A new systematic calculation of magnetization and specific heat contributions of vortex liquids and solids (not very close to the melting line) is presented. We develop an optimized perturbation theory for the Ginzburg-Landau description of thermal fluctuations effects in the vortex liquids. The expansion is convergent in contrast to the conventional high temperature expansion which is asymptotic. In the solid phase we calculate first two orders which are already quite accurate. The results are in good agreement with existing Monte Carlo simulations and experiments. Limitations of various nonperturbative and phenomenological approaches are noted. In particular we show that there is no exact intersection point of the magnetization curves both in 2D and 3D.

It was clearly seen in both magnetization [1] and specific heat experiments [2] that thermal fluctuations in high $T_c$ superconductors are strong enough to melt the vortex lattice into liquid over large portions of the phase diagram. The transition line between the Abrikosov vortex lattice and the liquid is located far below the mean field phase transition line. Between the mean field transition line and the melting point physical quantities like the magnetization, conductivity and specific heat depend strongly on fluctuations. Several experimental observations call for a refined precise theory. For example, a striking feature of magnetization curves intersecting at the same point $(T^*, H^*)$ was observed in a wide range of magnetic fields in both the layered [3] materials and the nonperturbative and phenomenological approaches are noted. In particular we show that there is no exact intersection point of the magnetization curves both in 2D and 3D.

Our starting point is the Ginzburg-Landau free energy:

$$F = L_c \int d^2x \frac{\hbar^2}{2m} |D\psi|^2 + a|\psi|^2 + \frac{b'}{2}|\psi|^4,$$

where $A = (By, 0)$ describes a nonfluctuating constant magnetic field in Landau gauge and $D \equiv \nabla - i\frac{\Phi_0}{\hbar c}A$. $\Phi_0 \equiv \frac{hc}{2e}, L_c$ is the width (for simplicity we write expressions for the 2D case, essential 3D complications are discussed separately). For simplicity we assume $a(T) = \alpha T_c (1-t), t \equiv T/T_c$. On LLL, the model after rescaling reduces to

$$f = \frac{1}{4\pi} \int d^2x \left[ a_T|\psi|^2 + \frac{1}{2} |\psi|^4 \right],$$

where the LLL reduced temperature $a_T \equiv -\sqrt{\frac{4\pi}{\omega} \left( \frac{1 - t - b}{2} \right)}$ is the only parameter in the theory [6]. Here $b \equiv \frac{\beta}{T_{c2}}$, $\omega \equiv (32\pi^3 e^2 k_B^2 T_c^2) / (e^2 k_B^2 L_c^2)$.

We will use a version of OPT, the optimized gaussian series [12]. It is based on the "principle of minimal sensitivity" idea [11], first introduced in quantum mechanics. Generally a perturbation theory starts from dividing the Hamiltonian into a solvable "large" part $K$ and a perturbation $V$. Since we can solve any quadratic Hamiltonian we have a freedom to choose "the best" such quadratic part. Quite generally such an optimization converts an asymptotic series into a convergent one (see a comprehensive discussion, references and a proof in [12]).

Due to the translational symmetry of the vortex liquid there is just one variational parameter, $\varepsilon$, in the free energy divided as follows:
where $a_H \equiv a_T - \varepsilon$. One reads Feynman rules from eq. (3): $K$ determines the propagator (just a constant), the first term in $V$ is a “mass insertion” vertex with a value of $\frac{\varepsilon}{4\pi}a_H$, while the four line vertex is $\frac{1}{8\pi}$. To calculate the effective free energy density $f_{eff} = -4\pi \ln Z$, one draws all the connected vacuum diagrams. We calculated directly diagrams up to the three loop order. However to take advantage of the existing long series of the non optimized gaussian expansion, we found a relation of the OPE to these series. Originally Thouless and Ruggeri calculated these series $f_{eff}$ to sixth order, but it was subsequently extended to 12th (9th in 3D) by Brezin et al and to 13th by Hu et al. It is usually presented using variable $x$ introduced by Thouless and Ruggeri 

$$f_{eff} = \frac{2\log \frac{\varepsilon_1}{4\pi} + 2 \sum_{n=1}^\infty c_n x^n}{\varepsilon_1}, \varepsilon = \frac{1}{2} (a_T + \sqrt{a_T^2 + 16})$$

(4)

$$x = \frac{\alpha}{\varepsilon_1}, \varepsilon_1 = \frac{1}{2} (\varepsilon_2 + \sqrt{\varepsilon_2^2 + 16\alpha})$$

Summing up all the insertions of the mass vertex is achieved by $\varepsilon_2 = \varepsilon + \alpha a_H$. Here $\alpha$ was introduced to keep track of order of the perturbation, so that expanding $f_{eff}$ to order $\alpha^{n+1}$, and then taking $\alpha = 1$ we obtain $\overline{f}_n(\varepsilon)$ (calculating $\overline{f}_n$ that way, we checked that indeed the first three orders agree with the direct calculation). The $n^{th}$ OPT approximant $\overline{f}_n(\varepsilon)$ is obtained by minimization of $\overline{f}_n(\varepsilon)$ with respect to $\varepsilon$:

$$\left( \frac{\partial}{\partial \varepsilon} - \frac{\partial}{\partial a_H} \right) \overline{f}_n(\varepsilon, a_H) = 0.$$  

(5)

The above equation is equal to $1/\varepsilon^{n+3}$ times a polynomial $g_n(z)$ of order $n$ in $z = \varepsilon - a_H$. That eq. (3) is of this type can be seen by noting that the function $f$ depends on the combination $\alpha/\varepsilon + a_H(\varepsilon^2)$ only. We were unable to prove this, but have checked it to the 40th order. This property greatly simplifies the task: one has to find roots of polynomials rather than solving transcendental equations. There are $n$ (real or complex) solutions for $g_n(z) = 0$. However (as in the case of anharmonic oscillator) the best results gives a real root with the smallest absolute value. We then obtain $\varepsilon(a_T) = \frac{1}{2} (a_T + \sqrt{a_T^2 - 4z_n})$ solving $z_n = \varepsilon \cdot a_H = \varepsilon a_T - \varepsilon^2$.

On Fig. 1 we present OPT for different orders including $n = 0$ (gaussian) together with several orders of the nonoptimized high temperature expansion. One observes that the OPT series converge above $a_T = -2.5$ and diverge below $a_T = -3.5$. The proof of convergence is analogous to that for the anharmonic oscillator, see ref. [12]. On the other hand, the nonoptimized series never converge despite the fact that above $a_T = 2$ first few approximants provide a precise estimate consistent with OPT. Above $a_T = 3$ the liquid becomes essentially a normal metal and fluctuations effects are negligible (see Fig. 2, 3). Therefore the information the OPT provides is essential to compare with experiments on magnetization and specific heat. If precision is defined as $(f_{12} - f_{10})/f_{10}$, we obtain $4.87\%, 1.27\%, 0.387\%, 0.222\%, 0.032\%$ at $a_T = -2, -1.5, -1, -0.5, 0$ respectively. For comparison with other theories and experiments on Fig. 2 and 3 we use the 10th approximant.

The calculation is basically the same in 3D, the only complication being extra integrations over momenta parallel to the magnetic field. However since the propagator factorizes, these integrations can be reduced to corresponding integrations in quantum mechanics of the anharmonic oscillator. The series converge above $a_T = -4.5$ and diverge below $a_T = -5.5$. The nonoptimized series are useful only above $a_T = -1$. The agreement is within the expected precision when we compare our results in 3D with ref. [13].

Now we turn to the vortex solids. Here the minimization is significantly more difficult due to reduced symmetry. Unlike in the liquid the field $\psi$ acquires a nonhomogeneous expectation value and can be expressed as $\psi(x) = v(x) + \chi(x)$, where $\chi$ describes fluctuations. Assuming hexagonal symmetry, it should be proportional to the mean field solution $v(x) = v\varphi_0(x)$ with a variational parameter $v$ taken real thanks global $U(1)$ gauge symmetry where $\varphi_k(x)$ is the quasi - momentum basis on LLL. Expanding $\chi$:

$$\chi(x) = \frac{1}{2\sqrt{2}} \int_k \exp[-i\theta_k/2]v\varphi_k(x)(O_k + iA_k).$$

(6)

where real fields $A_k = A_{k}^* (O_k = O_{k}^*)$ describing acoustic (optical) phonons of the flux lattice. The phase $\exp[-i\theta_k/2]$ defined, as in the low temperature perturbation theory developed recently, via $\gamma_k = |\gamma_k|\exp[i\theta_k]$, $\gamma_k \equiv \langle \varphi_0(x)\varphi_0(x)\varphi_k^*(x)\varphi_k^*(x) \rangle_{\varepsilon}$, is crucial for simplification of the problem. The most general quadratic form is

$$K = \frac{1}{8\pi} \int_k O_k G_{O_k}^{-1}(k)O_{-k} + A_k G_{A_k}^{-1}(k)A_{-k} + O_k G_{O_k}^{-1}(k)A_{-k} + A_k G_{A_k}^{-1}(k)O_{-k},$$

(7)

with matrix of functions $G(k)$ to be determined together with the constant $v$ by the variational principle. The corresponding gaussian free energy $f_{eff}$ is

$$a_T v^2 + \frac{\beta^4}{2} v^4 - 2$$
Observing that \( \beta \Delta \) is a constants (details will appear elsewhere). The matrix one just by a global gauge transformation. One can set

\[
\pm \sum_{n}^{\infty} (\langle |\gamma_k| \rangle (G \langle \rho \rangle - G \langle a \rangle)) k_l + 1/2\beta A \left( |\gamma_k| (G \langle \rho \rangle - G \langle a \rangle) \right)^2 + 4 |\gamma_k| G\langle a \rangle^2 \right) \frac{k}{k}
\]

where \( \langle \ldots \rangle \) \( \Delta \) denotes average over Brillouin zone \( \beta \equiv \langle \phi^2 \rangle \langle \phi \rangle \langle \phi \rangle \langle \phi \rangle \). \( \beta \Delta \) equals \( \beta \Delta \). The gap equations obtained by the minimization of the free energy look quite intractable, however they can be simplified. The crucial observation is that \( G \langle \rho \rangle = \beta \Delta = \beta \Delta \). The results show that \( G \langle \rho \rangle = \beta \Delta = \beta \Delta \). Therefore we conclude that the coincidence of the phenomenological approximant (gaussian) gives a rigorous upper bound. Like in 3D the intersection is approximate, although the approximation is quite good especially large (from several hundred \( T \)) to several \( T \) similar. This is seen on Fig.3 quite clearly. Instead of rising monotonously from \( C/\Delta C = 1 \) till melting as is predicted by OPT, their curve (dashed) first drops below 1 and only later develops a maximum above 1. In the liquid region it underestimates the specific heat. We conclude therefore that although the theory of Tesanovic et al. is very good at high temperatures they become of the order \( 5 - 10\% \) at \( aT = -3 \). An advantage of this theory is that it interpolates smoothly to the solid and never deviates more than \( 10\% \).

Experiments on great variety of layered high \( T \) cuprates (\( Bi \) or \( Ti \) based) show that in 2D, magnetization curves for different applied fields intersect at a single point (\( M^*, T^* \)). The range of magnetic fields is surprisingly large (from several hundred \( Oc \) to several \( Oc \)). This property fixes the scaled LLL magnetization defined as \( m(\alpha_T) = -\frac{d\chi(\alpha_T)}{d\alpha_T} = m_0 \frac{\sqrt{20}}{\mu_0 M} \). Demanding that the first two terms in \( 1/aT^2 \) expansion of \( m(\alpha_T) \) are consistent with the exact result, one obtains

\[
m(\alpha_T) = \frac{1}{4} \left( a_T - \sqrt{16 + a_T^2} \right) \]

The corresponding magnetization and specific heat are shown as a dashed lines on Fig.2 and 3 respectively. At large positive \( aT \), \( f_{eff} = 2\log aT + \frac{4}{aT^2} - \frac{16}{aT} + \frac{64}{aT^2} 
\]

and differs very little from the exact series \( 2\log aT + \frac{4}{aT^2} - \frac{16}{aT} + \frac{64}{aT^2} \). Its low temperature asymptotics is however less precise: \( \frac{\pi^2}{8} - \frac{2}{aT} + \frac{4}{aT^2} \) which has an opposite sign of the log term compared to the exact series \( -\frac{\pi^2}{8} + \frac{2}{aT} - \frac{4}{aT^2} \). This is seen on Fig.3 quite clearly. Instead of rising monotonously from \( C/\Delta C = 1 \) till melting as is predicted by OPT, their curve (dashed) first drops below 1 and then later develops a maximum above 1. In the liquid region it underestimates the specific heat. We conclude therefore that although the theory of Tesanovic et al is very good at high temperatures they become of the order 5–10% at aT = −3. An advantage of this theory is that it interpolates smoothly to the solid and never deviates more than 10%.

When it is plotted on Fig.2 (the dotted line), we find that at lower temperatures the magnetization is overestimated. The OPE results are consistent with the experimental data (points) within the precision range till the radius of convergence aT = −3. It is important to note that deviations of both the phenomenological formula eq. (8) and the Tesanovics’ are clearly beyond our error bars. Therefore we conclude that the intersection of all the lines at the same point (\( T^*, M^* \)) cannot be exact. Like in 3D the intersection is approximate, although the approximation is quite good especially at high magnetic fields.

Specific heat OPE result in 2D is compared on Fig. 3 with Monte Carlo simulation of the same model by Kato and Nagaosa (black circles) (and the phenomenological formula following from eq. (10), dotted line). The agreement is very good for both the low temperature and the high temperature OPT.

To summarize, we obtained the optimized perturbation theory results for the 2D and 3D LLL Ginsburg–Landau model in both vortex liquid and solid phases. The leading approximant (gaussian) gives a rigorous upper bound on energy, while the convergent series allow one to make several definitive qualitative conclusions. The intersection of the magnetization lines in only approximate not only in 3D, but also in 2D. The theory by Tesanovic [11]
describes the physics remarkably well at very high temperatures, but deviates on the 5-10% precision level at $\alpha_T = -2$ in 2D and has certain imprecise qualitative features in the solid phase. Comparison with Monte Carlo simulations and some experiments shows excellent agreement.

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FIG. 1. Optimized (solid lines) and nonoptimized (dashed lines) free energy approximants in 2D. Numbers indicate order of the approximant.

FIG. 2. The 2D scaled LLL magnetization. Comparison of data from Jin et al in ref. 3 with OPT calculation, Tesanovic et al result of ref. 10 (eq. 9) and phenomenological ”interception” theory eq. 10 are shown for comparison.

FIG. 3. Specific heat, 2D. Comparison of MC data with solid OPT (first two orders), liquid OPT (10th order). Tesanovic et. al. theory and phenomenological formula are also shown.