Precision Calculation of Magnetization and Specific Heat of Vortex Liquids and Solids in Type-II Superconductors

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A new systematic calculation of magnetization and specific heat contributions of vortex liquids and solids 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 the 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.

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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 rage of magnetic fields in both the layered [3] materials and the more isotropic ones [4]. To develop a quantitative theory of these fluctuations, even in the case of the lowest Landau level (LLL) corresponding to regions of the phase diagram "close" to H_{c2} [5], is a very nontrivial task and several approaches were developed.

Thouless and Ruggeri [6] proposed a perturbative expansion around a homogeneous (liquid) state in which all the "bubble" diagrams are resummed. Unfortunately, they proved that the series is asymptotic and although the first few terms provide accurate results at very high temperatures, the series becomes inapplicable for LLL dimensionless temperature $a_T \sim [T - T_{mf}(H)]/(TH)^{1/2}$ smaller than 2 in 2D quite far above the melting line (believed to be located around $a_T = -12$). Generally, attempts to extend the theory to lower temperatures by the Borel transform or Pade extrapolation were not successful [7]. Several nonperturbative methods have also been attempted including renormalization group [8] and the $1/N$ expansion [9]. Tesanovic and co-workers developed a theory based on separation of the two energy scales [10]: the condensation energy (98%) and the motion of the vortices (2%). The theory explains the intersection of the magnetization curves.

In the first part of this paper we apply optimized perturbation theory (OPT) first developed in field theory [11,12] to both the 2D and 3D LLL model. It allows one to obtain a convergent (rather than asymptotic) series for magnetization and specific heat of vortex liquids together with precision estimate. The radius of convergence is $a_T = -3$ in 2D and $a_T = -5$ in 3D. On the basis of this one can make several definitive qualitative conclusions.

Our starting point is the Ginzburg-Landau free energy:

$$F = L_c \int d^2x \, \frac{\hbar^2}{2m} |\mathbf{D}\psi|^2 + a|\psi|^2 + \frac{b'}{2}|\psi|^4, \quad (1)$$

where $\mathbf{A} = (By, 0)$ describes a nonfluctuating constant magnetic field in Landau gauge and $\mathbf{D} \equiv \nabla - i\frac{2\pi}{\Phi_0}\mathbf{A}$, $\Phi_0 \equiv \frac{hc}{2e}$, 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

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

where the LLL reduced temperature $a_T \equiv -\sqrt{\frac{4\pi}{b\omega}}\,\frac{1-t-b}{2}$ is the only parameter in the theory [6]. Here $b \equiv \frac{B}{H_{c2}}$, $\omega \equiv (32\pi^3 e^2\kappa^2\xi^2 T)/(c^2h^2L_z)$.

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]).

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Because of the translational symmetry of the vortex liquid there is just one variational parameter ε in the free energy divided as follows:

$$K = \frac{\varepsilon}{4\pi}|\psi|^2, \qquad V = \frac{1}{4\pi}\left[a_H|\psi|^2 + \frac{1}{2}|\psi|^4\right], \quad (3)$$

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 $\frac{1}{4\pi}a_H$, while the four line vertex is $\frac{1}{8\pi}$. To calculate the effective free energy density $f_{\rm eff} = -4\pi \ln Z$, 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 nonoptimized Gaussian expansion, we found a relation of the OPT to this series. Originally Thouless and Ruggeri calculated this series $f_{\rm eff}$ to sixth order, but it was subsequently extended to 12th (9th in 3D) by Brezin *et al.* and to 13th by Hu *et al.* [13]. It is usually presented using variable x introduced by Thouless and Ruggeri [6] $x = \frac{1}{\varepsilon^2}$, $\varepsilon = \frac{1}{2}(a_T + \sqrt{a_T^2 + 16})$ as follows: $f_{\rm eff} = 2\log\frac{\varepsilon}{4\pi^2} + 2\sum_{n=1}^{\infty} c_n x^n$. We can obtain all the OPT diagrams which do not appear in the Gaussian theory by insertions of bubbles and mass insertions from the diagrams contributing to the nonoptimized theory. Bubbles or "cacti" diagrams are effectively inserted by a technique known in field theory [14]:

$$f_{\rm eff} = 2\log\frac{\varepsilon_1}{4\pi^2} + 2\sum_{n=1}^{\infty} c_n x^n,$$
$$x = \frac{\alpha}{\varepsilon_1^2}, \qquad \varepsilon_1 = \frac{1}{2}(\varepsilon_2 + \sqrt{\varepsilon_2^2 + 16\alpha}). \quad (4)$$

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

$$\left(\frac{\partial}{\partial\varepsilon} - \frac{\partial}{\partial a_H}\right)\tilde{f}_n(\varepsilon, a_H) = 0. \quad (5)$$

The above equation is equal to $1/\varepsilon^{2n+3}$ times a polynomial $g_n(z)$ of order n in $z \equiv \varepsilon a_H$. That Eq. (5) is of this type can be seen by noting that the function f depends on the combination $\alpha/(\varepsilon + \alpha a_H)^2$ 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 [12]), the best results give 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 $z_n = \varepsilon a_H = \varepsilon a_T - \varepsilon^2$.

In 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 converges above $a_T = -2.5$ and diverges 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 converges despite the fact that above $a_T = 2$ the 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 Figs. 2 and 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 in Figs. 2 and 3 we use the 10th approximant.

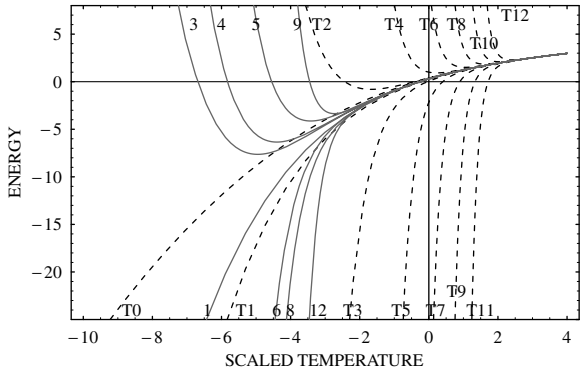

FIG. 1. Optimized (solid lines) and nonoptimized (dashed lines) free energy approximants in 2D. Numbers indicate the order of the approximant.

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 [6,11]. The series converges above $a_T = -4.5$ and diverges below $a_T = -5.5$. The nonoptimized series is useful only above $a_T = -1$. The agreement is within

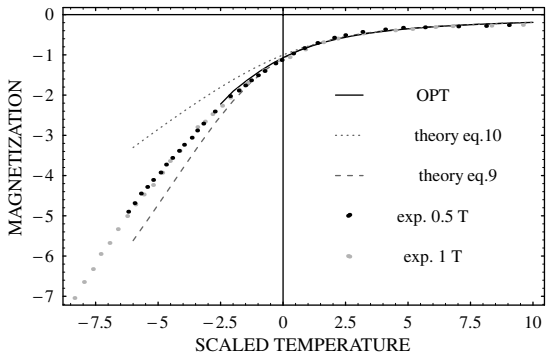

FIG. 2. The 2D scaled LLL magnetization. Comparison of data from Jin *et al.* in Ref. [3] with OPT calculation, Tesanovic *et al.* result of Ref. [10] [Eq. (9)] and phenomenological "interception" theory Eq. (10) are shown for comparison.

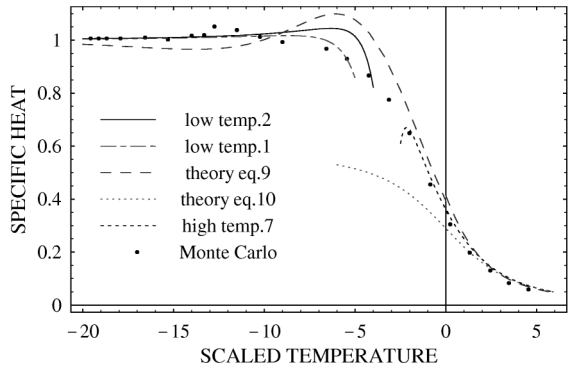

FIG. 3. Specific heat, 2D. Comparison of MC data with solid OPT (first two orders), liquid OPT (10th order). Tesanovic *et al.* theory and phenomenological formula are also shown.

the expected precision when we compare our results in 3D with Ref. [15].

Now we turn to the vortex solids. Here the minimization is significantly more difficult due to reduced symmetry. Unlike in the liquid the field ψ acquires a nonhomogeneous expectation value and can be expressed as $\psi(x) = v(x) + \chi(x)$, where χ describes fluctuations. Assuming hexagonal symmetry, it should be proportional to the mean field solution $v(x) = v\varphi_{k=0}(x)$ with a variational parameter v taken real thanks global $U(1)$ gauge symmetry where $\varphi_k(x)$ is the quasimomentum basis on LLL [5]. Expanding χ

$$\chi(x) = \frac{1}{2\pi\sqrt{2}} \int_k \exp[-i\theta_k/2]\varphi_k(x)\,(O_k + iA_k)\,, \quad (6)$$

where real fields $A_k = A^*_{-k}$ ($O_k = O^*_{-k}$) describe acoustic (optical) phonons of the flux lattice. The phase $\exp[-i\theta_k/2]$ defined, as in the low temperature perturbation theory developed recently [16], via $\gamma_k = |\gamma_k|\exp[i\theta_k]$, $\gamma_k \equiv \langle\varphi_0(x)\varphi_0(x)\varphi^*_k(x)\varphi^*_k(x)\rangle_x$, is crucial for simplification of the problem. The most general quadratic form is

$$K = \frac{1}{8\pi}\int_k O_k G^{-1}_{OO}(k)O_{-k} + A_k G^{-1}_{AA}(k)A_{-k} + O_k G^{-1}_{OA}(k)A_{-k} + A_k G^{-1}_{OA}(k)O_{-k}\,, \quad (7)$$

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

$$a_T v^2 + \frac{\beta_A}{2}v^4 - 2 - \langle\log[(4\pi)^2\det(G)] - a_T[G_{OO}(k) + G_{AA}(k)]\rangle_k + \langle v^2[(2\beta_k + |\gamma_k|)G_{OO}(k) + (2\beta_k - |\gamma_k|)G_{AA}(k)]\rangle_k + \langle\beta_{k-l}[G_{OO}(k) + G_{AA}(k)][G_{OO}(l) + G_{AA}(l)]\rangle_{k,l} + \frac{1}{2\beta_A}\{\langle|\gamma_k|[G_{OO}(k) - G_{AA}(k)]\rangle^2_k + 4\langle|\gamma_k|G_{OA}(k)\rangle^2_k\},$$

where $\langle\cdots\rangle_k$ denotes the average over Brillouin zone $\beta_k \equiv \langle\varphi^*_0(x)\varphi_0(x)\varphi^*_k(x)\varphi_k(x)\rangle_x$, $\beta_A = \beta_0$. The gap equations obtained by the minimization of the free energy look quite intractable, however, they can be simplified. The crucial observation is that $G_{OA}(k) = 0$ is a solution, and the general solution can be shown to differ from this simple one just by a global gauge transformation. One can set matrix G^{-1} as

$$\begin{pmatrix} E(k) + \Delta|\gamma_k| & 0 \\ 0 & E(k) - \Delta|\gamma_k| \end{pmatrix},$$

where Δ is a constant (details will appear elsewhere). The function $E(k)$ and the constant Δ satisfy

$$E(k) = a_T + 2v^2\beta_k + 2\left\langle\beta_{k-l}\left(\frac{1}{E_O(l)} + \frac{1}{E_A(l)}\right)\right\rangle_l, \quad (8)$$
$$\beta_A\Delta = a_T - 2\left\langle\beta_k\left(\frac{1}{E_O(k)} + \frac{1}{E_A(k)}\right)\right\rangle_k.$$

Observing that β_k has a very effective expansion in $\chi \equiv \exp[-a^2_\Delta/2] = \exp[-2\pi/\sqrt{3}] = 0.0265$, $\beta_k = \sum_{n=0}^\infty \chi^n\beta_n(k)$, $\beta_n(k) \equiv \sum_{|\mathbf{X}|^2=na^2_\Delta}\exp[i\mathbf{k}\cdot\mathbf{X}]$ and using the hexagonal symmetry of the spectrum, $E(k)$ can also be expanded in "modes" $E(k) = \sum E_n\beta_n(k)$. The integer n determines the distance of a points on the hexagonal lattice $\mathbf{X}$ from the origin. One estimates that $E_n \simeq \chi^n a_T$, therefore the coefficients decrease exponentially with n. For some integers, for example, $n = 2, 5, 6$, $\beta_n = 0$. We minimized numerically the Gaussian energy by varying v, Δ, and the first few modes of $E(k)$. In practice two modes are quite enough. The results show that around $a_T < -5$, the Gaussian liquid energy is larger than the Gaussian solid energy. So naturally when $a_T < -5$, one should use the Gaussian solid to set up a perturbation theory instead of the liquid one. The Gaussian energy in either liquid (see line T0 on Fig. 1) or solid is a rigorous upper bound on the free energy. We calculated the leading correction (without its minimization) in order to determine the precision of the Gaussian result (see Fig. 3 for the specific heat results). We obtain 0.2%, 0.4%, and 2% at $a_T = -30, -20, -12$, respectively.

In the rest of the paper we compare our results with other theories, simulations, and experiments. An analytic theory used successfully to fit the magnetization and the specific heat data [17]was developed in [10]. Their free energy density is

$$f_{\rm eff} = -\frac{a^2_T U^2}{4} + \frac{a_T U}{2}\sqrt{\frac{U^2a^2_T}{4} + 2} + 2\,\mathrm{arcsinh}\left[\frac{a_T U}{2\sqrt{2}}\right],$$
$$U = \frac{1}{2}\left[\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{\beta_A}} + \tanh\left[\frac{a_T}{4\sqrt{2}} + \frac{1}{2}\right]\left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{\beta_A}}\right)\right]. \quad (9)$$

The corresponding magnetization and specific heat are shown as dashed lines in Figs. 2 and 3, respectively. At large positive a_T, $f_{\rm eff} = 2\log a_T + \frac{4}{a_T^2} - \frac{16}{a_T^4} + \frac{320}{3a_T^6}$ and differs very little from the exact series $2\log a_T + \frac{4}{a_T^2} - \frac{18}{a_T^4} + \frac{1324}{9a_T^6}$. Its low temperature asymptotics is, however, less precise: $-\frac{a_T^2}{2\beta_A} - 2\log\frac{|a_T|}{4\pi^2}$, which has an opposite sign of the log term compared to the exact series [16] $-\frac{a_T^2}{2\beta_A} + 2\log\frac{|a_T|}{4\pi^2} - \frac{19.9}{a_T^2}$. This is seen in Fig. 3 quite clearly. Instead of rising monotonously from $C/\Delta C = 1$ until 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 $a_T = -3$. An advantage of this theory is that it interpolates smoothly to the solid and never deviates more than 10%.

Experiments on a great variety of layered high T_c cuprates (Bi or Tl [3] 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 Oe to several Tesla). This property fixes the scaled LLL magnetization defined as $m(a_T) = -\frac{df_{\rm eff}(a_T)}{da_T} = \frac{m_{ab}}{e^*h}\sqrt{\frac{4\pi}{b\omega}}\,M$. Demanding that the first two terms in $1/a_T^2$ expansion of $m(a_T)$ are consistent with the exact result, one obtains

$$m(a_T) = \frac{1}{4}\,(a_T - \sqrt{16 + a_T^2}\,). \qquad (10)$$

When it is plotted in Fig. 2 (the dotted line), we find that at lower temperatures the magnetization is overestimated. The OPE results are consistent with the experimental data [3] (points) within the precision range until the radius of convergence $a_T = -3$. It is important to note that deviations of both the phenomenological formula Eq. (10) and Tesanovic's are clearly beyond our error bars. Therefore we conclude that the coincidence of the intersection of all the lines at the same point (T^*, M^*) cannot be exact. As in 3D the intersection is approximate, although the approximation is quite good especially at high magnetic fields.

Specific heat OPE results in 2D is compared in Fig. 3 with Monte Carlo simulation of the same model by Kato and Nagaosa [18] (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 Ginzburg-Landau model in both vortex liquid and solid phases. The leading approximant (Gaussian) gives a rigorous upper bound on energy, while the convergent series allows one to make several definitive qualitative conclusions. The intersection of the magnetization lines is only approximate not only in 3D, but also in 2D. The theory by Tesanovic [10] describes the physics remarkably well at very high temperatures, but deviates on the 5%–10% precision level at $a_T = -2$ 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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