free energy, is a more stringent test of the method. In Fig. 1 we compare the analytic expression for $C(H,T)$ (8) and (9) with the Monte Carlo result of Ref. 20. (Similar results for specific heat have also been obtained in the Monte Carlo simulations of Ref. 21.) The agreement is very good demonstrating that the 98–2% procedure lives up to its name. Clearly, the agreement can be further improved by including some fitting parameters in the interpolation formula (9) or by devising a more accurate analytic expression for $U(g)$. Moreover, one could simply use $U(g)$ determined in a Monte Carlo simulation instead of the approximate form (9) as an input to Eqs. (5)–(8), resulting in virtually exact thermodynamics. An efficient way of doing this would be to combine the Monte Carlo data for $M(H,T)$ and Eq. (7) to extract $U(g)$, which can then be used in the specific heat and other thermodynamic functions. While such improvements would be useful they should still all lead to similar results at the 98% level as long as they are in agreement with the general properties of $U(g)$ outlined above Eq. (9). This is the basic message of the 98–2% method: Once we have succeeded in deriving $F(H,T,U)$ (5) the problem is as good as solved for most practical applications. It would take a determined effort to construct a physically plausible interpolation formula for $U(g)$ which makes the thermodynamic functions deviate from the exact solution by more than a few percent.

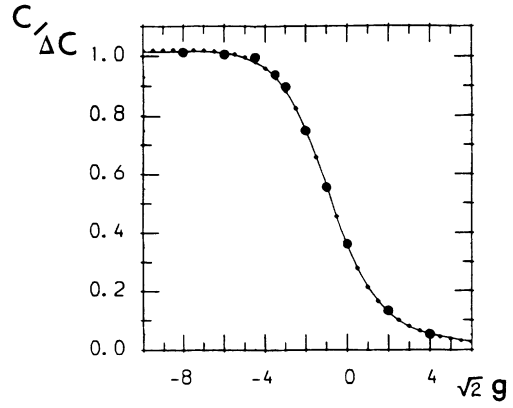

FIG. 1. The line with small dots represents the specific heat of the 2D GL-LLL model obtained in the numerical Monte Carlo simulation of Ref. 20 and normalized to the mean-field value, ΔC. Full black circles are evaluated from Eqs. (8) and (9).

It is appropriate at this point to comment on the relationship of our 98–2% method to other procedures for evaluation of thermodynamic functions, most of which are based on high-order perturbative expansions.[13] The perturbation theory, of course, makes no distinction between the explicit and the implicit (through U) g dependence manifested in our key results, Eqs. (5)–(8). One simply obtains $f(g)$ to a given order in $1/g^2$, in the perturbative limit $g \gg \sqrt{2}$. Various procedures utilizing Padé approximants are then employed to obtain $f(g)$ over the full range of g. The principal effort is therefore needlessly expended on obtaining the rapid variation of thermodynamic functions, the part of the problem that can be treated exactly. What is an interesting issue here is whether the perturbation theory can do a better job of treating the remaining lateral correlations, i.e., of calculating $s(U)$ (6). Just by looking at Eq. (6), whose

menacing appearance suggests that $s(U)$ is likely beyond reach of any perturbative scheme, one is tempted to give a negative answer. Let us nevertheless consider a relatively simple point concerning the limiting low-T result for $U(g)$, or $\langle\beta_A\rangle$, as obtained from a typical perturbative procedure.[13] The exact result is $\langle\beta_A\rangle \to 1.159$. There is nothing in the perturbative procedure outlined above which forces $\langle\beta_A\rangle$ to have this value in the low-T limit. (This statement is supported by the results of Brézin *et al.*,[13] who argued that $\langle\beta_A\rangle$ does not approach the correct low-T value even at arbitrary high orders in the perturbation theory.) In fact, depending on how high one goes in the perturbative expansion and which particular approximants one uses, $\langle\beta_A\rangle$ takes a series of different values within several percent of 1.159.[13] For example, the 11th-order expansion used by Hikami *et al.*[13] gives $\langle\beta_A\rangle = 1.159 \pm 0.03$, which appears as a particularly good result considering the said uncertainty. Actually, it is not. The above error bars of ± 0.03 arise naturally within the perturbative procedure. But, it is impossible for $\langle\beta_A\rangle$ to have a value less than 1.159 within the Hilbert space of the GL-LLL theory. Furthermore, this uncertainty of $\sim 2\%$ is the whole story. This is the full "dispersion" of lateral correlations. For $\langle\beta_A\rangle = 1.159$ one has a perfect triangular lattice of $\{z_i\}$ whereas for $\langle\beta_A\rangle \simeq 1.19$ one is already in the liquid state.[19–22] This $\sim 2\%$ uncertainty is conjectured to be inherent to any perturbative procedure.[15] It is due to an impossibility of enforcing the LLL constraint at any finite order in the perturbation theory. Therefore, the perturbative methods cannot be used to accurately account for the effects of lateral correlations which are essentially tied to this constraint. In contrast, the nonperturbative method of Ref. 17 used throughout this paper naturally enforces the LLL constraint. For example, it is obvious from the definition of $s(U)$ (6) that $U \to 1/\sqrt{1.159}$ in the low-T limit. The interpolation formula for $U(g)$ (9) simply incorporates this fact. We should finally observe that the high-order perturbative expansion, if augmented (entirely by hand) by the external condition requiring $\langle\beta_A\rangle \to 1.159$ in the low-T limit, will also provide a good description (albeit unnecessarily complicated and entirely numerical) of the 98% of the thermodynamics.

The above detailed discussion of the 2D case gives us confidence in the accuracy of our procedure and we will now proceed to use it with impunity in the study of general layered systems. It is important to recognize that there is no reason to expect the 98–2 % procedure to be any more or less justified in layered or 3D systems than it is in 2D. The lateral correlations in all cases should account only for several percent of the answer. Just how good the approximation will be can only be answered *a posteriori*, by comparison to experiments and numerical simulations. All we can say in advance is that in layered systems with weak interlayer coupling we expect the 98–2 % method to work as well as in 2D.

We now turn to the case of a general layered system. The variables in (1) are rescaled as follows: $r \to \sqrt{2\pi\ell^2}r$, $\Psi_n \to (2\pi\ell^2 d 2\beta/T)^{-1/4}\Psi_n$. Introducing new dimensionless coupling constants $g = \tilde{\alpha}\sqrt{2\pi\ell^2 d/2\beta T}$ and $g_\eta = \eta\sqrt{2\pi\ell^2 d/2\beta T}$ we obtain

$$\frac{F}{T} = \sum_n \int d\mathbf{r}\Big[g|\Psi_n(\mathbf{r})|^2 + g_\eta|\Psi_{n+1}(\mathbf{r}) - \Psi_n(\mathbf{r})|^2 + \frac{1}{4}|\Psi_n(\mathbf{r})|^4\Big]. \quad (10)$$

It is clear from the above expression that there is no single-parameter scaling in this general case. Various thermodynamic quantities depend on two different coupling constants, g and g_η. Only if g_η is very small or very large will a single-parameter scaling be restored corresponding to 2D and 3D cases, respectively. Whether one should use the quasi-2D or the 3D scaling forms or simply use general expressions obtained from (10) depends on material parameters as well as on where one is in the H-T phase diagram. It would be useful to have a criterion which can tell us what is the effective dimensionality of the scaling functions. Such a criterion can be formulated in the following way: We make the replacement $\overline{|\Psi_n|^4} \to \langle\beta_A\rangle(\overline{|\Psi_n|^2})^2$ directly in the free-energy functional (10). In this way the lateral correlations have been completely eliminated from the problem, and, naturally, the resulting model describes different physics than the original GL-LLL theory. The interesting point, however, is that the quartic interaction term is now also degenerate on the LLL manifold. Therefore, we have obtained a 1D layered version of the $O(2N)$ vector model, which can be solved exactly by the $1/N$ expansion. Observe that this vector model gives the same results as the Hartree-Fock approximation but with $\langle\beta_A\rangle$ set to its true thermodynamic value instead of $\langle\beta_A\rangle = 2$. We will now make an assumption that the *longitudinal* correlations of this vector model represent a good approximation to the *longitudinal* correlations of the GL-LLL theory in the critical region. Note that this assumption will not be true far below the nominal critical region, near and below the phase transition of the GL-LLL theory. Since the vector model can be solved exactly we will use the dimensionality criterion for this model as a good substitute for the same criterion in the GL-LLL theory.

After the above replacement has been made we rescale Ψ_n by $\sqrt{U}$ and obtain the resulting 1D layered $O(2N)$ vector model

$$\frac{F}{T} = \sum_n \int d\mathbf{r}\Big[\Big(gU + \frac{1}{2}\langle\overline{|\Psi|^2}\rangle\Big)|\Psi_n(\mathbf{r})|^2 + g_\eta U|\Psi_{n+1}(\mathbf{r}) - \Psi_n(\mathbf{r})|^2\Big] - \sum_n \frac{N}{4}(\langle\overline{|\Psi|^2}\rangle)^2. \quad (11)$$

We expand the order parameter as $\Psi_n(\mathbf{r}) = \sum_{m,k}\frac{1}{\sqrt{N_\zeta}}\exp(ikn)\varphi_m(\mathbf{r})b_{mk}$, where $\varphi_m(\mathbf{r})$ is a normalized LLL function and N_ζ is the number of layers in the system. The free-energy functional of our vector model is then expressed as follows:

$$\frac{F}{T} = \sum_{m,k}\{[gU + \tfrac{1}{2}\langle\overline{|\Psi|^2}\rangle + 2g_\eta U\sin^2(k/2)]|b_{mk}|^2\} - \frac{NN_\zeta}{4}(\langle\overline{|\Psi|^2}\rangle)^2. \quad (12)$$

From here we find

$$\langle|b_{mk}|^2\rangle = \frac{1}{gU + \frac{1}{2}\langle\overline{|\Psi|^2}\rangle + 2g_\eta U \sin^2(k/2)} \quad . \tag{13}$$

The self-consistency equation reads

$$\langle\overline{|\Psi|^2}\rangle = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{1}{gU + \frac{1}{2}\langle\overline{|\Psi|^2}\rangle + 2g_\eta U \sin^2(k/2)} = \frac{1}{\sqrt{(gU + \frac{1}{2}\langle\overline{|\Psi|^2}\rangle)(gU + \frac{1}{2}\langle\overline{|\Psi|^2}\rangle + 2g_\eta U)}} \quad . \tag{14}$$

This can be rewritten as

$$\langle\overline{|\Psi|^2}\rangle^2 \left(gU + \frac{\langle\overline{|\Psi|^2}\rangle}{2}\right)\left(gU + \frac{\langle\overline{|\Psi|^2}\rangle}{2} + 2g_\eta U\right) = 1 \quad . \tag{15}$$

This is a quartic algebraic equation whose solution gives $\langle\overline{|\Psi|^2}\rangle$ as a function of g and g_η. We can use (15) to devise the criterion for effective dimensionality of the GL-LLL theory. In the limit $g_\eta \to 0$, Eq. (15) becomes the self-consistency condition of the 0D $O(2N)$ vector model. Thus, provided $gU + \langle\overline{|\Psi|^2}\rangle/2 \gg 2g_\eta U$ is satisfied, we can use a quasi-2D version of the GL-LLL theory and the corresponding 2D scaling functions. If, on the other hand, $gU + \langle\overline{|\Psi|^2}\rangle/2 < 2g_\eta U$, an anisotropic homogeneous GL-LLL description becomes appropriate with the 3D single-parameter scaling. In all other cases we must use the general model (10). The above dimensionality criterion is easily recast into the more familiar form, comparing the effective superconducting correlation length, $\xi_\zeta(T,H) = d\sqrt{2g_\eta U/(gU + \langle\overline{|\Psi|^2}\rangle/2)}$, to the interlayer separation, d. Note that ξ_ζ remains finite throughout the critical region, even below $H_{c2}(T)$.

Let us first consider the case of a homogeneous, (an-)isotropic superconductor, which is the other example of the single-parameter scaling. For this description to be applicable we must have $g_\eta U > gU + \langle\overline{|\Psi|^2}\rangle/2$, as explained above. The free-energy functional is obtained from (1) by taking the limit of strong interlayer coupling, $g_\eta \to \infty$, expanding $\sin^2(k/2)$ and keeping only the leading k^2 term. The partition function can be written as

$$Z = \int_{\mathcal{H}_0} \mathcal{D}\Psi(\mathbf{r},\zeta) \exp\left[-\frac{1}{T}\int d\mathbf{r}\int d\zeta\{\tilde{\alpha}|\Psi(\mathbf{r},\zeta)|^2 + \gamma|\partial_\zeta\Psi(\mathbf{r},\zeta)|^2 + \tfrac{1}{2}\beta|\Psi(\mathbf{r},\zeta)|^4\}\right], \tag{16}$$

where $\tilde{\alpha} = \alpha(T)[1 - H/H_{c2}(T)]$; $\alpha(T)$, γ, and β are now the 3D versions of the GL coefficients; $\alpha(T) = \alpha'(T - T_{c0})$; ζ is the coordinate along $\mathbf{H}$ and the functional integral is again restricted to the subspace $\mathcal{H}_0$ of the LLL. We will employ here the continuous version of the nonlinear representation for $\Psi(\mathbf{r},\zeta)$, namely $\Psi(\mathbf{r},\zeta) = \Phi(\zeta)\prod_i[z - z_i(\zeta)]\exp(-|z|^2/4)$. This form enables us to take advantage of the LLL degeneracy, through the $1/N$ expansion discussed previously. With these new variables the partition function (16) becomes

$$Z = \prod_i \int \frac{\mathcal{D}z_i(\zeta)}{N!} \int \mathcal{D}\Phi(\zeta) \prod_\zeta \prod_{i<j} |z_i(\zeta) - z_j(\zeta)|^2 \times [\Phi(\zeta)\Phi^*(\zeta)]^N \exp\left[-\frac{2\pi\ell^2 N}{T}\int d\zeta\left(\tilde{\alpha}|\Phi(\zeta)|^2\overline{f^2(\zeta)} + \gamma\overline{|\partial_\zeta[\Phi(\zeta)f(\zeta)]|^2} + \frac{\beta}{2}|\Phi(\zeta)|^4\overline{f^4(\zeta)}\right)\right], \tag{17}$$

where the functional integrals, $\prod_\zeta$, ∂_ζ, etc., are all defined on a set of discrete intervals of size Λ. Formally, at the end of the calculation, the limit $\Lambda \to 0$ is to be taken in all final results. This limit, however, is not entirely trivial and will be discussed shortly. It is convenient to recast (17) in a dimensionless form by rescaling $z \to \sqrt{2\pi}\ell z$, $\zeta \to \Lambda\zeta$, $\Phi \to (2\pi\ell^2\Lambda 2\beta/T)^{-1/4}\Phi$:

$$Z = \int \mathcal{D}\Phi(\zeta)\int \mathcal{D}U(\zeta)\int \mathcal{D}\Gamma(\zeta)\int \mathcal{D}W(\zeta)\exp\left[-N\int d\zeta\left(-\ln|\Phi(\zeta)|^2 + g|\Phi(\zeta)|^2 + g_\zeta|\Phi(\zeta)|^2\Gamma(\zeta) + g_\zeta|\partial_\zeta\Phi(\zeta)|^2 + g_\zeta\Phi^*(\zeta)[\partial_\zeta\Phi(\zeta)]W(\zeta) + (\text{c.c.}) + \frac{1}{4U^2(\zeta)}|\Phi(\zeta)|^4 - s[U(\zeta),\Gamma(\zeta),W(\zeta)]\right)\right] \equiv \int \mathcal{D}\Phi(\zeta)\int \mathcal{D}U(\zeta)\int \mathcal{D}\Gamma(\zeta)\int \mathcal{D}W(\zeta)\exp\left[-N\int d\zeta f[\Phi(\zeta),U(\zeta),\Gamma(\zeta),W(\zeta)]\right], \tag{18}$$

where $g = \tilde{\alpha}(T)\sqrt{2\pi\ell^2\Lambda/2\beta T}$, $g_\zeta = (\gamma/\Lambda^2)\sqrt{2\pi\ell^2\Lambda/2\beta T}$, and we have introduced $s[U,\Gamma,W]$ as

$$\exp N\int d\zeta s[U(\zeta),\Gamma(\zeta),W(\zeta)] \equiv \prod_i \int \frac{\mathcal{D}z_i(\zeta)}{N!}\exp\int d\zeta\left[-\frac{1}{2}N\ln\overline{f^4(\zeta)} + 2\sum_{i<j}\ln|z_i(\zeta) - z_j(\zeta)|\right] \times \prod_\zeta \delta\left(\frac{\overline{f^2(\zeta)}}{\sqrt{\overline{f^4(\zeta)}}} - U(\zeta)\right)\delta\left[\left|\partial_\zeta\left(\frac{f(\zeta)}{\sqrt{\overline{f^2(\zeta)}}}\right)\right|^2 - \Gamma(\zeta)\right]\delta^{(2)}\left[\frac{f(\zeta)}{\sqrt{\overline{f^2(\zeta)}}}\partial_\zeta\left(\frac{f^*(\zeta)}{\sqrt{\overline{f^2(\zeta)}}}\right) - W(\zeta)\right]. \tag{19}$$

In the limit $N \to \infty$ (which is associated with the thermodynamic limit) the functional integration over $\Phi(\zeta)$, $U(\zeta)$, $\Gamma(\zeta)$, and $W(\zeta)$ can be carried out in the saddle-point approximation by the method of steepest descents. Only the configuration which minimizes $f[\Phi, U, \Gamma, W]$ contributes to the partition function. Such configuration is found by taking the functional derivatives of f with respect to all of its arguments, setting the derivatives equal to zero and solving the resulting system of functional equations. Again, as in 2D, this is not possible in general since we do not know the functional $s[U, \Gamma, W]$. However, the plausible *ansatz* for this solution is that $W(\zeta) = 0$ and Φ, U, and Γ are uniform. After minimizing $f[\Phi, U, \Gamma, W = 0]$ with respect to Φ (which again can be done since s does not depend on it) we obtain the free energy $F(H,T) = NL_z f(g, U, \Gamma)$, where

$$f(g,U,\Gamma) = -\frac{1}{2}G^2U^2 + \frac{1}{2}GU\sqrt{G^2U^2+2} + \sinh^{-1}(GU/\sqrt{2}) - s(U,\Gamma) \qquad (20)$$

and $G \equiv g + g_\zeta \Gamma$. f depends on g explicitly and implicitly, through U and Γ. Also, note that the $\ln U$ term produced by integration over Φ has been absorbed in $s(U,\Gamma)$.

The rapid change in the thermodynamic quantities taking place in the critical region is again due to the change in Φ, which we were able to integrate out exactly. The changes in U and Γ are comparatively far slower and we can account for them in some average way. The question of U is straightforward, just like in the 2D case. However, when trying to construct the interpolation formula for Γ, which describes the average bending of $\{z_i(\zeta)\}$, one encounters an unpleasant snag: The exact free energy (20) is actually divergent in the $\Lambda \to 0$ limit. This is a standard ultraviolet divergence which has nothing to do with type-II superconductors. It is a general property of the GL-type functionals. The gradient terms are simply unable to prevent highly nonuniform configurations from contributing to the partition function. While such terms cost considerable energy, the entropy gained is much higher causing the said divergence. Actually, in the GL-LLL theory this divergence is milder than in the zero-field GL theory in the same number of dimensions. This is because the LLL constraint regularizes the theory in the xy plane leaving only the gradients along $\mathbf{H}$ to do the damage. [The divergence will arise from $s(U,\Gamma)$ which is unbounded for $\Gamma \to \infty$.] Of course, this divergence is only a mathematical nuisance since in condensed matter physics there are no ultraviolet divergences: It simply indicates that final results depend on some short lengthscale which serves as a natural cutoff and which should arise from the full theory in which the nonlocality is fully included instead of being treated by the gradient expansion.[24] We will discuss this point again shortly. For now we observe that the shortest lengthscale in the problem is the interlayer separation and/or lattice spacing of the underlying crystalline structure. Clearly, Λ cannot be smaller than this lattice spacing. Still, the choice of Λ requires some care and it contains physical information. For example, setting Λ to equal the interlayer separation is a wrong choice if one is interested in an effectively 3D system (of course, it is the right choice for a quasi-2D system). If we do that we will include those configurations in the partition function which are really a part of the "normal" electronic background and which cannot be described by the GL-like free-energy functional. In fact, in problems of this kind the cutoff is typically chosen to equal the BCS coherence length. Still, within the GL-LLL theory even this choice is not appropriate. If the BCS coherence length is used as a cutoff the resulting free energy will not have a single-parameter scaling. This is the consequence of including in the entropy the configurations whose energy is actually higher than the cyclotron gap: Such configurations have been integrated out in the GL-LLL theory. Therefore, the proper choice for the cutoff in the GL-LLL theory must respect the fact that we are restricting ourselves to only those configurations of $\Psi(\mathbf{r}, \zeta)$ whose "kinetic" energy along the ζ axis is at most of the order of the cyclotron gap. With such a choice, the free energy (20) will generically obey a single-parameter scaling (G will be a function of g only) and will represent a genuine LLL contribution, while the contributions to the free energy arising from higher LL's, together with everything else, form a slowly varying background. In essence, to within factors of order unity, this will lead to Λ being equal to the true (not mean-field) superconducting correlation length perpendicular to the layers, ξ_ζ. Throughout the nominal critical region this correlation length remains finite and can be quite short, even below $H_{c2}(T)$. Only far below $H_{c2}(T)$, as one is approaching the phase transition, can this correlation length become very long. This regime, however, does not concern us in this paper.

The role of Λ clarified, we now specify U and Γ. U again changes from $1/\sqrt{2}$ far above $H_{c2}(T)$ to 0.928 far below $H_{c2}(T)$. We therefore again resort to our simple interpolation formula

$$U(g) \cong 0.818 - 0.110 \times \tanh\left(\frac{G+K}{M}\right), \qquad (21)$$

where K and M can be used as fitting parameters, but, for simplicity, we can still take $K \sim \sqrt{2}$ and $M \sim 2\sqrt{2}$, just like in 2D (note, however, that the coupling constant g is different). We see that now U is actually a function of $G = g + g_\zeta \Gamma$ and is thus defined through Γ. This choice of $U(g)$ is dictated by the fact that lateral correlations arise through the quartic term of the GL-LLL theory and their strength should therefore be a function of the size of $|\Phi|^2$ which itself is given by G. Γ starts from $\sim (\tilde{\alpha}/\gamma)$ (in dimensionful form) far above $H_{c2}(T)$ and is ultimately driven to zero for $T \to 0$. This change is expected to be smooth and slow through the critical region. In this paper, we adopt a simple choice for Γ, based on our expectation that the longitudinal correlations of the GL-LLL theory are not very different from the those of the vector model (11), as long as one is in the neighborhood of the nominal critical region. In this vector model (11) Γ can be easily calculated:

$$g_\zeta \Gamma = \frac{Q - \tan^{-1} Q}{2\tan^{-1} Q}\left[g + \sqrt{g^2 + \frac{\tan^{-1} Q}{\pi U^2}}\right], \qquad (22)$$

where Q is a number corresponding to the cutoff in the k space along the ζ axis, in units of Λ. This number should not be too different from π but otherwise can be adjusted at will, reflecting the unfortunate and unavoidable dependence of thermodynamics on the ultraviolet cutoff. Λ itself is given by

$$\Lambda^{\frac{3}{2}} = 2\gamma\sqrt{\frac{2\pi\ell^2}{2\beta T}}\left[g+\sqrt{g^2+\frac{\tan^{-1}Q}{\pi U^2}}\right]^{-1} . \tag{23}$$

The reader should be reminded here that Λ is, within factors of order unity, equal to the superconducting correlation length, ξ_ζ. As stated previously, we are assuming ξ_ζ of the GL-LLL model to be well approximated by the same quantity in the corresponding vector model. Also note that the above expression for Γ (22) involves U which is itself specified through Γ in Eq. (21). Therefore, Eq. (21) is actually a rather complicated implicit expression for $U(g)$. Often, in view of the overall accuracy of the 98–2% method, such complications will be unnecessary and one can simply set $U \sim 0.8$ wherever it appears on the right-hand side of (21). This gives us a simple expression for $U(g)$ which is then used in Eq. (22) to determine $\Gamma(g)$. The expression for Λ in terms of g can now be used to derive the relation between g and the conventional 3D scaling variable, $t \equiv [T-T_c(H)]/(HT)^{\frac{2}{3}}$:

$$g\left[g+\sqrt{g^2+\frac{\tan^{-1}Q}{\pi U^2}}\right]^{\frac{1}{3}} = Bt, \quad B=\alpha'\left(\frac{\gamma\phi_0^2}{2\beta^2}\right)^{\frac{1}{3}} . \tag{24}$$

This relationship is not as simple as in 2D (where $g \propto t$) because the definition of g contains Λ which itself is a function of g. As discussed earlier, the above expressions are obtained in our basic approximation, which we know is rather good in 2D and quasi-2D layered systems. Obviously, in 3D there is an added uncertainty which enters through correlations between Γ and U contained in $s(U,\Gamma)$, which we have in effect replaced by their average when we used the vector model expression for Γ (22). However, since the most important integration over Φ was again carried out exactly and no rapid changes in Γ are expected in the nominal critical region, our procedure should still be accurate to within several percent.

The free-energy functional in 3D is now written as

$$f(g) = -\frac{1}{2}G^2U^2+\frac{1}{2}GU\sqrt{G^2U^2+2} + \sinh^{-1}(GU/\sqrt{2}) - s'(U) , \tag{25}$$

where

$$G = g+\frac{Q-\tan^{-1}Q}{2\tan^{-1}Q}\times\left[g+\sqrt{g^2+\frac{\tan^{-1}Q}{\pi U^2}}\right],$$

and $U(g)$ is given in (21) [as in 2D, $s'(U)$ can be determined by working backwards from (21)]. All other thermodynamic functions can now be determined by taking appropriate derivatives of $f(g)$. The magnetization, $M(H,T)$, and the specific heat, $C(H,T)$, have the following form:

$$\frac{4\pi MH'_{c2}}{(TH)^{2/3}\alpha'}(4\beta\gamma\phi_0^2)^{1/3} = \left(g+\sqrt{g^2+\frac{\tan^{-1}Q}{\pi U^2}}\right)^{\frac{1}{3}} \times\left[GU^2-U\sqrt{G^2U^2+2}\right] , \tag{26}$$

$$\frac{C}{T}\frac{\beta}{\alpha'^2} = \frac{1}{2}(1+\tfrac{1}{3}gR)^{-1}\left\{\left[U^2-\frac{GU^2}{\sqrt{G^2U^2+2}}\right]\times[1+I(1+gR)] +\frac{R}{3}\left[GU^2-U\sqrt{G^2U^2+2}\right]\right\} , \tag{27}$$

where

$$R\equiv\left(g^2+\frac{\tan^{-1}Q}{\pi U^2}\right)^{-\frac{1}{2}} , \quad I\equiv\frac{Q-\tan^{-1}Q}{2\tan^{-1}Q} .$$

To keep the expression manageable, we have included only the leading derivatives in the specific heat (the terms containing dU/dg and the like have been omitted). We have also expressed all of the thermodynamic functions in terms of the single coupling constant g: The connection between g and the conventional scaling variable t is given by Eq. (24).

In Fig. 2 we compare the above theoretical result for specific heat with recent measurements of Welp *et al.* performed on the Y-Ba-Cu-O system. The reader should note that these authors use a somewhat different scaling form for $C(H,T)$ [they plot $(C/T)H^{1/3}T^{2/3}$ versus the scaling variable t] instead of the 3D form given above. After adjusting for this difference the agreement between

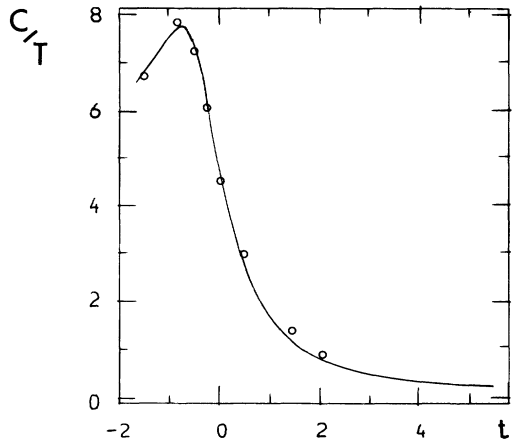

FIG. 2. The open circles are the measured specific heat values of the 1-2-3 Y-Ba-Cu-O system at 70 kG vs the 3D scaling variable, $t=[T-T_c(H)]/(TH)^{2/3}$, as shown in Fig. 4 of Welp *et al.* (Ref. 3). The line is obtained from our Eq. (27). As indicated in the text, 3D scaling is satisfactory near the peak but not farther above the peak testifying to the layered nature of the system.

theory and experiment appears to be rather good. One should note, however, that Y-Ba-Cu-O is a layered system and, while it might behave as an anisotropic 3D superconductor in the low-field region of the H-T phase diagram, the 3D scaling will fail at higher fields. In fact, if one considers all the data of Ref. 3 the agreement with the 3D scaling forms cannot be characterized as very good. This is why we have concentrated on the behavior of $C(H,T)$ near the peak, where the 3D scaling seems to work better. Farther above the peak it appears that the quasi-2D scaling becomes more accurate,[7] reflecting the layered structure of Y-Ba-Cu-O.

If the effective dimensionality is not three according to the criterion derived from (15) but g_η is not very small either, we have the general case in which there is no single-parameter scaling. We can find the expression for the free energy by following the 3D derivation step by step and simply using the discretized version of the ζ dependence in all the variables. In this way we obtain

$$f(g,g_\eta,U,\Gamma) = -\frac{1}{2}G^2U^2+\frac{1}{2}GU\sqrt{G^2U^2+2} + \sinh^{-1}(GU/\sqrt{2}) - s(U,\Gamma), \tag{28}$$

which is exactly the same expression as (20) but now $G \equiv g+g_\eta\Gamma$, g, and g_η are defined above Eq. (10), and $s(U,\Gamma)$ is a discretized version of (19). As before, $U(g,g_\eta)$ and $\Gamma(g,g_\eta)$ are obtained by minimizing the above expression with respect to U and Γ. The magnetization and specific heat are then given by

$$\frac{M(H,T)}{\sqrt{HT}}\frac{d\phi_0 H'_{c2}}{A} = GU^2 - U\sqrt{G^2U^2+2}\quad , \tag{29}$$

$$C(H,T)\frac{d\phi_0}{2TA^2} = \frac{1}{2}\left(1-\frac{GU}{\sqrt{G^2U^2+2}}\right)\left[U^2\left(1+g_\eta\frac{\partial\Gamma}{\partial g}\right)+\left(\sqrt{G^2U^2+2}-GU\right)\left|\frac{dU}{dG}\right|\right]\quad , \tag{30}$$

where again $M(H,T)$ is the exact form and only the leading terms are kept in the expression for $C(H,T)$. We take $U(G)$ to be the same as in Eq. (21). Note that the last term in (30) is the derivative of $U(G)$ with respect to $G \equiv g+g_\eta\Gamma(g,g_\eta)$ (of course, G itself is different than in the 3D case). Finally, $\Gamma(g,g_\eta)$ is specified the same way as in 3D, by connection to the vector model. We have

$$g_\eta\Gamma(g,g_\eta) = \frac{1}{U(G)\langle|\overline{\Psi}|^2\rangle} - g + \frac{\langle|\overline{\Psi}|^2\rangle}{2U(G)}\quad , \tag{31}$$

where $\langle|\overline{\Psi}|^2\rangle$ is the solution of Eq. (15). From (31) one obtains $\Gamma(g,g_\eta,U)$. The fact the Γ and U are coupled can be handled just like in the 3D case, by replacing $U \sim 0.8$ on the right-hand side of Eq. (21), i.e., by using $G = g+g_\eta\Gamma(g,g_\eta,U=0.8)$ in Eq. (21). [See discussion below Eq. (23).] Since there is no single-parameter scaling the whole procedure is now somewhat more complicated and it is probably most efficient to implement numerically by first solving the self-consistency equation (15), then obtaining $\Gamma(g,g_\eta)$ and $U(g,g_\eta)$ from (31) and (21), and finally the free energy (28) and other thermodynamic functions (29) and (30).

Before we conclude it is useful to discuss one general point: All our results have been derived within the GL-LLL theory, which is assumed to describe the critical behavior near $H_{c2}(T)$. While this assumption is both intuitively clear [the reader should be reminded that the Abrikosov mean-field solution near $H_{c2}(T)$ lies entirely in the LLL] and widely used with much quantitative success, it naturally has its limitations and it is useful to spell out explicitly what these are. We start by observing that in the GL-LLL theory we make two different and independent assumptions. One is that a GL-type free-energy functional can be used to describe fluctuations. The other one is that it suffices to focus only on the LLL configurations and that other LL manifolds can be ignored. Let us now discuss the validity of these two assumptions in order: GL first and the LLL second. We will discuss a 2D system in the perpendicular field but our discussion can be readily generalized to a 3D case. The first assumption (GL) is actually somewhat of an illusion. To appreciate this imagine that we start from the original *microscopic* problem of the electrons interacting via some effective attractive interaction. We can write down the formal functional integral expression for the partition function of this system. Then, we can eliminate the electronic fields altogether in favor of the bosonic Hubbard-Stratonovich field which describes Cooper pairs. This is an exact transformation of the original problem and it simply amounts to expressing the partition function, which is the trace of the Boltzmann operator, in a different basis. The integration over the electronic fields generates familiar log determinants in the exponent which makes the resulting bosonic theory rather complicated. However, if we now make the assumption that the overall amplitude of the bosonic field is small we can expand the log determinant and stop at the quartic terms. A rather general description of the critical behavior in a 2D type-II superconductor in a magnetic field is then provided by the partition function of the form

$$Z = \int \mathcal{D}\Psi(\mathbf{r})\exp\left[-\frac{d}{T}\int d\mathbf{r}\int d\mathbf{r}'\left(\Psi^*(\mathbf{r})K_2(\mathbf{r},\mathbf{r}')\Psi(\mathbf{r}') + \frac{1}{2}\int d\mathbf{r}''\int d\mathbf{r}'''\Psi^*(\mathbf{r})\Psi(\mathbf{r}') \times K_4(\mathbf{r},\mathbf{r}',\mathbf{r}'',\mathbf{r}''')\Psi^*(\mathbf{r}'')\Psi(\mathbf{r}''')\right)\right], \tag{32}$$

where K_2 and K_4 are some general nonlocal kernels respecting all the symmetries of the problem and containing all the effects of the external field (the fluctuations in the magnetic field itself can be ignored for strongly type-II systems). The explicit form of these kernels can be derived from the original electronic propagators.[24–27] The only assumption used in (32) is that it is safe to neglect terms which are of higher order in Ψ than quartic and that the quantum fluctuations of Ψ can be ignored. This should be justified in the critical region as long as the Ginzburg fluctuation parameter, θ, is small. It is well known that θ is indeed very small for all interesting superconductors including the high-temperature superconductors (HTS) (although, of course, it is considerably larger in HTS than in most conventional superconductors). It is less known that θ itself can actually be measured directly from the so-called crossing point T^* (see Fig. 3) in the magnetization.[14] The relation between the two is $(T_{c0}-T^*)/T^*=\theta$, where T_{c0} is the *mean-field* transition temperature for $H=0$. T_{c0} itself can be obtained either by fitting the measured magnetization to the expression (7) or by some independent method like the Aslamazov-Larkin fit to the zero-field fluctuation conductivity. The largest θ obtained in this way is found in the Bi(2:2:1:2) system,[5] $\theta \cong 0.045$, which is therefore expected to be the strongest "fluctuator" among HTS. [For comparison, $\theta \cong 0.027$ in Bi(2:2:2:3) and ~ 0.010 in 1-2-3.] This ability to measure θ directly instead of relying on various indirect measurements of coherence length and other parameters is quite significant. It tells us the following: If we assume that the fluctuation behavior can be represented by some Ψ^4 theory then there is basically a single parameter, θ, measuring the strength of fluctuations, the width of the critical region, the size of the higher-order terms dropped in the expansion of the log determinant, and the significance of quantum fluctuations. If we now find that θ is indeed small this makes the whole procedure self-consistent and justifies the approximations made along the way. Consequently, the partition function (32) describes superconducting fluctuations at *any* H and T, as long as one is near $H_{c2}(T)$ and not at very low temperatures. (So that the quantum fluctuations can be ignored—they can be easily included in the GL-LLL theory, if needed.) Of course, this does not mean that one should use (32) religiously in all circumstances: For example, the physics at energy scales higher than the BCS condensation energy ($\sim \sqrt{\theta}T_{c0}$) is not well described by (32). Rather, it implies that the reasoning which led to (32) is likely to be valid and should serve as a starting point for inclusion of higher-order effects and corrections.

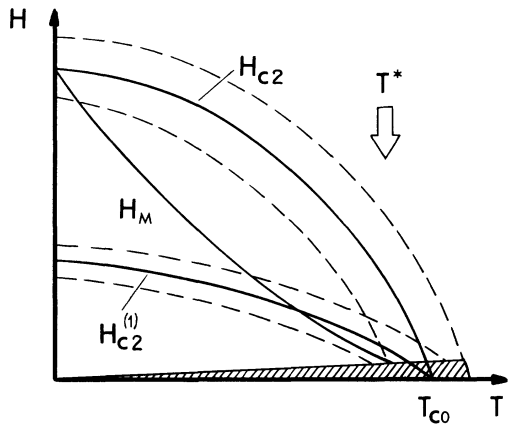

FIG. 3. An artist's representation of the H-T phase diagram. The nominal boundaries of the critical region around $H_{c2}(T)$ are denoted by dashed lines. The width of the critical region is given by θ, where $\theta \ll 1$ is the Ginzburg fluctuation parameter. The GL-LLL description is valid everywhere near $H_{c2}(T)$, as long as one is above the "critical region" of the next lowest LL, shown by the dashed lines surrounding $H_{c2}^{(1)}(T) \simeq (1/3)H_{c2}(T)$. When critical regions of the LLL and higher LL's start overlapping the simple GL-LLL approach becomes inappropriate and we may have to include several LL's in our description of fluctuations. The low-field regime of critical behavior is confined to the shaded area containing the $(H=0, T=T_{c0})$ point and bounded from above by the $HT_{c0}=(\theta/16)TH_{c2}(0)$ line (see text). In this regime the LL structure is destroyed by the quartic interaction term. The arrow indicates the $T=T^*=(1-\theta)T_{c0}$ line along which the magnetization $M(H,T)$ (6) is essentially independent of H, (Refs. 14 and 28), as observed experimentally. The $H_M(T)$ line is the "vortex melting" transition which takes place only far below the nominal critical region.

We now observe that the eigenfunctions of K_2 form macroscopically degenerate LL manifolds for particles of charge $2e$. This is an exact result in a translationally invariant system[24,25,27] (the underlying crystalline lattice or weak disorder do not make a practical difference for our present purposes). Furthermore, interaction K_4, being of range given by the magnetic length which is the shortest relevant length in the problem, can be replaced by some effective local interaction of strength β without a loss in generality or accuracy. So, finally, we have

$$Z=\prod_j \int \mathcal{D}\Psi_j(\mathbf{r}) \exp\left[-\frac{d}{T}\int d\mathbf{r}\left(\sum_j \tilde{\alpha}_j|\Psi_j(\mathbf{r})|^2 + \frac{1}{2}\beta|\Psi(\mathbf{r})|^4\right)\right] , \tag{33}$$

where j is the LL index, $\Psi_j(\mathbf{r})$ belongs to the jth LL manifold and $\tilde{\alpha}_j(H,T)$ is the corresponding eigenvalue of K_2. While it has a GL-type appearance the partition function (33) has a rather different physical meaning. For example, note that $\Psi(\mathbf{r})$ is a bosonic quantum field obtained by the transformation of the original microscopic problem. It is *not* the fluctuating superconducting order parameter that is featured in the true GL approach. In fact, no assumptions have been made about the presence of any phase transitions in (32) and, as already explained, the rapid variation of thermodynamic quantities through the nominal critical region is not associated with the proximity of the superconducting transition—it is instead the remnant of the transition that takes place in that region above the dimension four. No gradient expansions of slowly varying quantities have been made. The fully nonlocal kernels K_2 and K_4 have been derived from the microscopic model and $\tilde{\alpha}_j$ and β are thus not some unknown coefficients of the GL functional written solely on the basis of symmetry. They can be explicitly evaluated

within a given microscopic model of superconductivity. The correct way to think of (33) is as a true microscopic representation of the original electronic problem as long as the conditions under which it has been derived are satisfied. The labels "GL theory" for our starting point (1) and "fluctuating order parameter" for the Cooper pair quantum field $\Psi(\mathbf{r})$ are used in this paper for purely historical reasons; they have been used by everyone else over the years.

This brings us to the justification of the LLL part of the GL-LLL theory. The above form of the partition function makes the qualitative effect of finite magnetic field particularly evident. The fluctuating complex field $\Psi(\mathbf{r})$ (often referred to as the xy order parameter when the amplitude fluctuations are ignored) has been "compartmentalized" into different LL manifolds. It is clear that (33) exhibits two physically distinct regimes: If the "cyclotron gap" between different LL manifolds is small compared to the quartic interaction term, LL's will be strongly mixed and all LL's will be required to describe fluctuation effects. This is the low-field regime: The integrity of LL's is destroyed by the quartic term and there will be no sign of the LL structure in the fluctuation spectrum. In this regime one might try to describe the physics of fluctuations by some "semiclassical" modification to the $H = 0$ case, with the xy form of the order parameter still relatively intact, such as the frequently used London description. The situation is entirely different in the opposite limit where the LL splitting is larger than the interaction term. The xy order parameter is then completely "blown up" by the magnetic field and the critical behavior will bear a clear signature of the LL structure. A finite number of LL's will be sufficient to describe the fluctuations. In practice this number will be rather small, probably always less than three and always dominated by the LLL (see Fig. 3). In this high-field regime the GL-LLL theory becomes an accurate description of the critical behavior and there will be no connection to the low-field regime. The quantitative criterion which distinguishes between these two regimes can be arrived at by using already familiar rescaling which in effect sets $\beta \to 1/2$ and $\tilde{\alpha}_j \to g_j$ in Eq. (33), with $g_j = \tilde{\alpha}_j \sqrt{2\pi\ell^2 d/2\beta T}$. If we now introduce dimensionless quantities $\tau = T/T_{c0}$ and $h = H/H_{c2}(0)$, we obtain $g_j = [\tau - \tau_j(h)]/\sqrt{\theta\tau h}$, where $\theta \ll 1$ is the Ginzburg fluctuation parameter. The $H_{c2}(T)$ curve $[h_0(\tau)]$ follows from $\tau = \tau_{j=0}(h)$, while $\tau = \tau_{j>0}(h)$ leads to $h_j(\tau) \simeq h_0(\tau)/(2j+1)$.[25] The critical region around $H_{c2}(T)$, determined by $g_0 \in [-\sqrt{2}, \sqrt{2}]$, is depicted in Fig. 3. The width of this region in the H-T phase diagram is determined by θ and it narrows for T near T_{c0} and near zero ($\sim \theta$) and bulges in between ($\sim \sqrt{\theta}$). To keep things simple we have ignored such subtleties in Fig. 3. In this region the gap to higher LL's, $g_{j>0} \propto 1/\sqrt{\theta}$, is much larger than unity and the quartic interaction will not be effective in mixing higher LL's. Consequently, higher LL's can be integrated out providing a part of the structureless background. Thus, we are left with the renormalized GL-LLL theory.[14] This picture becomes inadequate, however, when the "critical regions" of higher LL's (defined by $g_j \in [-\sqrt{2}, \sqrt{2}]$) start overlapping with that of the LLL, which will occur above the shaded area surrounding the $T = T_{c0}$, $H = 0$ point (Fig. 3). In this regime additional LL's have to be included in the description of fluctuations: First the $j = 1$ level, then $j = 2$, and so on. While the study of fluctuations with several LL's included deserves further attention it is likely to yield results qualitatively and quantitatively similar to the GL-LLL theory since the LLL contribution is always dominant.

This incremental inclusion of LL's cannot go on forever. As the field gets lower one finally crosses into the shaded region of Fig. 3 where the quartic interaction in (33) strongly mixes LL manifolds and renders the LL description useless.[29] Here, some low-field approach, completely different from the GL-LLL theory, must be used, as discussed above. The boundary of this low-field region can be obtained by comparing the "cyclotron gap" between LL's with the size of the quartic interaction term and setting the ratio of the two to unity. This gives $h \cong (\theta/16)\tau$ as the upper boundary of the shaded area in Fig. 3. Such a boundary is naturally only a crossover between two qualitatively different regimes but the factor of $1/16$ is real. For example, we could choose to absorb it in the definition of θ but then $1/16$ would resurface in the expression for T^*. Since in all superconductors θ is much less than unity ($\theta \sim 10^{-2}$ in HTS and is only smaller in most other superconductors) the shaded region is rather small and the GL-LLL description of critical behavior, fortified if necessary by a next LL or two, will be valid almost everywhere. For example, in Bi(2:2:1:2) the shaded region in Fig. 3 is confined to fields < 0.8 Tesla. Furthermore, the reader should note that the GL-LLL theory will also be valid far below the nominal critical region around $H_{c2}(T)$ [say, near $H_M(T)$ in Fig. 3] as long as one is outside the "critical region" for the next LL, $g_1 \in [-\sqrt{2}, \sqrt{2}]$, which in practice means above $\sim (1/3)H_{c2}(T)$. Below this line we may have to include the next LL. Again, however, as long as one is above the shaded region, the LL description remains in force. At fields far *above* the critical region around $H_{c2}(T)$ the GL-LLL will also eventually break down with trivial consequences: The contributions of all LL's become of similar size but the fluctuation effects in this limit are vanishingly small. Finally, for $T > T_{c0}$, the LL description has a rather narrow region of validity as is clear from the above discussion.

In passing, we should observe that, while attempting to calculate the contribution of fluctuations to various physical quantities, the summations over all LL's frequently lead to divergences. These are again those (trivial) ultraviolet divergences, present in the zero-field case as well, which we have already discussed in the context of the 3D GL-LLL theory. These "divergent" contributions, when correctly regularized, are simply part of the uninteresting background. The challenge is to properly isolate the rapidly changing part of the thermodynamics containing the real low-energy physics. This is exactly what the GL-LLL theory accomplishes in the critical region near $H_{c2}(T)$.

In conclusion, we have constructed thermodynamic scaling functions for the critical region near $H_{c2}(T)$. A clear physical picture was used, taking advantage of the

weakness of lateral correlations to solve the GL-LLL theory at the 98% level of nominal accuracy. The weakness of these peculiar lateral correlations is a purely geometric effect of the LLL and can be traced back to the constraint that the external magnetic field places on the fluctuating order parameter. This 98–2 % method was found to be very accurate in quasi-2D systems, at the level of a few percent, just as advertised. Consequently, the problem of the "smooth" thermodynamics near $H_{c2}(T)$ in layered systems with weak interlayer coupling, superconducting thin films and superconducting superlattices, is basically solved for most practical purposes. Further improvements might concentrate on including the effects of higher LL's which should become important at lower fields. Following the same method, we have also derived the scaling functions for an (an-)isotropic 3D superconductor. The agreement with the available experimental results is good but just how accurate the 98–2 % method is in 3D is difficult to assess before more experiments on purely 3D systems become available. Similarly, it would be desirable to compare our results to numerical Monte Carlo simulations, which have not been done yet for a 3D superconductor near $H_{c2}(T)$. We expect, however, that the 98–2 % method will live up to its name in the 3D case as well.

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