First principles theory of fluctuations in vortex liquids and solids.

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Abstract

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.
Thermal fluctuations play much larger role in high $T_c$ superconductors than in the low temperature ones because the Ginzburg parameter $G_i$ characterizing fluctuations is much larger. In the presence of magnetic field the importance of fluctuations in high $T_c$ superconductors is further enhanced. Strong magnetic field effectively suppresses long wavelength fluctuations in direction perpendicular to the field reducing dimensionality of the fluctuations by two \cite{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 Ginzburg - Landau description \cite{2}. However it proved to be extremely difficult to develop a quantitative theory in the interesting region below this line, even neglecting fluctuation of magnetic field and within the lowest Landau level (LLL) approximation.

To approach the region below the mean field transition line $T < T_{mf}(H)$ Thouless \cite{3} proposed a perturbative approach around homogeneous (liquid) state was in which all the ”bubble” diagrams are resummed. The series provide accurate results at high temperatures, but for LLL dimensionless temperature $a_T \equiv (T - T_{mf}(H))/(TH)^{2/3} \lesssim -2$ become inapplicable (see dotted lines on Fig.2,3 which represent successive approximants). Generally attempts to extend the theory to lower temperature by Pade extrapolation were not successful and require additional external information about the low temperatures \cite{6}. Alternative, more direct approach to low temperature fluctuations physics might have been to start from the Abrokovov 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.

Long time ago Eilenberger calculated spectrum of harmonic excitations of the triangular vortex lattice \cite{4}. Subsequently Maki and Takayama \cite{5} noted that the gapless mode is softer then the usual Goldstone mode expected as a result of spontaneous breaking of translational
invariance. The propagator for the "phase" excitations behaves as $1/(k_x^2 + c(k_x^4 + k_y^4))$. 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 divergencies at higher orders rendering the perturbation theory around the vortex state doubtful. For example contributions to energy depicted on Fig. 1A and 1D are respectively $\log^2(L)$ and $L^4$ divergent ($L$ being an IR cutoff) and at higher orders divergencies 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 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 [10] and it was abandoned. However a closer look at the diagrams like Fig.1D (see some details below) reveals that in fact one encounters actually only logarithmic divergencies. This makes the divergencies similar to so called "spurious" divergencies in the theory of critical phenomena with broken continuous symmetry. In that case one can prove [10] that they exactly cancel at each order provided we are calculating a symmetric quantity.

In this note I show that all the IR divergencies 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 fluctuating $D = 3$ GL model in 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 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
\[
G = \frac{\hbar^2}{2m_{ab}} |(\vec{\nabla} - \frac{ie^*}{c} \vec{A})\psi|^2 + \frac{\hbar^2}{2m_c} |\partial_z \psi|^2 + a|\psi|^2 + \frac{b}{2}|\psi|^4 \tag{1}
\]

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

\[
\psi(x) = \upsilon \varphi(x) + \frac{1}{2\pi} \int d^2k \varphi_k(x) \sqrt{\frac{\gamma_k}{2|\gamma_k|}} (O_k + iA_k) \tag{2}
\]

\[
\varphi_k = \sqrt{\frac{2}{\sqrt{\pi}a_\Delta}} \sum_{l=-\infty}^{\infty} \exp \left\{ i \left[ \frac{\pi l (l-1)}{2} + \frac{2\pi}{a_\Delta} l(x - k_y) - xk_z \right] - \frac{1}{2} \left( y + k_y - \frac{2\pi}{a_\Delta} l \right)^2 \right\}
\]

Unit of length will be the magnetic length \(l_H \equiv \sqrt{\hbar c/eH}\) and \(a_\Delta \equiv \sqrt{4\pi/\sqrt{3}}\) is the lattice spacing. The \(k = 0\) component \(\varphi_0(x) \equiv \varphi(x)\) is "a vacuum" with its VEV denoted by \(\upsilon\). The integration is over 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 usual solids with some peculiarities due to 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 free energy, quadratic terms in fields define propagators, while cubic and quartic are interactions. The phase factors containing a function \(\gamma_k \equiv \int_x \varphi^*(x)\varphi(x)\varphi_k(x)\varphi_{-k}(x)\) 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 \(P_{O,A}(k,k_z) = 2a + 2bv^2(2\beta_k \pm |\gamma_k|) + k_z^2\) (to simplify intermediate expressions an isotropic case \(m_{ab} = m_c\) is considered, results are generalized later). Functions \(\gamma_k = \lambda(-k, k)\) and \(\beta_k \equiv \int_x \varphi^*(x)\varphi(x)\varphi^*_k(x)\varphi_k(x) = \lambda(0, k)\) as well as all the three and four leg vertices can be expressed via single function of two quasimomenta

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

For example the \(A_{k_1}A_{k_2}A_{-k_1-k_2}\) vertex is:

\[
ibv \text{Re} [\lambda(k_1, k_2)] = \frac{ibv}{2} \beta^A_{02}(k_1^x k_1^y + k_2^x k_2^y) + O(k^4), \tag{4}
\]
where $\beta_A^4 \equiv (\frac{2\pi}{a\Delta})^4 \sum_{l,m} l^s m^t (-)^{lm} \exp \left[ -\frac{(2\pi)^2}{2a\Delta} (l^2 + m^2) \right]$. If the fluctuations were absent the expectation value $v_0^2 = \frac{a}{\beta_A^b}$ would minimize $G_0 = -av^2 + \frac{b}{2} \beta_A v^4$ where $\beta_A \equiv \beta_{00}^A = 1.16$.

The propagators entering Feynman diagrams therefore are:

$$P_{O,A}(k) = \frac{1}{M_{O,A}^2(k) + k^2}; M_{O,A}^2(k) \equiv \frac{2a}{\beta_A} (-\beta_A + 2\beta_k \pm \gamma_k)$$ (5)

Expanding around $k = 0$ using explicit expressions for $\gamma_k$ and $\beta_k$ one observes that constant and the $k^2$ terms vanish, so that the (only) leading quartic term is $M_A^2(k) = \frac{\beta_A^4}{2\beta_A} |k|^4$.

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

$$G_1 = \frac{1}{2} \frac{1}{(2\pi)^{3/2}} \int_{k_x} \int_{k_y} \{ \log[P_O(k)] + \log[P_A(k)] \}$$ (6)

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

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

Due to 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 Mermin - Wagner theorem [8] is applicable. It however does not necessarily means that perturbation theory starting from ordered ground state is inapplicable. The way to proceed in these situations have been found while considering simpler models like $\varphi^4$ model $F = \frac{1}{2}(\nabla \varphi_i)^2 + V(\varphi_i^2)$ in $D = 2$ with number of components larger then 1, say $i = 1, 2$ [12]. Considering statistical sum, one first integrates exactly zero modes existing due to continuous symmetry (translations in our case) and then develops a perturbation theory via steepest descent method for the rest of the variables. When the zero mode is taken out, there appears a single configuration with lowest energy and steepest descent is well defined. For invariant quantities like energy this procedure simplifies: one actually can forget for a moment about integration over 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.1D actually converges. To see this one writes explicitly its expression in terms of function $\lambda$

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

$$I_D(q,p) \equiv -\lambda(p,-q)\lambda(p,q) + 4\lambda(p+q,p)\lambda(p+q,q) \frac{\gamma_{p+q}}{|\gamma_{p+q}|} -$$

$$-2\lambda(p+q,-q)\lambda(p,-q) \frac{\gamma_{p+q}^*}{|\gamma_{p+q}|} + + 2\lambda(q+p,p) \frac{\gamma_{q+p}^*}{|\gamma_{q+p}|} + c.c$$

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

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

The leading divergence $\sim \int_p \int_q I_a(q,p) \frac{1}{p^2 + |q| p^* + q^2 + |q+p|^2}$, is determined by the asymptotics of $I_D(q,p)$ as both $p$ and $q$ 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.([2]), so that expansion of $I_D(q,p)$ starts from terms quartic in $p$ and $q$ 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 $p$, $q$ or $p+q$ vanishes. The corresponding expressions are $\sim \int_k \int I_D^o(I) \frac{1}{k^2 M_A(k)^2},$ with $I_D^o = 0, I_D^1 = \beta_1^2 - \beta_1 |\gamma_1|$ and $I_D^3 = -\beta_1^2 + \beta_1 |\gamma_1|$ respectively. Here $k$ denotes an IR divergent momentum while integration over $l$ is nonsingular. Although the second and the third contributions are divergent their sum is convergent.

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

$$\frac{b}{\sqrt{2\pi}} \int_p \frac{1}{M_A(p)} \int_q \frac{3\beta A - |\gamma q|}{M_A(q)} + \frac{|\gamma q|}{M_A(q)},$$

$$\frac{b}{\sqrt{2\pi}} \int_p \frac{1}{M_A(p)} \int_q \frac{2\beta A - |\gamma q| - 3\beta A}{M_A(q)}$$

for diagrams Fig.1 a, b and e respectively. In addition to direct contributions from $G_2$ Fig.1 there is also a "correction term" due to correction in the value
of $v$ from eq.(7) inserted into the lower order contributions to free energy $G_0$ and $G_1$. It’s divergent part is \(-\frac{b}{\sqrt{22\pi}} \int_p \frac{1}{M_A(p)} \int_q \left[ \frac{2\beta_k - |\gamma_q| - \beta_A}{M_A(q)} - \frac{2\beta_k + |\gamma_q|}{M_0(q)} \right]\). Both the leading divergencies $\log^2 L$ and the next to leading ones $\log L$ cancel between the four contributions. Similar cancellations of all the logarithmic IR divergencies occur in scalar models with Goldstone bosons in $D = 2$ and $D = 3$ (where the divergencies 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 $m_c \neq m_{ab}$:

$$G = \frac{\pi \hbar^2}{e H k_B T \sqrt{m_{ab}}} g; g = -\frac{1}{2\beta_A} a_T^2 + c_1 \sqrt{|a_T|} + c_2 \frac{1}{|a_T|} \tag{9}$$

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

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

and specific heat normalized to the mean field value

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

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

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

The coefficients were constrained from both low and high temperature sides. It has been already noted \[8\] 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 1T, 2T and 5T results for YBCO). I used just three leading terms in high temperature expansion shown on Fig.2 and 3 by 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 order of two loops that perturbation theory around Abrikosov lattice is consistent. All the IR divergencies 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 range of validity of the perturbative results and nonperturbative effects. As can be seen from Fig.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 small magnetization jump (not seen on Fig.2’s scale) 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 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 YBCO was attempted in ref. [11,15]. The present simple interpolation formula eq. (12) works equally well.

Author is very grateful to L. Bulaevsky for encouragement and numerous discussions, R. Sasik for providing original MC data and explaining details of his MC simulation, Y. Kluger and other members of T11 and T8, especially A. Balatsky for discussions and hospitality in Los Alamos where part of this work was done. Work was supported by grant NSC of
Taiwan.
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Figure Captions

Fig. 1.
Contributions to the free energy at the two loop level.

Fig. 2.
Scaled magnetization defined in eq.(10). Dashed (dotted) lines are successive low (high) temperature approximants, while the solid line is the interpolation. Points are the MC results.

Fig. 3
Scaled specific heat defined in eq.(11). Same notations as in Fig.2.