First-principles theory of fluctuations in vortex liquids and solids

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Consistent perturbation theory for thermodynamical quantities in type-II superconductors in magnetic field at low temperatures is developed. It is complementary to the existing expansion valid at high temperatures. Magnetization and specific heat are calculated to two-loop order and compare well to existing Monte Carlo simulations and experiments. [S0163-1829(99)01829-9]

Thermal fluctuations play much larger role in high-T_c superconductors than in the low-temperature ones because the Ginzburg parameter G characterizing fluctuations is much larger. In the presence of magnetic field the importance of fluctuations in high-T_c superconductors is further enhanced. A strong magnetic field effectively suppresses long-wavelength fluctuations in a direction perpendicular to the field reducing dimensionality of the fluctuations by two.[1] Under these circumstances, fluctuations influence various physical properties and even lead to new observable qualitative phenomena like vortex lattice melting into vortex liquid far below the mean-field phase transition line. It is quite straightforward to systematically account for the fluctuations effect on magnetization, specific heat or conductivity perturbatively above the mean-field transition line using the Ginzburg-Landau (GL) description.[2] However, it proved to be extremely difficult to develop a quantitative theory in the interesting region below this line, even neglecting fluctuation of the magnetic field and within the lowest-Landau-level (LLL) approximation.

To approach the region below the mean-field transition line $T<T_{\mathrm{mf}}(H)$ Thouless[3] proposed a perturbative approach around homogeneous (liquid) state was in which all the ''bubble'' diagrams are resumed. The series provides accurate results at high temperatures, but for LLL dimensionless temperature $a_T \equiv [T-T_{\mathrm{mf}}(H)]/(TH)^{2/3} \lesssim -2$ become inapplicable (see dotted lines in Figs. 2 and 3 which represent successive approximants). Generally, attempts to extend the theory to lower temperature by Padé extrapolation were not successful and require additional external information about the low temperatures.[6] Alternative, a more direct approach to low-temperature fluctuation physics might have been to start from the Abrokosov solution at zero temperature and then take into account perturbatively deviations from this inhomogeneous solution. Experimentally it is reasonable since, for example, specific heat at low temperatures is a smooth function and the fluctuations contribution experimentally is quite small. This contrasts sharply with theoretical expectations.

A long time ago Eilenberger calculated the spectrum of harmonic excitations of the triangular vortex lattice.[4] Subsequently Maki and Takayama[5] noted that the gapless mode is softer than the usual Goldstone mode expected as a result of spontaneous breaking of translational invariance. The propagator for the ''phase'' excitations behaves as $1/[k_z^2+c(k_x^4+k_y^4)]$. The influence of this unexpected additional ''softness'' apparently goes even beyond enhancement of the contribution of fluctuations at leading order. It leads to disastrous infrared divergences at higher orders rendering the perturbation theory around the vortex state doubtful. For example, contributions to energy depicted in Figs. 1(a) and 1(d) are, respectively, $\log^2(L)$ and L^4 divergent (L being an IR cutoff) and at higher orders divergences get worse. Also qualitatively one argues[7] (in a way similar to that used frequently to understand the Mermin-Wagner theorem[8]) that lower critical dimensionality for melting of the Abrikosov lattice is $D=3$ and consequently a vortex lattice in clean materials exists in the thermodynamic limit only at $T=0$. One therefore tends to think that nonperturbative effects are so important that such a perturbation theory should be abandoned[9] and it was abandoned. However, a closer look at diagrams like Fig. 1(d) (see some details below) reveals that in fact one encounters actually only logarithmic divergences. This makes the divergences similar to so-called ''spurious'' divergences in the theory of critical phenomena with broken continuous symmetry. In that case one can prove[10] that they exactly cancel at each order provided we are calculating a symmetric quantity.

In this paper I show that all the IR divergences in free energy or other quantities invariant under translations cancel to the two-loop order. I calculate magnetization and specific heat to this order, interpolate with existing high-temperature expansion, and compare with Monte Carlo (MC) simulation[11] of the same system and experiments. Qualitatively physics of a fluctuating $D=3$ GL model in the magnetic field turns out to be similar to that of spin systems (or scalar fields) in $D=2$ possessing a continuous symmetry. In particular, although within perturbation theory in the thermodynamic limit the ordered phase (solid) exists only at $T=0$, at low temperatures liquid differs very little in most aspects from solid. One can effectively use properly modified perturbation theory to quantitatively study various properties of the vortex-liquid phase.

The GL free energy is

$$G=\frac{\hbar^2}{2m_{ab}}\left|\left(\vec{\nabla}-\frac{ie^*}{c}\vec{A}\right)\psi\right|^2+\frac{\hbar^2}{2m_c}|\partial_z\psi|^2+a|\psi|^2+\frac{b}{2}|\psi|^4. \tag{1}$$

Here $\vec{A}=(-By,0)$ describes a nonfluctuating almost constant magnetic field in the c direction. Within the LLL approximation ψ can be expanded in a basis of quasimomentum $\mathbf{k}$ eigenfunctions

$$\psi(x)=v\varphi(x)+\frac{1}{2\pi}\int d^2k\varphi_{\mathbf{k}}(x)\sqrt{\frac{\gamma_{\mathbf{k}}}{2|\gamma_{\mathbf{k}}|}}(O_k+iA_k), \tag{2}$$

$$\varphi_{\mathbf{k}}=\sqrt{\frac{2}{\sqrt{\pi}a_\Delta}}\sum_{l=-\infty}^{\infty}\exp\left\{i\left[\frac{\pi l(l-1)}{2}+\frac{2\pi}{a_\Delta}l(x-k_y)-xk_x\right]-\frac{1}{2}\left(y+k_x-\frac{2\pi}{a_\Delta}l\right)^2\right\}.$$

The unit of length will be the magnetic length $l_H\equiv\sqrt{c\hbar/eH}$ and $a_\Delta\equiv\sqrt{4\pi/\sqrt{3}}$ is the lattice spacing. The $\mathbf{k}=0$ component $\varphi_0(x)\equiv\varphi(x)$ is ''a vacuum'' with its vacuum expectation value denoted by v. The integration is over the Brillouin zone. Instead of one complex field two real fields O and A were introduced. They are somewhat analogous to acoustic and optical phonons in the usual solids with some peculiarities due to the strong magnetic field studied in detail by Moore.[6] For example, the A mode corresponds to shear of the two-dimensional lattice. Substituting Eq. (2) into the free energy, quadratic terms in fields define propagators, while cubic and quartic are interactions. The phase factors containing a function $\gamma_{\mathbf{k}}\equiv\int_x\varphi^*(x)\varphi^*(x)\varphi_{\mathbf{k}}(x)\varphi_{-\mathbf{k}}(x)$ are introduced in order to diagonalize the resulting quadratic part $P_O^{-1}(k)O_k^*O_k+P_A^{-1}(k)A_k^*A_k$, where $P_{O,A}^{-1}(\mathbf{k},k_z)=2a+2bv^2(2\beta_{\mathbf{k}}\pm|\gamma_{\mathbf{k}}|)+k_z^2$ (to simplify intermediate expressions an isotropic case $m_{ab}=m_c$ is considered, results are generalized later). Functions $\gamma_{\mathbf{k}}=\lambda(-\mathbf{k},\mathbf{k})$ and $\beta_{\mathbf{k}}\equiv\int_x\varphi^*(x)\varphi(x)\varphi_{\mathbf{k}}^*(x)\varphi_{\mathbf{k}}(x)=\lambda(0,\mathbf{k})$ as well as all the three- and four-leg vertices can be expressed via a single function of two quasimomenta

$$\lambda(\mathbf{k}_1,\mathbf{k}_2)=\sum_{l,m}(-)^{lm}\exp\left\{i\frac{2\pi}{a_\Delta}[lk_1^y+mk_2^y]-\frac{1}{2}\left[\left(k_2^x-\frac{2\pi}{a_\Delta}l\right)^2+\left(k_1^x-\frac{2\pi}{a_\Delta}m\right)^2\right]\right\}. \tag{3}$$

For example, the $A_{k1}A_{k2}A_{-k1-k2}$ vertex is

$$ibv\,\mathrm{Re}[\lambda(\mathbf{k}_1,\mathbf{k}_2)]=\frac{ibv}{2}\beta_{02}^A(k_1^xk_1^y+k_2^xk_2^y)+O(k^4), \tag{4}$$

where $\beta_{st}^A\equiv(2\pi/a_\Delta)^4\Sigma_{l,m}l^sm^t(-)^{lm}\exp\{-[(2\pi)^2/2a_\Delta^2](l^2+m)^2\}$. If the fluctuations were absent the expectation value $v_0^2=a/\beta_Ab$ would minimize $G_0=-av^2+(b/2)\beta_Av^4$ where $\beta_A\equiv\beta_{00}^A=1.16$. The propagators entering Feynman diagrams, therefore, are

$$P_{O,A}(k)=\frac{1}{M_{O,A}^2(\mathbf{k})+k_z^2};$$

$$M_{O,A}^2(\mathbf{k})\equiv\frac{2a}{\beta_A}(-\beta_A+2\beta_{\mathbf{k}}\pm\gamma_{\mathbf{k}}). \tag{5}$$

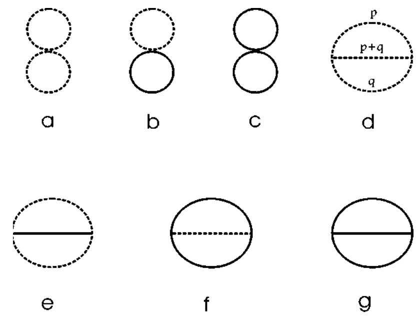

FIG. 1. Contributions to the free energy at the two-loop level.

Expanding around $\mathbf{k}=0$ using explicit expressions for $\gamma_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ one observes that the constant and the k^2 terms vanish, so that the (only) leading quartic term is $M_A^2(\mathbf{k})=(\beta_{22}^A/2\beta^A)\,|\mathbf{k}|^4$.

At the one-loop level the fluctuation contribution to the free energy is

$$G_1=\frac{1}{2}\frac{1}{(2\pi)^{3/2}}\int_{k_z}\int_{\mathbf{k}}\{\ln[P_O(k)]+\ln[P_A(k)]\}. \tag{6}$$

One should minimize G_0+G_1 with respect to v leading to the correction to its value

$$v_1^2=\frac{1}{(2\pi)^{3/2}}\int_{k_z}\int_{\mathbf{k}}[P_O(k)+P_A(k)]=\frac{1}{2(2\pi)^{1/2}}\int_{\mathbf{k}}\left[\frac{1}{M_O(\mathbf{k})}+\frac{1}{M_A(\mathbf{k})}\right]. \tag{7}$$

Due to the additional softness of the A mode the second ''bubble'' integral diverges logarithmically in the infrared. This means that for the infinite cutoff fluctuations destroy the inhomogeneous ground state, namely the state with lowest energy is a homogeneous liquid.[13] Since the divergence is logarithmic we are at lower critical dimensionality in which an analog of the Mermin-Wagner theorem[8] is applicable. It, does however, not necessarily mean that perturbation theory starting from the ordered ground state is inapplicable. The way to proceed in these situations have been found while considering simpler models like the φ^4 model $F=\frac{1}{2}(\nabla\varphi_i)^2+V(\varphi_i^2)$ in $D=2$ with a number of components larger then 1, say $i=1,2$.[12] Considering the statistical sum, one first integrates exactly zero modes existing due to continuous symmetry (translations in our case) and then develops a perturbation theory via the steepest descent method for the rest of the variables. When the zero mode is taken out, a single configuration appears with the lowest energy and the steepest descent is well defined. For invariant quantities such as energy, this procedure simplifies to: one actually can forget for a moment about integration over the zero mode and proceed with the calculation as if it is done in the ordered phase. The invariance of the quantities ensures that the zero-mode integration trivially factorizes. This is no longer true for noninvariant quantities for which the machinery of ''collective coordinates method'' should be used.[14]

To the two-loop order one gets several classes of diagrams, see Fig. 1. The leading-order propagators are denoted by dashed and solid lines for the ''supersoft'' A and ''hard''

B modes, respectively. The (naively) most divergent diagram Fig. 1(d) actually converges. To see this one writes explicitly its expression in terms of the function λ

$$\frac{b^2 v^2}{2(2\pi)^{3/2}} \int_q \int_p I_D(\mathbf{q},\mathbf{p}) P_A(p) P_A(q) P_A(p+q); \qquad (8)$$

$$I_D(\mathbf{q},\mathbf{p}) \equiv -\lambda(\mathbf{p},-\mathbf{q})\lambda(\mathbf{p},\mathbf{q}) + 4\lambda(\mathbf{p}+\mathbf{q},\mathbf{p})\lambda(\mathbf{p}+\mathbf{q},\mathbf{q}) \times \frac{\gamma_{\mathbf{p}+\mathbf{q}}}{|\gamma_{\mathbf{p}+\mathbf{q}}|} - 2\lambda(\mathbf{p}+\mathbf{q},-\mathbf{q})\lambda(\mathbf{p},-\mathbf{q}) \frac{\gamma_{\mathbf{p}} \gamma^*_{\mathbf{p}+\mathbf{q}}}{|\gamma_{\mathbf{p}} \gamma_{\mathbf{p}+\mathbf{q}}|} + 2\lambda(\mathbf{q},-\mathbf{p})^2 \frac{\gamma_{\mathbf{p}} \gamma_{\mathbf{q}} \gamma^*_{\mathbf{p}+\mathbf{q}}}{|\gamma_{\mathbf{p}} \gamma_{\mathbf{q}} \gamma_{\mathbf{p}+\mathbf{q}}|} + \text{c.c.}$$

The integrals over p_z and q_z can be explicitly performed using a formula

$$\frac{1}{2\pi} \int_p \int_q \frac{1}{p^2+M_1^2} \frac{1}{q^2+M_2^2} \frac{1}{(p+q)^2+M_3^2} = \frac{\pi}{2} \frac{1}{M_1 M_2 M_3} \frac{1}{M_1+M_2+M_3}.$$

The leading divergence

$$\sim \int_{\mathbf{p}} \int_{\mathbf{q}} I_a(\mathbf{q},\mathbf{p}) \frac{1}{\mathbf{p}^2 \mathbf{q}^2 |\mathbf{q}+\mathbf{p}|^2} \frac{1}{\mathbf{p}^2+\mathbf{q}^2+|\mathbf{q}+\mathbf{p}|^2},$$

is determined by the asymptotics of $I_D(\mathbf{q},\mathbf{p})$ as both $\mathbf{p}$ and $\mathbf{q}$ approach zero. If $I_D \sim 1$, it would diverge as L^4. However, the vertex is ''supersoft'' at small quasimomenta $\sim p^2$ according to Eq. (4), so that the expansion of $I_D(\mathbf{q},\mathbf{p})$ starts from terms quartic in $\mathbf{p}$ and $\mathbf{q}$ and there is no singularity at the origin. This goes beyond the usual ''softness'' of interactions of the Goldstone modes ($\sim p$). Nonleading divergences can be found by analyzing contributions coming from three regions on which one of the line momenta $\mathbf{p}$, $\mathbf{q}$ or $\mathbf{p}+\mathbf{q}$ vanishes. The corresponding expressions are

$$\sim \int_{\mathbf{k}} \int_{\mathbf{l}} I_D^i(\mathbf{l}) \frac{1}{\mathbf{k}^2 M_A(\mathbf{l})^3},$$

with $I_D^1 = 0$, $I_D^2 = \beta_{\mathbf{l}}^2 - \beta_{\mathbf{l}} |\gamma_{\mathbf{l}}|$ and $I_D^3 = -\beta_{\mathbf{l}}^2 + \beta_{\mathbf{l}} |\gamma_{\mathbf{l}}|$, respectively. Here $\mathbf{k}$ denotes an IR divergent momentum while integration over $\mathbf{l}$ is nonsingular. Although the second and the third contributions are divergent their sum is convergent.

Standard methods similar to the one used above can be applied to evaluate IR divergences of other superficially less divergent diagrams. There are no power divergences—only $\log^2 L$ and $\log L$. The results are

$$\frac{b}{\sqrt{2}\pi} \int_{\mathbf{p}} \frac{1}{M_A(\mathbf{p})} \int_{\mathbf{q}} \left[\frac{\beta_A - |\gamma_{\mathbf{q}}|}{M_A(\mathbf{q})} + \frac{|\gamma_{\mathbf{q}}|}{M_O(\mathbf{q})} \right],$$

$$\frac{b}{\sqrt{2}2\pi} \int_{\mathbf{p}} \frac{1}{M_A(\mathbf{p})} \int_{\mathbf{q}} \frac{2\beta_{\mathbf{q}} + |\gamma_{\mathbf{q}}| - 3\beta_A}{M_A(\mathbf{q})},$$

$$\frac{b}{\sqrt{2}2\pi} \int_{\mathbf{p}} \frac{1}{M_A(\mathbf{p})} \int_{\mathbf{q}} \frac{2\beta_{\mathbf{k}} - |\gamma_{\mathbf{q}}|}{M_O(\mathbf{q})}$$

for Figs. 1(a), 1(b), and 1(e), respectively. In addition to direct contributions from G_2 (Fig. 1), there is also a ''correction term'' due to the correction in the value of v from Eq. (7) inserted into the lower order contributions to free energy G_0 and G_1. Its divergent part is

$$-\frac{b}{\sqrt{2}2\pi} \int_{\mathbf{p}} \frac{1}{M_A(\mathbf{p})} \int_{\bar{q}} \left[\frac{2\beta_{\mathbf{k}} - |\gamma_{\mathbf{q}}| - \beta_A}{M_A(\mathbf{q})} - \frac{2\beta_{\mathbf{k}} + |\gamma_{\mathbf{q}}|}{M_O(\mathbf{q})} \right].$$

Both the leading divergences $\log^2 L$ and the next-to-leading ones $\log L$ cancel between the four contributions. Similar cancellations of all the logarithmic IR divergences occur in scalar models with Goldstone bosons in $D=2$ and $D=3$ (where the divergences are known as ''spurious'').

The finite result for the Gibbs free energy to two loops (finite parts of the integrals were calculated numerically) is restoring the original units and reintroducing the asymmetry $m_c \neq m_{ab}$:

$$G = \frac{\pi\hbar^2}{eHk_B T \sqrt{m_{ab}}} g; \quad g = -\frac{1}{2\beta_A} a_T^2 + c_1 \sqrt{|a_T|} + c_2 \frac{1}{|a_T|}, \qquad (9)$$

where numerical values of the coefficients are $c_1 = 3.16$ and $c_2 = 7.5$. The dimensionless entropy (LLL scaled magnetization)

$$s = -\frac{dg}{da_T} = \left(\frac{\pi^2 c^5 m_{ab}^3 b}{8e^5 k_B^2 m_c} \right)^{1/3} \frac{M}{(TH)^{2/3}} = \frac{1}{\beta_A} a_T + \frac{c_1}{2} \frac{1}{|a_T|} - c_2 \frac{1}{a_T^2}, \qquad (10)$$

and specific heat normalized to the mean-field value

$$\frac{1}{\beta_A} \frac{C}{\Delta C} = -\frac{d^2 g}{da_T^2} = 1 + \frac{c_1}{4} \frac{1}{|a_T|^{3/2}} + 2c_2 \frac{1}{a_T^3}, \qquad (11)$$

for successive partial sums are plotted in Figs. 2 and 3 (dashed lines). Qualitatively they are in accord with numerous experiments and MC simulations.[11] At low temperature magnetization is a bit larger than that of the mean field, while dimensionless specific heat characteristically grows before dropping fast around $a_T = -5$. To make a more detailed comparison, I interpolated between the results of low-temperature expansion and those of high-temperature expansion using the following rational form for the free energy in terms of the often-used variable x defined implicitly by $x = y^2$, $a_T = 4(2y)^{2/3}(1 - 1/8y^2)$:

$$g = 4(2y)^{2/3} \frac{1 + a_1 y + \cdots + a_{n+2} y^{n+2}}{1 + b_1 y + \cdots + b_n y^n}. \qquad (12)$$

The coefficients were constrained from both the low- and high-temperature sides. It has been already noted[6] that constraining from both sides the Padé approximants, just by the first term at low energy, improves otherwise unsatisfactory magnetization and specific heat.

Adding two more terms on the low-temperature end makes it very close to the MC results (stars triangles, and diamonds correspond to the 1, 2, and 5 T results for Y-Ba-Cu-O). I used just three leading terms in the high-

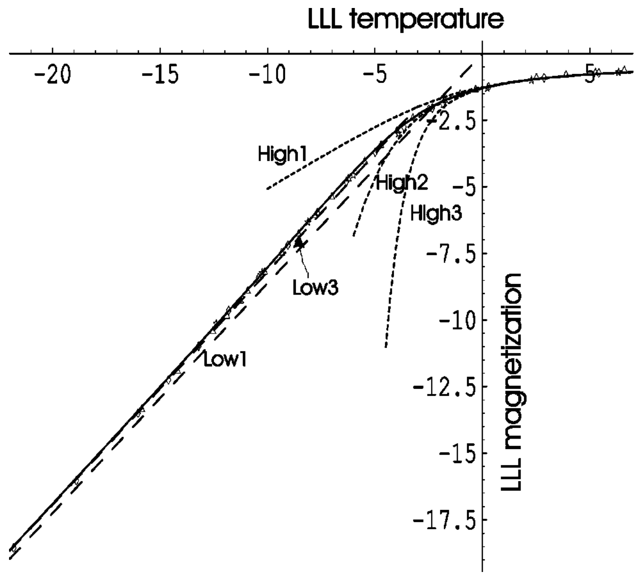

FIG. 2. Scaled magnetization defined in Eq. (10). Dashed (dotted) lines are successive low- (high-) temperature approximants, while the solid line is the interpolation. The points are the MC results.

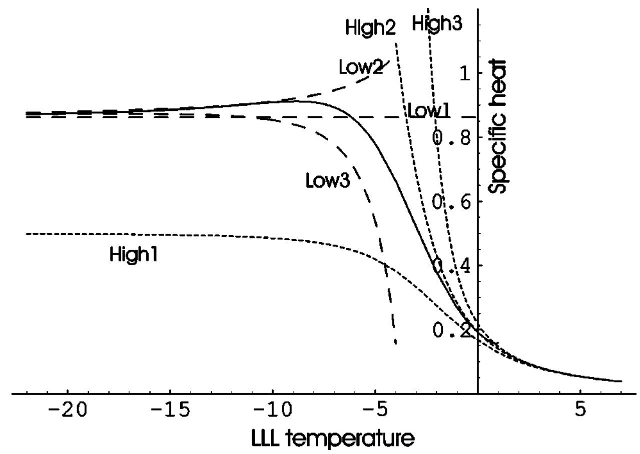

FIG. 3. Scaled specific heat defined in Eq. (11). The same notations as in Fig. 2.

temperature expansion shown in Figs. 2 and 3 by the dotted lines. Using more terms does not modify significantly the result. Although magnetization curve Eq. (12) agrees with that of Ref. 15, the specific heat is not.

To summarize, it is established up to the order of two loops that perturbation theory around the Abrikosov lattice is consistent. All the IR divergences cancel due to soft interactions of the soft mode. Perturbative results as well as interpolation with the high-temperature expansion agree very well with the direct MC simulation.

Now I comment on the range of validity of the perturbative results and nonperturbative effects. As can be seen from Figs. 2 and 3, the range of validity of the low-temperature expansion presented in this paper is below $a_T = -10$, while that of the high-temperature expansion is above $a_T = -2$. Both exclude the range in which a small magnetization jump (not seen in the scale of Fig. 2) due to vortex melting is seen experimentally and in the numerical simulation. Since the MC simulation is the only systematic tool available in the intermediate region [the theory of Tešanović *et al.*[15] captures the major (98%) contribution, but does not treat the small (2%) effect including melting], one might have two possibilities to discuss such a singularity within the present framework. One possibility is that the jump is due to finite-size effects and disappears in the thermodynamic limit (value of the cutoff in the simulation is only $L \sim 25$). Another is that some nonperturbative effects can stabilize the vortex lattice. Quantitative comparison with experiments on Y-Ba-Cu-O was attempted in Refs. 11 and 15. The present simple interpolation formula Eq. (12) works equally well.

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