Supercooled vortex liquid and quantitative theory of melting of the flux line lattice in type II superconductors.

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Abstract

A metastable homogeneous state exists down to zero temperature in systems of repelling objects. Zero "fluctuation temperature" liquid state therefore serves as a (pseudo) "fixed point" controlling the properties of vortex liquid below and even around melting point. There exists Madelung constant for the liquid in the limit of zero temperature which is higher than that of the solid by an amount approximately equal to the latent heat of melting. This picture is supported by an exactly solvable large $N$ Ginzburg - Landau model in magnetic field. Based on this understanding we apply Borel - Pade resummation technique to develop a theory of the vortex liquid in type II superconductors. Applicability of the effective lowest Landau level model is discussed and corrections due to higher levels is calculated. Combined with previous quantitative description of the vortex solid the melting line is located. Magnetization, entropy and specific heat jumps along it are calculated. The magnetization of liquid is larger than that of solid by 1.8% irrespective of the melting temperature. We compare the result with experiments on high $T_c$ cuprates $YBa_2Cu_3O_7$, $DyBCO$, low $T_c$ material $(K,Ba)BiO_3$ and with Monte Carlo simulations.

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I. INTRODUCTION AND THE MAIN IDEA

Abrikosov flux lines (vortices) created by magnetic field in type II superconductors strongly interact with each other creating highly correlated configurations like the vortex lattice. In high $T_c$ cuprates thermal fluctuations at relatively large temperatures are strong enough to melt the lattice. Several remarkable experiments demonstrated that the vortex lattice melting in high $T_c$ superconductors is first order with magnetization jumps [1] and spikes in specific heat [2]. Magnetization and entropy jumps were measured using local Hall probes [1], SQUID [3,4], torque magnetometry [5,6] and integrating the specific heat spike [2,7]. It was found that in addition to the spike there is also a jump in specific heat in YBCO which was measured as well [2,7,8]. These precise measurements pose a question of accurate quantitative theoretical description of thermal fluctuations in vortex matter.

The melting line in high $T_c$ cuprates has been studied mainly not very far from $T_c$. In this part of the phase diagram the Ginzburg - Landau (GL) approach is generally appropriate to describe thermal fluctuations near $T_c$ [9,10]. The GL model is however highly nontrivial even within the lowest Landau level (LLL) approximation valid at relatively high fields. This simplified model has only one parameter: the dimensionless LLL scaled temperature $a_T \sim (T - T_{mf}(H))/(TH)^{2/3}$ (defined precisely in eq.(13a) below). Over the last twenty years great variety of theoretical methods were applied to study this model. Brezin, Nelson and Thiaville [11] applied the renormalization group (RG) method on the one loop level description of the vortex liquid. No nontrivial fixed points of the (functional) RG equations were found and they concluded therefore that the transition from liquid to the solid is first order [12]. Another often used approach applicable also beyond the range of validity of GL model is to use elasticity theory description of the vortex lattice and Lindermann criterion to determine the location of melting line [13]. However all those approaches do not provide a quantitative theory of melting since these are one phase theories and in order, for example, to calculate discontinuities at first order transition accurate description of both phases is necessary.

Two perturbative approaches were developed and greatly improved recently to describe both the solid and the liquid phases in the LLL GL model. The perturbative approach on the liquid side was pioneered long ago by Thouless and Ruggeri [14]. They developed a perturbative expansion around a homogeneous (liquid) state in which all the ”bubble” diagrams are resumed. Unfortunately they found that the series are asymptotic and although first few terms provide accurate results at very high temperatures, the series become inapplicable for $a_T$ less than $-2$, which is quite far above the melting line (believed to be located around $a_T \sim -10$). We recently obtained the optimized Gaussian series [15] which are convergent rather than asymptotic with radius of convergence of $a_T = -5$ still unfortunately above the melting point.

On the solid side, long time ago Eilenberger and Maki and Takayama [16] calculated the fluctuations spectrum around Abrikosov’s mean field solution. They noticed that the vortex lattice phonon modes are softer than that of the acoustic phonons in atomic crystals and this leads to infrared (IR) divergences in certain quantities. This was initially interpreted as ”destruction of the vortex solid by thermal fluctuations” and the perturbation theory was abandoned. However the divergences look suspiciously similar to ”spurious” IR divergences in the critical phenomena theory and recently it was shown that
all these IR divergences cancel in physical quantities [17]. The series therefore are reliable, and were extended to two loops, so that the LLL GL theory on the solid side is now precise enough even around melting point. Therefore the missing part is a theory in the region $-10 < a_T < -5$ on the liquid side. Moreover this theory should be very precise since free energies of solid and liquid happen to differ only by few percents around melting. Closely related to melting is the problem of nature of the metastable phases of the theory. While it is clear that the overheated solid becomes unstable at some finite temperature, it not generally clear whether the overcooled liquid becomes unstable at some finite temperature (like water and other molecular liquids, which however has a crucial attractive component of the intermolecular force) or exists all the way down to $T = 0$ as a metastable state. The Gaussian (Hartree - Fock) variational calculation, although perhaps of a limited precision, is usually a very good guide as far as qualitative features of the phase diagram are concerned. Such a calculation in the liquid was performed long ago [14], while a significantly more complicated one sampling also inhomogeneous states (vortex lattice) was obtained recently [18,19]. The gaussian results are as follows. The free energy of the solid state is lower than that of the liquid for all temperatures lower than melting temperature $a^m_T$. The solid state is therefore the stable one below $a^m_T$, becomes metastable at somewhat higher temperatures and is destabilized at $a_T = -5$. The liquid state becomes metastable below the melting temperature, but unlike the solid, does not loose metastability all the way down to $a^m_T = -\infty$ ($T = 0$). The excitation energy of the supercooled liquid approaches zero as a power $\varepsilon \sim 1/a_T^2$. This general picture is supported in section III by an exactly solvable large $N$ Ginzburg - Landau model of vortex matter in type II superconductors. Meantime in different area of physics similar qualitative results were obtained. It was shown by variety of analytical and numerical methods that liquid (gas) phase of the classical one component Coulomb plasma exists as a metastable state down to very low temperature possibly $T = 0$ [20]. The quantum one component plasma - electron gas also shows similar feature [21]. One considers quantum fluctuations instead of the thermal ones (an analog of inverse temperature is coupling $r_s$, see section III). It seems plausible to speculate that the same phenomenon would happen in any system of point like or line like objects interacting via purely repulsive forces. In fact the vortices in the London approximation are a sort of repelling lines with the force even more long range than Coulombic. This was an additional strong motivation to consider the above scenario in vortex matter. In section III we provide both theoretical and phenomenological evidence that the above scenario is the correct one. Assuming absence of singularities on the liquid branch allows to develop an essentially precise theory of the LLL GL model in vortex liquid (even including supercooled liquid) using methods of theory of critical phenomena [22,23]. The generally effective mathematical tool to approach a nontrivial fixed point (in our case at zero temperature) is the Borel - Pade (BP) transformation [23]. Before embarking on this program in following sections, we address several subtleties which prevented the use and acceptance of the BP method in the past and then combine it with the recently developed LLL theory of solids to calculate the melting line and the magnetization and the specific heat jumps across the line. Very early on Ruggeri and Thouless [14] tried to use BP (unfortunately a "constrained" one, so that it interpolates smoothly with the solid, assumption we believe is
incorrect) to calculate the specific heat without much success. It was shown by Wilkin and
Moore [24] that the constrained BP does not converge, while the results for unconstrained
BP were inconclusive. They attributed this to the limited order of expansion known at
that time. Subsequent attempts to use BP for the calculation of the melting line using
longer series also ran into problems. Hikami, Fujita and Larkin [25] tried to find the
melting point by comparing the BP energy with the one loop solid energy and obtained
\[ a_T = -7. \]
However their one loop solid energy was incorrect and, in any case, it was not
precise enough (as will become clear below the two loop contribution cannot be neglected).
The LLL GL model was also studied numerically in both Lawrence - Doniach model (a
good approximation of the 3D GL for large number of layers) [26,27] and in 2D [28] and by
a variety of nonperturbative analytical methods. Among them the density functional [29],
\[ 1/N \] [30–32], dislocation theory of melting [33] and others [34].
As we show in this paper, the BP liquid free energy combined with the correct two loop
solid energy computed recently gives scaled melting temperature \[ a_T^m = -9.5 \] and in
addition predicts other characteristics of the model. The magnetization of liquid is larger
than that of solid by 1.8% irrespective of the melting temperature (the specific heat jump
is about 6% and decreases slowly with temperature in \( YBCO \)). Brief account of these
results was published [18].
In addition to the theory of melting, we considered overcooled liquid and calculated
magnetization and specific heat curves. Since the metastable overcooled liquid state exists
all the way down to zero temperature, we can define liquid Madelung energy. Looking at
the melting process from the low temperature side for both the liquid and the solid we find
that the Madelung energy of liquid is larger than that of the solid approximately by the
latent heat of melting. Our magnetization curves agree quite well with Monte Carlo
simulations of the LLL GL [26], and almost perfectly for specific heat in 2D by Kato and
Nagaosa in ref. [28].
In addition we consider in this paper several ”phenomenological” issues, some matter of
significant disagreement. First is the range of applicability of the LLL model. We find that
in order to describe experimental reversible magnetization of \( YBCO \) at lower fields, higher
Landau levels (HLL) corrections should be incorporated. We therefore clarify in section V
the role of the HLL modes. Experimentally it was claimed that one can establish the LLL
scaling for fields above \( 3T \) [35]. A glance at the data however shows that in normal state
(above \( T_c \) ) the LLL scaling for magnetization curves is generally very bad. Most of the
HLL effects can be taken into account by just renormalizing parameters of the LLL model.
Therefore one should use the ”effective LLL” in which HLL were ”integrated out”. To
clarify this often salient feature we explicitly perform this integration within a self
consistent approach in section V. It was noted by Koshelev [36] and others that, to
calculate magnetization, one has to carefully account for renormalization of the free energy
since it is field dependent. Then we calculated the leading correction the effective LLL and
compared with experiments. It is found that although the LLL contribution to
magnetization is much larger that the experimentally observed one above \( T_c \), it is nearly
cancelled by the HLL contributions. This explains the breaking of the LLL scaling in the
normal state.
The paper is organized as follows. The model is defined and its applicability range
discussed in section II. In section III, supercooled liquid in general repulsive system will be
discussed. We provide evidence for the scenarios outlined above using both a solvable (for
a large number of components) Ginzburg - Landau model and analyzing numerical results
in other systems. In section IV the LLL model is solved and the melting theory of vortex
lattice is presented and compared to experiments. In section V, the HLL corrections are
discussed and the magnetization curves are compared with experiments.
Phenomenological issues are addressed in sections IIB (assumptions), IVC (melting line,
Ginzburg parameter fit for various materials), IVD (magnetization, entropy jumps), IVE
(specific heat jumps) and VD (reversible magnetization curve), so readers not interested in
theoretical details can directly proceed to these sections.

II. THE GL MODEL AND ITS BASIC ASSUMPTIONS.

A. The GL model

On the mesoscopic scale a 3D superconducting materials with not very strong asymmetry
along the z axis are effectively described by the following Ginzburg-Landau free energy
functional:

\[ F[\psi, \psi^*, A] = \int d^3x \frac{\hbar^2}{2m_{ab}} |D\psi|^2 + \frac{\hbar^2}{2m_c} |\partial_z \psi|^2 - a(T)|\psi|^2 + \frac{b'}{2} |\psi|^4 + \frac{(B - H)^2}{8\pi} \]  

involving the order parameter field \( \psi \) and magnetic field \( B \). The external constant
magnetic field is described by the vector potential in Landau gauge \( A_0 = (Hy, 0, 0) \). The
covariant derivative is defined by \( D \equiv \nabla - 2\pi i A/\Phi_0, \Phi_0 \equiv \hbar c/e^* (e^* = 2e) \). The
microscopic thermal fluctuations are integrated out and, as a consequence, coefficients \( a, b' \)
and \( m \) depend on temperature. Mesoscopic thermal fluctuations of the order parameter
are described by the partition function:

\[ Z = \int D\psi D\psi^* DA \exp \left\{ -\frac{F[\psi, \psi^*, A]}{T} \right\} \]

Our aim is to quantitatively describe the effects of thermal fluctuations of high \( T_c \) cuprates
of the \( YBCO \) type and some other ”strongly fluctuating” 3D materials.

B. Assumptions

The use of the above GL energy hinges upon several physical assumptions. They are listed
below.

1. Continuum 3D model

We use the anisotropic GL model despite the well established layered structure of the high
\( T_c \) cuprates for which models of the Lawrence - Doniah type are more appropriate. Effects
of layered structure are dominant in \( BSCCO \) or \( Tl \) compounds (anisotropy very large:
\( \gamma \equiv \sqrt{m_c/m_{ab}} > 1000 \) ) and noticeable for cuprates with anisotropy of order \( \gamma = 50 \) like
\( LaBaCuO \), strongly underdoped \( YBCO \) (see however [37]) or \( Hg1223 \). The requirement,
that the 3D GL can be effectively used, therefore limits us to optimally doped \( YBCO_{7-\delta} \)
(or slightly overdoped or underdoped) for which the anisotropy parameter is not very large.
\( \gamma = 4 - 8 \ [38] \)), \( DyBCO \) and possibly \( Hg1221 \) which has a slightly larger anisotropy. There is no such problem in recently discovered isotropic "fluctuating" superconductor \((K, Ba)BiO_3 \ [39]\).

(2) \textbf{Range of validity of the mesoscopic (GL) approach}

The GL approach generally is an effective mesoscopic approach. It is applicable when one can neglect higher order terms in the functional eq.(1) typically generated, when one "integrates out" microscopic degrees of freedom. The leading higher dimensional terms we neglect (as "irrelevant") are \( |\psi|^6 \) and higher (four) derivative terms like \( |D^2 \psi|^2 \). This naively leads to a condition that \( 1 - t - b < 1 \). Here and in what follows

\[
t \equiv T/T_c; \quad b \equiv H/H_{c2} \approx B/H_{c2}. \tag{3}
\]

The applicability line \( 1 - t - b < 0.2 \) for \( YBCO \) is plotted in Fig. 1. We also will consider a model invariant under rotations in the \( ab \) plane. Noninvariant models sometimes can be rescaled it to \( m_a \simeq m_b = m_{ab} \ [10] \). For several physical questions those assumptions are not valid because neglected "irrelevant" terms might become "dangerous". For example the question of the structural phase transition into the square lattice is clearly of this type [40]. It is known that even assuming \( m_a/m_b = 1 \) in low temperature vortex lattices in \( YBCO \), rotational symmetry is broken down to the fourfold symmetry by the four derivative terms. However there is no significant correction to, for example, the magnetization from those higher dimension terms.

(3) \textbf{Expansion of parameters around} \( T_c \)

Generally parameters of the GL model of eq.(1) are complicated functions of temperature which are determined by the details of the microscopic theory. We expand the coefficient \( a(T) \) near \( T_c \):

\[
a(T) = T_c[\alpha(1 - t) - \alpha'(1 - t)^2 + ...]. \tag{4}
\]

The second and higher terms in the expansion are omitted and therefore, when temperature deviates significantly from \( T_c \), one cannot expect the model to have a good precision. We note that recently measured \( H_{c2}(T) \) is linear in \( T \) in a wide region near \( T_c \) in both \( YBCO \) and \((K, Ba)BiO_3 \ [41,39]\).

(4) \textbf{Constant nonfluctuating magnetic field}

For strongly type II superconductors like the high \( T_c \) cuprates not very far from \( H_{c2}(T) \) (this easily covers the range of interest in this paper, for the detailed discussion of the range of applicability beyond it see ref. [42]) magnetic field is homogeneous to a high degree due to superposition from many vortices. Inhomogeneity is of order \( 1/\kappa^2 \sim 10^{-3} \).

Since the main subject of this study is thermal fluctuation effects of the order parameter field, one might ask whether thermal fluctuations of the electromagnetic field should be also taken into account. Halperin, Lubensky and Ma considered this question long time ago [43]. The conclusion was that they are completely negligible for very large \( \kappa \). Upon discovery of the high \( T_c \) cuprates, the issue was reconsidered [44] and the same result was obtained to a very high precision. Therefore here magnetic field is treated both as constant and nonfluctuating \((B = H)\) and the last term in eq.(1) can be omitted (to precision of order \( 1/\kappa^2 \)). However when we calculate the magnetization, \( M = (B - H)/4\pi \) which is of order \( 1/\kappa^2 \), higher order correction must be considered.
Recently it was claimed that the “vortex loops” fluctuations are important and even might lead to additional phase transition at field of order $Gi H_{c2}$ [45]. This is of order $100G$ for the materials of interest listed in Table 2 and therefore is irrelevant for physics discussed in this paper. Note that $Gi$ in the papers discussing the vortex loops [46] physics is assumed to be much larger. We discuss this issue in section IV.

(5) Disorder.

Point-like disorder is always present in YBCO. For example magnetization becomes irreversible. Melting line of the optimally doped or underdoped samples bends towards lower fields [7] and signs of the second order transition appear at $12T$ [47]. However in some samples like fully oxidized $YBa_2Cu_3O_7$ [6] and $DyBa_2Cu_3O_7$ [8,48] the disorder effects are minor especially at temperature close to $T_c$. In the maximally oxidized YBCO [6] the second order transition associated with disorder is not seen even at highest available fields (30T). Certain aspects of the disorder problem were addressed in the framework of GL theory [49], elasticity theory [50] and phenomenological approach based on the Lindermann criterion [13].

C. Landau level modes in the quasi momentum basis

Assuming that all the requirements are met we now divide the fluctuations into the LLL and HLL modes. Throughout most of the paper will use the coherence length $\xi = \sqrt{\hbar^2/(2m_{ab}T_c)}$ as a unit of length, $T_c$ as unit of temperature and $\frac{dH_{c2}(T_c)}{dT_c}T_c = \frac{\Phi_0}{2\pi \xi^2}$ as a unit of magnetic field. As we mentioned above, we assume constant magnetic induction $B = b H_{c2}$ which is slightly different from the external magnetic field $H = h H_{c2}$. After rescaling eq.(1) by $x \rightarrow \xi x, y \rightarrow \xi y, z \rightarrow \xi z, \psi^2 \rightarrow 2aT_c \psi^2 (\gamma \equiv \sqrt{m_c/m_{ab}})$ one obtains the Boltzmann factor:

$$f = \frac{F}{T} = \frac{1}{\omega} \int d^3x \left[ \frac{1}{2} |D\psi|^2 + \frac{1}{2} |\partial_z \psi|^2 - \left( a_h + \frac{b}{2} \right) |\psi|^2 + \frac{1}{2} |\psi|^4 + \frac{\kappa^2}{4} (b - h)^2 \right],$$

(5)

where dimensionless parameter

$$\omega = \sqrt{2Gi} \pi^2 t$$

(6)

characterizes the strength of thermal fluctuations. The commonly used dimensionless Ginzburg number is defined by

$$Gi \equiv \frac{1}{2} \left( \frac{32\pi e^2 \kappa^2 \xi T_c}{c^2 \hbar^2} \right)^2.$$

(7)

And

$$a_h = \frac{1 - t - b}{2}.$$

(8)

defines the distance from the mean field transition line. It is convenient to expand the order parameter field in a complete basis of noninteracting theory: the Landau levels. In the hexagonal lattice phase the most convenient basis is the quasi-momentum basis:
Here $\psi^n_k(x, y, z)$ is the eigenstate of the $n^{th}$ Landau level $\varepsilon_n = (n + 1/2)b$ with two dimensional quasi-momentum $k$ with the hexagonal symmetry:

$$
\psi(x, y, z) = \frac{1}{\sqrt{2}} \sqrt{\frac{2}{\pi}} \frac{1}{3} \int_k \sum_{n=0}^{\infty} e^{-ikz} \varphi^n_k(x, y) \psi^n(k, k_z). \tag{9}
$$

The function $\varphi_A \equiv \varphi^n_k=0$ describes the Abrikosov lattice solution [9].

Even in the liquid state which is more symmetric than the hexagonal lattice, we find it convenient to use this basis.

Naively, if the magnetic field is sufficiently high, the energy gap of the order $b$ separating the $n = 0$ LLL modes from the HLL is very large it is reasonable to keep only the LLL modes in eq.(5). The dominance of the LLL modes for melting was discussed in ref.[11], and Pierson and Valls in ref. [35] and we will discuss it in more detail in section V. In the rest of this section, we consider the LLL GL model.

D. The LLL scaling

Using the LLL condition $|D\psi|^2 = b|\psi|^2$, the free energy simplifies:

$$
f = \frac{1}{\omega} \int d^3x \left[ \frac{1}{2} |\partial_z \psi|^2 - a_h |\psi|^2 + \frac{1}{2} |\psi|^4 + \frac{\kappa^2 (b-h)^2}{4} \right]. \tag{11}
$$

There is no longer a gradient term in directions perpendicular to the field and consequently the model possesses the LLL scaling [51]. After additional rescaling

$x \rightarrow x/\sqrt{b}, y \rightarrow y/\sqrt{b}, z \rightarrow z \left( \frac{b\omega}{4\pi \sqrt{2}} \right)^{-1/3}, \psi \rightarrow \left( \frac{b\omega}{4\pi \sqrt{2}} \right)^{1/3} \psi$, the dimensionless free energy takes a form:

$$
f = \frac{1}{4\pi \sqrt{2}} \int d^3x \left[ \frac{1}{2} |\partial_z \psi|^2 + a_T |\psi|^2 + \frac{1}{2} |\psi|^4 + \kappa^2 \left( \frac{b\omega}{4\pi \sqrt{2}} \right)^{-4/3} \frac{(b-h)^2}{4} \right]. \tag{12}
$$

Minimizing it with respect to $b$ leads to magnetization $b - h$ of the order $\frac{1}{\kappa^2}$. This means that in the strongly type II limit ($\kappa >> 1$) the last term is of the order $1/\kappa^2$ and can be neglected. The theory has a single dimensionless parameter, the Thouless scaled temperature defined by:

$$
a_T = - \left( \frac{b\omega}{2^{5/2}\pi} \right)^{-2/3} a_h. \tag{13a}
$$

8
The Gibbs free energy density in the newly scaled model is defined as:

\[
g(\alpha_T) = -\frac{4\pi\sqrt{2}}{V} \log \int D\psi D\psi^* \exp \{-f[\psi]\};
\] (14)

which is also a function of \(\alpha_T\) only (\(4\pi\sqrt{2}\) is the scaled “temperature”). The relation to the original Gibbs free energy is:

\[
G(T, H) = \frac{H^2_c}{2\pi \kappa^2} \left( \frac{b\omega}{2^{5/2} \pi} \right)^{4/3} g(\alpha_T).
\] (15)

### III. OVERCOOLED LIQUID AND THE T=0 FIXED POINT OF THE LLL MODEL

#### A. Mean field approximation: absence of the finite temperature pseudo critical point for the vortex liquid.

The energy of the hexagonal solid in mean field (neglecting mesoscopic thermal fluctuations) is [9]:

\[
g_{\text{sol}}^M = -\frac{a_T^2}{2\beta_A}; \quad G_{\text{sol}}^M = -\frac{H^2_c}{4\pi \kappa^2 \beta_A} a_h^2
\] (16)

where \(\beta_A = 1.1596\) and the subscript “\(\hat{M}\)” underlies similarity to the Madelung energy of atomic solids. The major fluctuations contribution to the solid free energy is due to the “phonon” modes. In harmonic approximation it is proportional to the fluctuation temperature \(T = a_T^{-3/2}\):

\[
g_1^{\text{sol}} = 2.848 |a_T|^{1/2}; \quad G_1^{\text{sol}} = C_1^{\text{sol}} T;
\] (17)

\[
C_1^{\text{sol}} = 2.848 \frac{H_c^2 B}{8\kappa^2 T_c} \sqrt{|a_h|}.
\]

At low fluctuation temperatures one can neglect the \(T\) dependence of \(a_h \simeq -(1 - b)/2\). Solid becomes unstable at \(a_T = -5\) according to the self consistent (gaussian) approximation [19].

In the (homogeneous) liquid state order parameter vanishes and the contributions to free energy come solely from fluctuations. The gaussian (“mean field”) approximation to the free energy [14] is

\[
g = 4\sqrt{\varepsilon} - 4/\varepsilon,
\] (18)

where the excitation energy \(\varepsilon\) is given by a solution of the cubic ”gap equation”

\[
\varepsilon^{3/2} - a_T \sqrt{\varepsilon} - 4 = 0.
\] (19)

The liquid state becomes metastable below the melting temperature, but unlike the solid above melting, does not loose metastability at certain ”spinodal” point [52]. It persists all
the way down to \( T = 0 \). The excitation energy of the supercooled liquid approaches zero as a power \( \varepsilon \sim (a_T^3)^{\frac{16}{3}} \). For \( a_T \to -\infty \), the scaled energy eq.(18) has an expansion in \( \frac{1}{a_T^3} \propto T^2 \) for small fluctuation temperature \( T \) (the radius of convergence of the expansion extending to \( a_T = -3 \)). Therefore the liquid despite having energy larger than that of solid becomes (pseudo) critical [53] at zero temperature. Physical quantities ”around” this point exhibits a power behavior with characteristic (pseudo) critical exponents. The metastable liquid state has a distinct Madelung energy

\[
G_{\text{M}}^{\text{liq}} = -\frac{H_2^2}{8\pi \kappa^2}a_T^2.
\]

As temperature increases the difference between the solid and the liquid becomes smaller and vanishes at melting. Generally one expects a linear correction at small \( T \):

\[
G^{\text{liq}} = G_{\text{M}}^{\text{liq}} + C_1^{\text{liq}}T.
\]

Since the expansion of the mean field free energy is in \( T^2 \): \( C_1^{\text{liq}} = 0 \). Comparing the solid free energy eqs.(16,17) with eq.(21), we get the melting temperature \( a_T^m = -6.3 \). We therefore conclude that in this approximation the supercooled liquid state exists down to its pseudo critical point at zero temperature. Moreover the pseudo critical point might govern the behavior of the liquid phase to temperature as high as the melting point.

**B. The large N approximation and the Lopatin - Kotliar model of the Abrikosov lattice melting**

It is important to confirm the above scenario in an exactly solvable model. The simplest model of this kind is the multicomponent GL model. The LLL GL theory can be generalized (in several different ways) to an \( N \) component order parameter field \( \psi^a, a = 1, \ldots, N \):

\[
f = \frac{1}{4\pi \sqrt{2}} \int d^3x \left[ \frac{1}{2} |\partial_z \psi^a|^2 + a_T |\psi^a|^2 + \frac{\nu}{2N} |\psi^a|^2 |\psi^b|^2 + \frac{1 - \nu}{2N} \psi^a \psi^{*a} \psi^b \psi^{*b} \right].
\]

The large \( N \) limit of this theory can be solved in a way similar to that in the \( N \) component scalar models widely used in theory of critical phenomena [22]. The simplest case \( \nu = 1 \) has been considered in ref. [30]. It was found that the homogeneous state is stable at all temperatures. Under assumption that the conventional Abrikosov lattice takes over at low temperatures it supported the original conjecture by Brezin et al. [11] that melting of the flux lattice is a first order phase transition. However it was shown (by explicit numerical evaluation) in [12] that the low temperature ground state in that model is not the Abrikosov lattice state in which just one component has a nonzero expectation value (similar to the one component Abrikosov lattice). The ”true” ground state has infinite degeneracy. Different ground states at large \( N \) are markedly different from the hexagonal lattice. The case \( \nu = 2 \), in which the Abrikosov lattice state is a stable ground state, was first introduced in [32] (in what follows it will be referred to as the LK model). Eq.(22) is a slight generalization including both models studied in ref. [30,32]. We find that in fact all models with \( \nu \geq 2 \) possess such a stable lattice state.
A straightforward method to develop the $1/N$ expansion with the last component of $\psi^N$ having the expectation value $\propto \varphi_A \equiv \varphi_{k=0}^N$, describing the hexagonal lattice (see see eq.(10)), is to shift this field $\psi^N(x,y,z) \to \psi^N(x,y,z) + \sqrt{Nc}\varphi_A(x,y)$, where $c$ is a (real) constant. Then one introduces Hubbard - Stratonovich (HS) fields $\rho, \chi$ [32] via free energy:

$$f[\psi^a, \rho, \chi] = \frac{1}{4\pi\sqrt{2}} \left\langle \frac{1}{2} |\partial_x \psi^a|^2 + (\nu \rho + a_T)|\psi^a|^2 + \nu c^2|\varphi_A|^2|\psi^a|^2 + \frac{1 - \nu}{2} \left[(c^2\varphi_A^2 + \chi)|\psi^a|^2 + cc\right] \right\rangle_x$$

$$- \frac{N}{4\pi\sqrt{2}} \left\langle \frac{\nu}{2} \rho^2 + \frac{1 - \nu}{2} |\chi|^2 \right\rangle_x + N \int f_{nf} + ...$$

(23)

Here the "nonfluctuating part" is the Abrikosov free energy density

$$f_{nf} = \frac{1}{4\pi\sqrt{2}} \left[ a_T c^2 + \frac{\beta_A}{2} c^4 \right].$$

(24)

We omitted several cubic terms which do not influence the leading order in $1/N$.

Integrating over the fluctuating the $\psi^a$ fields one obtains the effective scaled Gibbs energy density (the calculation is very similar to that in [19], where technical details can be found):

$$\frac{g_{eff}}{N} = a_T c^2 + \frac{\beta_A}{2} c^4 - \left\langle \frac{\nu}{2} \rho^2 + \frac{1 - \nu}{2} |\chi|^2 \right\rangle_x + 2 \left\langle \sqrt{\epsilon_O(k)} + \sqrt{\epsilon_A(k)} \right\rangle_k.$$  

(25)

The spectrum has two branches:

$$\epsilon_{O,A}(k) = a_T + v \left( \beta_k c^2 + \rho_k \right) \pm \left| (1 - v) \left( c^2\gamma_k + \chi_k \right) \right|.$$  

(26)

To have a stable perturbative Abrikosov solution, the spectrum should be positive definite for $\rho_k = \chi_k = 0$. Thus we demand $-\nu/2 + (\nu - 1) \geq 0$ or $\nu \geq 2$, as stated above. Here both HS fields

$$\rho_k = \left\langle \rho(x)|\varphi_k(x)|^2 \right\rangle_x; \quad \chi_k = \left\langle \chi(x)\varphi_k^*(x)\varphi_k^*(x) \right\rangle_x$$

(27)

and the constant $c$ should minimize free energy $g_{eff}$.

**C. The inhomogeneous (solid) solution**

The minimization with respect to $\rho(x)$ and $\chi(x)$ leads to

$$\rho(x) = \left\langle |\varphi_k(x)|^2 \left\{ [\epsilon_O(k)]^{-1/2} + [\epsilon_A(k)]^{-1/2} \right\} \right\rangle_k$$

$$sign (1 - \nu) \chi(x) = \left\langle \varphi_k(x)\varphi_{-k}(x) \frac{c^2\gamma_k + \chi_k}{c^2\gamma_k + \chi_k} \left\{ [\epsilon_O(k)]^{-1/2} - [\epsilon_A(k)]^{-1/2} \right\} \right\rangle_k,$$

which, in terms of Fourier harmonics of the hexagonal lattice, takes a form:

$$\rho_l = \left\langle \beta_{l-k} \left\{ [\epsilon_O(k)]^{-1/2} + [\epsilon_A(k)]^{-1/2} \right\} \right\rangle_k$$

$$sign (1 - \nu) \chi_l = \left\langle \gamma_{l-k} \frac{c^2\gamma_k + \chi_k}{c^2\gamma_k + \chi_k} \left\{ [\epsilon_O(k)]^{-1/2} - [\epsilon_A(k)]^{-1/2} \right\} \right\rangle_k.$$
The lattice functions $\beta_k, \gamma_k, \gamma_{k,l}$ are defined in appendix of [19]. The only consistent solution preserving the hexagonal symmetry is $\chi_k = \chi_c \gamma_k$, and the above equation will simplify to:

$$\text{sign} \left( 1 - \nu \right) \chi_c \beta_A = \left\langle \text{sign} \left( c^2 + \chi_c \right) \eta_k \left\{ \left[ \epsilon_O(k) \right]^{-1/2} - \left[ \epsilon_A(k) \right]^{-1/2} \right\} \right\rangle_k. \quad (30)$$

For the LK model [32], $\nu = 2$, this leads to: $\chi_c \beta_A = \left\langle \eta_k \left\{ \left[ \epsilon_A(k) \right]^{-1/2} - \left[ \epsilon_O(k) \right]^{-1/2} \right\} \right\rangle_k.$

Finally the set of the minimization equations ($\chi \geq 0$) is

$$0 = a_T + \beta_A c^2 + 2 \left\langle \beta_k \left\{ \left[ \epsilon_O(k) \right]^{-1/2} + \left[ \epsilon_A(k) \right]^{-1/2} \right\} \right\rangle_k +$$

$$\left\langle \eta_k \left\{ \left[ \epsilon_O(k) \right]^{-1/2} - \left[ \epsilon_A(k) \right]^{-1/2} \right\} \right\rangle_k$$

$$\chi_c \beta_A = \left\langle \eta_k \left\{ \left[ \epsilon_A(k) \right]^{-1/2} - \left[ \epsilon_O(k) \right]^{-1/2} \right\} \right\rangle_k \quad (31)$$

$$\rho_l = \left\langle \beta_{l-k} \left\{ \left[ \epsilon_O(k) \right]^{-1/2} + \left[ \epsilon_A(k) \right]^{-1/2} \right\} \right\rangle_k$$

and

$$\epsilon_{O,A}(k) = a_T + 2\beta_k c^2 + 2\rho_k \pm \left( c^2 + \chi_c \right) \gamma_k. \quad (32)$$

Following formulas will be useful for the calculation of the free energy:

$$\left\langle \rho^2 \right\rangle = \left\langle \beta_{l-k} \left\{ \left[ \epsilon_O(k) \right]^{-1/2} + \left[ \epsilon_A(k) \right]^{-1/2} \right\} \left\{ \left[ \epsilon_O(l) \right]^{-1/2} + \left[ \epsilon_A(l) \right]^{-1/2} \right\} \right\rangle_{k,l}$$

$$\left\langle |\chi|^2 \right\rangle = \frac{1}{\beta_A} \left[ \left\langle \eta_k \left\{ \left[ \epsilon_A(k) \right]^{-1/2} - \left[ \epsilon_O(k) \right]^{-1/2} \right\} \right\rangle_k \right]^2 \quad (33)$$

The equations in eq.(31) can be solved using mode expansion [32,19]. The spectrum can be written as follows

$$\epsilon_O(k) = E(k) + \Delta \eta_k, \epsilon_A(k) = E(k) - \Delta \eta_k, \quad (34)$$

with $E(k)$ expanded in modes

$$E(k) = \sum E_n \beta_n(k), \quad (35)$$

where

$$\beta_k = \sum_{n=0}^{\infty} \exp[-2\pi n/\sqrt{3}] \beta_n(k), \quad \beta_n(k) \equiv \sum_{|\mathbf{x}|^2=4\pi n/\sqrt{3}} \exp[i \mathbf{k} \cdot \mathbf{x}]. \quad (36)$$

The integer $n$ determines the distance of a points on reciprocal lattice from the origin. The effective ”expansion parameter” is $\exp[-2\pi/\sqrt{3}] = 0.0265$ and coefficients decrease exponentially with $n$ [19]as can be seen from Table 1.
Table 1

| $a_T$   | $g$     | $E_1$          | $E_2$          | $E_3$          | $\Delta$     |
|---------|---------|----------------|----------------|----------------|-------------|
| -4.6179| -3.43164| 0.728715       | -0.0022412     | -0.00001227    | 0.6167      |
| -5      | -4.96636| 1.92669        | 0.0717767      | 0.00003881     | 2.0331      |
| -10     | -34.3165| 6.29543        | 0.355908       | 0.00023872     | 7.2718      |
| -20     | -159.826| 13.8477        | 0.842385       | 0.0058357      | 16.3036     |

The solution disappears at $a_T = -4.6179$. At this point the solid is no longer a metastable state. $\epsilon_A(k)$ is a gapless mode and $\epsilon_A(k) \to const. k^2$ for $k \to 0$. For perturbative spectrum, $\epsilon_A(k) \to const. k^4$ for $k \to 0$.

D. Melting in the LK model

The energy corresponding to the solid solution of the minimization equation eq.(31) calculated from

$$g_{eff} = a_T c^2 + \frac{\beta_A}{2} c^4 - \left( \rho^2 - \frac{1}{2} |\chi|^2 \right)_x + 2 \left( \sqrt{\epsilon_O(k)} + \sqrt{\epsilon_A(k)} \right)_k$$

is given in Table 1. The convergence of the mode expansion is exponential.

For liquid, we impose rotationally invariant Ansatz with $c^2 = 0$, $\chi = 0$ and obtain the gap equation

$$\rho = \frac{2}{\sqrt{a_T + 2\rho}},$$

which minimizes energy

$$g_{liq} = -\rho^2 + 4\sqrt{a_T + 2\rho}.$$  \hspace{1cm} (39)

The results for both the liquid and the solid free energy are plotted on Fig.2. The melting point appears at $a_T = -5.15$.

It is well approximated in the whole region by its low temperature expansion in powers of $|a_T|^{-3/2}$ (which is proportional to the ”fluctuation temperature” $T$ assuming that at low temperatures $a_h \simeq -(1 - b)/2$)

$$\frac{g_{sol}}{a_T^2} = c_{M}^{sol} + c_1^{sol} T + c_2^{sol} T^2 \ldots, T \equiv |a_T|^{-3/2}, \hspace{1cm} (40)$$

$$c_{M}^{sol} = -\frac{1}{2\beta_A}; c_1^{sol} = 2.84835; c_2^{sol} = -2.54087.$$  

The first two terms are the same as for the one component model, while the two loop correction is different.

Similarly the liquid energy can be expanded, but this time in powers of square of the ”fluctuation temperature $T$.
Here the first term is the "Madelung energy" of liquid at zero fluctuation temperature. Note that, as in the mean field approximation to the one component theory, there is no term linear in $T$ (the harmonic approximation). This means that the specific heat vanishes at zero temperature. Retaining just the Madelung and the harmonic term for solid we estimate the melting temperature in the linear approximation:

$$T_m = \frac{c_{\text{sol}}^M - c_{\text{liq}}^M}{c_{\text{liq}}^M - c_{\text{sol}}^M}$$

The latent heat in the same approximation is:

$$\Delta U = c_{\text{sol}}^M - c_{\text{liq}}^M.$$

Numerically this melting temperature $T_m = 0.064$ corresponding to $a_T = -6.25$ and the latent heat $\Delta U = 0.18$ should be compared with the exact results: $T_m = 0.086$ ($a_T = -5.15$), $\Delta U = 0.122945$.

To conclude obtains the first order melting. Supercooled liquid persists as a metastable state all the way to zero temperature. We emphasize that this means that the matching of the (Borel - Pade approximant to) liquid to solid energy at $T = 0$ employed in [14] to improve convergence of the series is not only ineffective [24], but should lead to an incorrect result. Liquid and solid energies are different in the limit of zero fluctuation temperature.

**E. General hypothesis about melting of lattices made of repelling objects**

In atomic liquids, an attractive long range force is generally present. As a result the supercooled liquid state loses its metastability at an end point (spinodal) [52]. Lovett argued on general grounds long time ago [54] (stability analysis of approximate set of relations between density correlators) that for certain purely repelling interactions the spinodal point disappears (shifted to zero temperature) and is recovered when the attractive interaction is introduced. The existence of a metastable overcooled liquid down to zero temperature for repelling particles therefore might be quite general. The best studied example of mutually repelling particles is the classical one component Coulomb plasma. We assume that, as in the vortex system at low temperature, the supercooled liquid has a Madelung energy and moreover its free energy has a low temperature expansion. The free and internal energies at low temperatures can be expanded as:

$$F_{\text{sol,liq}} = C_{M}^\text{sol,liq} + C_{1}^\text{sol,liq}T_f + C_{2}^\text{sol,liq}T_f^2 - \frac{3}{2}T_f \log T_f + ...$$

$$U_{\text{sol,liq}} = C_{M}^\text{sol,liq} + \frac{3}{2}T_f - C_{2}^\text{sol,liq}T_f^2 + ..., $$

where scaled temperature $T_f$ is inverse of to the dimensionless plasma parameter $\Gamma = \left( \frac{4\pi n_s}{3} \right)^{1/3} e^2 / T$ for density $n_s$. Existent Monte Carlo simulations of the internal energy in
the stable and metastable region of the 3D one component Coulomb plasma [55] can be well fitted (see solid line on Fig. 3) by

\[ C_{\text{liq}}^{M} = -0.89186, \quad C_{2 \text{liq}}^{M} = -23.89. \]  

(45)

It underestimates the internal energy at higher temperatures. Note that this fit is quite different from a variety of the fractional power expressions used at higher temperatures. One of the more successful (not very far from the melting point) liquid theories based on density functional approach is [56]:

\[ U_{\text{liq}} = -0.9 + 0.388 \frac{T^3}{T_f^{3/5}} \]  

(46)

(dashed line in Fig. 3). Note however that these expression cannot be continued to \( T = 0 \), since finite packing parameter is assumed. Unfortunately the coefficient \( C_{\text{liq}}^{1} \) cannot be deduced from internal energy only, while free energy is not available at large coupling. In the solid the analytical calculation gives [57]

\[ C_{\text{sol}}^{M} = -0.895929, \quad C_{1 \text{sol}}^{M} = -1.8856, \quad C_{2 \text{sol}}^{M} = -10.84. \]  

(47)

This was corroborated by recent simulations [58]. Using the linear in \( T \) approximation eq.(43) we obtain latent heat \( \Delta U = 0.0041 \), which should be compared with MC simulation result [59] \( \Delta U = 0.043 \). From the measured melting temperature [57] \( T_m = 1/172 \) and coefficients fitted above one deduces

\[ C_{\text{liq}}^{1} = -2.5. \]  

(48)

One observes that even at melting the linear approximation is justified (the \( C_{\text{liq}}^{2} \) contribution to free energy account for less than 10% of the linear one). It would be very interesting to simulate the 3D Coulomb plasma at even stronger coupling \( \Gamma > 200 \) to verify the existence of expansion of supercooled liquid free energy as in eq.(44). We expect that other liquids with purely repulsive interactions like the Yukawa (screened Coulomb) studied recently in connection with ”dusty plasma” or colloid suspensions physics [60] or even hard core repulsion lead to qualitatively similar result. An intriguing question is whether structure function is universal in the zero temperature limit of the liquid phase. Since ideal liquid is (pseudo) critical, certain universal properties are expected. Even more closely related to the vortex system is the quantum one component plasma - electron gas. The quantum particle is described by a fluctuating line very analogous to a thermally fluctuating vortex line. Here we consider 2D electron gas at zero temperature

\[ H = -\frac{\hbar^2}{2m} \sum_i v^2_i + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|r_i - r_j|}. \]  

(49)

The path integral of this system is quite analogous to a system of repelling flux lines. The quantum fluctuations in 2DEG replace the thermal fluctuations of the vortex system. In quantum partition function

\[ Z = \int D\Psi D\Psi^* \exp \left[ \frac{i}{\hbar} A(\Psi, \Psi^*) \right] \]  

(50)
with the fermionic (Grassmannian) field $\Psi$ replacing the bosonic field in eq. (2). The (Wigner) solid solution can be well approximated by the expansion in quantum fluctuations $T_q = 1/\sqrt{T_s} = h^{(\pi n_s)^{1/4}}$ [21],

$$E^{\text{sol}} = C_M^{\text{sol}} + C_1^{\text{sol}} T_q + C_2^{\text{sol}} T_q^2,$$

where $C_M^{\text{sol}} = -2.2122, C_1^{\text{sol}} = 1.6284, C_2^{\text{sol}} = 0.058$. For unpolarized liquid, a very good fit in wide range of densities is [21]:

$$E^{\text{liq}} = -\frac{8\sqrt{2}}{3\pi} + T_q^2 + \frac{a_0(T_q + a_1)}{T_q^3 + a_1 T_q^2 + a_2 T_q + a_3},$$

$$a_0 = -0.3568, a_1 = 1.13, a_2 = 0.9052, a_3 = 0.4165.$$

The fit in the low temperature region

$$E^{\text{liq}} = C_M^{\text{liq}} + C_1^{\text{liq}} T_q + ...$$

gives liquid Madelung energy $C_M^{\text{liq}} = -2.18154$, while leading correction is $C_1^{\text{liq}} = 1.45266$. The transition to Wigner crystal occurs at $T_q^m = 0.174$ corresponding to $r_s = 33$. Variational MC simulation [21] indicates that the transition occurs at $r_s = 37$.

**IV. BORREL - PADE METHOD APPLIED TO THE LLL MODEL. MELTING LINE, MAGNETIZATION AND SPECIFIC HEAT.**

**A. The BP method applied to liquid energy**

As we have seen above, within mean field the liquid branch exhibits a pseudo critical point [53] at $T = 0$. It is well known that in the theory of critical phenomena one can obtain an accurate description in the critical region by applying the Borel - Pade methods to perturbation expansion at ”weak coupling” [23]. In technical terms there exists a renormalization group flow from the weak coupling fixed point towards the strongly coupled one [22]. We therefore start with (the renormalized) weak coupling (high temperature or non-ideal gas) expansion.

The liquid LLL (scaled) free energy is written as [14]

$$g_{\text{liq}} = 4\varepsilon^{1/2}[1 + h(x)].$$

(51)

The function $h$ can be expanded as

$$h(x) = \sum c_n x^n,$$

(52)

where the ”small parameter” $x = \frac{1}{2}\varepsilon^{-3/2}$ is defined as a solution of the Gaussian gap equation for the excitation energy $\varepsilon$, eq.(72). The coefficients $c_n$ can be found in [25]. The consecutive approximants are plotted on Fig.4 as dashed lines ($T_1$ to $T_9$, $T_0$ being equivalent to the Gaussian mean field). One clearly sees that the series are asymptotic and can be used only at $a_T > -2$. One can improve on this by optimizing the variational
parameter $\varepsilon$ at each order instead of fixing it at the first order calculation. The procedure is rather involved, see [61], however the optimized perturbation series is convergent with radius of convergence about $a_T = -5$ (see dash dotted lines 1 to 9 on Fig.4). Now we construct the BP series and compare them with the optimized perturbation series results for $a_T > -5$.

We will denote by $h_k(x)$ the $[k, k-1]$ BP transform [23] of $h(x)$ (other BP approximants violate the correct low temperature asymptotics). The BP transform is defined as

$$h_k = \int_0^{\infty} \tilde{h}_k(xt) \exp(-t) \, dt$$

(53)

where $\tilde{h}_k$ is the $[k, k-1]$ Pade transform of $\sum_{n=1}^{2k-1} \frac{c_n x^n}{n!}$, namely a rational function $\sum_{i=1}^{k} a_i x_i / \sum_{i=1}^{k-1} b_i x_i$ with the same expansion at small $x$ as the original function.

For $k = 4$ and $k = 5$, the liquid energy converges to required precision (0.1%), see Fig. 4. On this Figure only $k = 3$ and 5 are shown since $k = 4$ practically coincides with the latter. In what follows we will use $h_5$ as the best available approximation of the liquid branch. The liquid energy completely agrees with the optimized Gaussian expansion results [15] till its radius of convergence at $a_T = -5$. We therefore conclude that $k = 5$ is quite sufficient for our purposes.

Since the metastable liquid state exists at all temperatures one can consider the $T = 0$ limit. One finds:

$$\frac{g^{\text{liq}}(a_T)}{g^{\text{sol}}(a_T)} \to 0.964$$

(54)

for $a_T \to -\infty$. For $g^{\text{sol}}(a_T)$, the leading term in this limit is $-\frac{a_T^2}{2\beta_A}$, which is the Madelung energy of the solid. The leading term for $g^{\text{liq}}(a_T)$ is $-0.964 \frac{a_T^2}{2\beta_A}$. Usually the Madelung energy for the solid phase of the point particle system is realized by minimizing the potential energy of the system (the minimum is often obtained by taking the hexagonal lattice for the repulsive system in 2D). In this vortex system, we can have the supercooled liquid down to $a_T \to -\infty$ ($T \to 0$). The leading term for the overcooled liquid energy, or the Madelung energy of the liquid is therefore equal to $-0.964 \frac{a_T^2}{2\beta_A}$, which is slightly larger than the Madelung energy of the solid. This limit, the ”ideal liquid”, however cannot be thought as a minimization of a potential energy.

**B. Melting line. Comparison with Monte Carlo simulations and Lindemann criterion.**

The solid energy to two loops is [17,19]:

$$g_{\text{sol}} = -\frac{a_T^2}{2\beta_A} + 2.848 |a_T|^{1/2} + \frac{2.4}{a_T}$$

(55)

where $\beta_A = 1.1596$. On Fig. 1 of ref. [18] we plot the energies of solid and liquid. They are very close near melting (see the difference on inset of this figure). We find that the melting point is:
\[ a_T^m = -9.5. \]

The available 3D Monte Carlo simulations [26] unfortunately are not precise enough to provide an accurate melting point since the LLL scaling is violated and one gets values of \( a_T^m = -14.5, -13.2, -10.9 \) at magnetic fields 1, 2, 5T respectively. We found also that the theoretical magnetization calculated by using parameters given by ref. [26] is in a very good agreement with the Monte Carlo simulation result of ref. [26]. However the determination of melting temperature needs higher precision, and the sample size (\( \sim 100 \) vortices) used in ref. [26] may be not large enough to give an accurate determination of the melting temperature (due to boundary effects, LLL scaling will be violated too). The situation in 2D is better since the sample size is much larger. We performed similar calculation for the 2D LLL GL liquid free energy, combined it with the earlier solid energy calculation [17,19]

\[
g_{\text{sol}} = -\frac{a_T^2}{2\beta_A} + 2 \log \frac{|a_T|}{4\pi^2} - \frac{19.9}{a_T^2} - 2.92. \tag{57} \]

and find that the melting point \( a_T^m = -13.2 \). It is in good agreement with MC simulations [28].

Phenomenologically melting line can be located using Lindemann criterion or its more refined version using Debye - Waller factor. The more refined criterion is required since vortices are not point like. It was found numerically for Yukawa gas [60] that the Debye - Waller factor \( e^{-2W} \) (ratio of the structure function at the second Bragg peak at melting to its value at \( T = 0 \)) is about 60\% at the melting point. Using methods of [62], one obtains for the 3D LLL GL model

\[
e^{-2W} = 0.59. \tag{58} \]

C. Fitting of the melting line. Values of the Ginzburg numbers of various superconductors

In this subsection we use the above results to fit experimental melting line of several ”fluctuating” superconductors. As an example on Fig.2 of ref. [18] we presented the fitting of the melting line of fully oxidized \( YBa_2Cu_3O_7 \) [6]. Melting lines of two different samples of the optimally doped untwinned [2,38] near \( T_c \) (YBa2Cu3O7−δ), \( DyBa_2Cu_3O_7 \) [8] and \((K, Ba)BiO_3 \) [39] are also fitted extremely well. The results of fitting are given in Table 2

(To remind our convention, \( H_{c2} \) is defined as \( T_c \frac{dH_{c2}(T)}{dT} \bigg|_{T=T_c} \) rather than (often inaccessible) \( H_{c2}(T = 0) \)).

| material         | \( T_c \) | \( H_{c2} \) | \( G_i \) | \( \kappa \) | \( \gamma \) | reference |
|------------------|----------|---------------|----------|-------------|-------------|-----------|
| \( YBCO_{7-\delta} \) | 93.1     | 167.5         | 1.9 \times 10^{-4} | 48.5        | 7.76        | [2]       |
|                  | 92.6     | 190           | 2 \times 10^{-4}    | 50          | 8.3         | [38]      |
| \( YBCO_7 \)     | 88.2     | 175.9         | 7.0 \times 10^{-5}  | 50          | 4           | [6]       |
| \( DyBCO_{0.67} \) | 90.1     | 163           | 3.2 \times 10^{-6}  | 33.77       | 5.3         | [8]       |
| \((K, Ba)BiO_3\) | 31       | 26            | 5.3 \times 10^{-5}  | 107         | 1           | [39]      |
Our value for the Ginzburg number of YBCO and DyBCO estimated here are generally lower than the ones commonly believed in the literature. Often quoted value for YBCO is of order $G_i = 0.01$ (see page 1134 of commonly used ref. [10]). The direct calculation from eq.(7) gives $G_i = 0.003$ for $\lambda = 1400 \text{ A}$, $\xi = 15 \text{ A}$, and $\gamma = 7$ ($\kappa = 93.3$). Note however that these values are estimated from measurements at very low temperature. Our values of $\lambda$ and $\xi$ are fitted to the vortex physics experiments near $T_c$ and extrapolating using (admittedly questionable) two liquid model to $T = 0$ give $\lambda = 931 \text{ A}$, $\xi = 18.7 \text{ A}$. Our values of $\frac{dH_c(T)}{dT}$ near $T_c$ are consistent with recent measurement [41] (about 2) and smaller than earlier ones. There is no consensus on values of $\kappa$ measured using the microwave technique at very low temperatures, however they are also generally smaller than 100 (smaller than 70 at $T = 0$ and decreasing with temperature according to ref. [63] and from 50 to 60 in ref. [64]). This explains the difference of order of magnitude in $G_i$ between the often used values and our fitting results (small $\kappa$ will lead a small $G_i$ as $G_i \propto \kappa^4 \xi^2 \gamma^2$). We emphasize that the actual small parameter in the theory is not $G_i$ but rather $\omega = \sqrt{2G_i \pi}$ (see eq.(5)). Even for Ginzburg number as small as $2 \times 10^{-4}$ this quantity is 0.2. As a result the effect of thermal fluctuations is important on a significant portion of the phase diagram.

Recently it was found that thermal fluctuation are quite significant even in a low $T_c$ material ($K,Ba$)BiO$_3$. This is despite its lower critical temperature and very small anisotropy (and thereby very small Ginzburg number $5.3 \times 10^{-5}$). Since this material is not a "strange metal" nor d-wave superconductor, its $H_{c2}$ is directly accessible and there is no problem with direct estimate of $G_i$. $\omega = 0.1$ for ($K,Ba$)BiO$_3$ is not much smaller than that of YBCO. There is therefore no surprise (contrary to a statement in ref. [39]) that fluctuation effects are still experimentally observable in ($K,Ba$)BiO$_3$. In order to be able safely ignore thermal fluctuations the fluctuation parameter $\omega$ should be of order 0.01 in which case $G_i$ should be smaller than $5 \times 10^{-7}$. These are the cases of most low $T_c$ materials.

### D. Magnetization jump at melting

The scaled magnetization (of liquid or solid) is defined by:

$$m(a_T) = -\frac{d}{da_T} g(a_T), \quad (59)$$

while the LLL contribution to the magnetization is

$$M_{LLL} = \frac{H_{c2}}{4\pi\kappa^2} \frac{a_h}{a_T} m(a_T). \quad (60)$$

Using expressions eqs.(55) for solid and eqs. (51,53) for liquid the magnetization jump $\Delta M$ at the melting point $a_T^m = -9.5$ divided by the magnetization at the melting on the solid side is

$$\frac{\Delta M}{M_s} = \frac{\Delta m}{m_s} = 0.018. \quad (61)$$
It is indeed small and is compared on Fig. 2 of ref. [18] (right inset) with experimental results of fully oxidized $YBa_2Cu_3O_7$ [6] (rhombs) and optimally doped untwinned $YBa_2Cu_3O_{7−δ}$ [4] (stars). The agreement is quite good. If the HLL contribution is significant (see next section) eq.(61) is expected to be violated.

E. Specific heat jump at melting

In addition to the delta function like spike at melting for specific heat experiments, the experiments also show specific heat jump. The theory allows us to quantitatively estimate it. The specific heat contribution due to the vortex matter is $C = −T \frac{∂^2}{∂T^2} G(T, H)$. The normalized specific heat is defined as

$$ c = \frac{C}{C_{mf}}, $$

where $C_{mf} = \frac{\beta H^2}{4\pi^2 \lambda^2_{AF} T_c^2}$ is the mean field specific heat of solid. Substituting the definition of the scaled free energy eq.(15) and scaled temperature eq.(13a), we obtain:

$$ c = \frac{-16\beta_A}{9t^2} \left( \frac{b\omega}{4\pi\sqrt{2}} \right)^{4/3} g(a_T) + \frac{4\beta_A}{3t^2} (b-1-t) \left( \frac{b\omega}{4\pi\sqrt{2}} \right)^{2/3} g'(a_T) $$

$$ -\frac{\beta_A}{9t^2} (2-2b+t)^2 g''(a_T) $$

Using our expressions for energy of liquid and solid we obtain the following specific heat jump at melting:

$$ \Delta c = 0.0075 \left( \frac{2-2b+t}{t} \right)^2 - 0.20 Gt^{1/3} \left( b-1-t \right) \left( \frac{b}{t^2} \right)^{2/3}. \quad (62) $$

Using the parameters of $YBCO_{7−δ}$ obtained by fitting the melting line, Table 2, we compare eq.(62) with the experimental result of ref. [2] in Fig. 2 of ref. [18] (right inset). Note that error bars are very large and also that disorder might be important [49], so that the agreement of the theoretical and experimental result of specific jump is not good as that of magnetization jump.

V. HIGHER LANDAU LEVELS CONTRIBUTIONS. EFFECTIVE LLL MODEL.

A. Where is the LLL approximation really valid?

Contributions of HLL are important phenomenologically in two sections of the phase diagram. The first is at temperature above the mean field critical temperature $T_c(H)$ inside the liquid phase. The second is far below the melting point deep inside the solid phase. Naively in the solid phase, when ”distance from the mean field transition line” is smaller than the ”inter Landau level gap”, $1-t-b < 2b$, one expects that higher Landau
harmonics can be neglected. More careful examination shows that a weaker condition $1 - t - b < 12b$ should be used for a validity test of the LLL approximation \cite{42} to calculate the mean field contributions in vortex solid. Additional factor 6 comes from the hexagonal symmetry of the lattice since contributions of higher Landau levels (HLL), first to fifth HLL do not appear in perturbative calculation. In the liquid state the question has been studied by Lawrie \cite{65} using the Hartree-Fock (gaussian) approximation. The result was that the region of validity is limited, but quite wide, see Fig.1.

In this section we will incorporate the leading HLL correction using Gaussian approximation and then compare the theoretical results with experimental magnetization curves.

B. Gaussian Approximation in the liquid phase

The free energy density beyond the LLL approximation is:

$$G = -\frac{\omega H_{c2}^2}{2\pi\kappa^2 vol} \log \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \exp \left( -\frac{1}{\omega} \int d^3x \left( \frac{1}{2} |\nabla\psi|^2 - a_h |\psi|^2 + \frac{1}{2} |\psi|^4 \right) \right),$$

(63)

where $vol$ denotes volume. In the framework of the Gaussian (Hartree-Fock) approximation free energy is divided into an optimized quadratic part $K$, and a ”small” part $V$. Then $K$ is chosen in such a way that the gaussian energy is minimal. The gaussian energy is a rigorous lower bound on energy. Due to translational symmetry of the vortex liquid, an arbitrary $U(1)$ symmetric quadratic part $K$ has only one variational parameter $\varepsilon$:

$$K = \frac{1}{\omega} \int d^3x \left( \frac{1}{2} (|\nabla\psi|^2 - b|\psi|^2) + \frac{1}{2} |\partial_z \psi|^2 + \varepsilon |\psi|^2 \right).$$

(64)

The small perturbation is therefore:

$$V = \frac{1}{\omega} \int d^3x \left[ (-a_h - \varepsilon) |\psi|^2 + \frac{1}{2} |\psi|^4 \right].$$

(65)

The Gaussian energy consists of two parts. The first is the ”Trace log” term:

$$-\frac{\omega H_{c2}^2}{2\pi\kappa^2 vol} \log \left[ \int \mathcal{D}\psi \exp(-K) \right] = \frac{\omega H_{c2}^2}{2\pi\kappa^2} b \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} \sqrt{n b + \varepsilon},$$

(66)

The second is proportional to the expectation value of $v$ in a solvable model defined by $K$

$$\frac{\omega H_{c2}^2}{2\pi\kappa^2} \langle V \rangle = \frac{\omega H_{c2}^2}{2\pi\kappa^2} [(-a_h - \varepsilon) b \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} \frac{1}{\sqrt{n b + \varepsilon}}$$

$$+\omega \left( \frac{b}{2\sqrt{2\pi}} \sum_{n=0}^{\infty} \frac{1}{\sqrt{n b + \varepsilon}} \right)^2].$$

(67)

Both are divergent in the ultraviolet in a sense that at large $n$ the sums diverge.

Introducing an UV momentum cutoff in a sense that at large $n$ the sums diverge.

Introducing an UV momentum cutoff which effectively limits the number of Landau levels to $N_f = \frac{A}{b} - 1$, the Trlog term diverges as:

21
\[
\frac{1}{\sqrt{2\pi}} b \sum_{n=0}^{\infty} \sqrt{nb + \varepsilon} = \frac{1}{\sqrt{2\pi}} \left( \frac{2}{3} \Lambda^{3/2} + \left( \varepsilon - \frac{b}{2} \right) \Lambda^{1/2} \right) + u(\varepsilon, b) \quad (68)
\]

with the last term, function \( u \) being finite. The "bubble" integral diverges logarithmically:

\[
\frac{b}{2\sqrt{2\pi}} \sum_{n=0}^{\infty} \frac{1}{\sqrt{nb + \varepsilon}} = \frac{1}{\sqrt{2\pi}} \Lambda^{1/2} + u', \quad (69)
\]

where \( u' \equiv \frac{\partial}{\partial \varepsilon} u(\varepsilon, b) \). Substituting eq. (68) into the gaussian energy one obtains (in units of \( \frac{\omega H^2}{2\pi \kappa^2} \)):

\[
g_{\text{Gauss}} = \frac{1}{\sqrt{2\pi}} \frac{2}{3} \Lambda^{3/2} + \omega \left( \frac{1}{\sqrt{2\pi}} \Lambda^{1/2} \right)^2 + \left( -a_h - \frac{b}{2} \right) \frac{1}{\sqrt{2\pi}} \Lambda^{1/2} - a_h u' \\
+ 2\omega \frac{1}{\sqrt{2\pi}} \Lambda^{1/2} u' - \varepsilon u' + \omega (u')^2 + u. \quad (70)
\]

The first term does not depend on parameters of the system and can be ignored (the renormalization of the reference energy density), while the second is \( \omega \) dependent and indicates that \( T_c \) present inside \( a_h \) is renormalized. Defining \( a_h = a_h^r + 2\omega \frac{1}{\sqrt{2\pi}} \Lambda^{1/2} \), the above energy becomes:

\[
g_{\text{Gauss}} = -\omega \left( \frac{1}{\sqrt{2\pi}} \Lambda^{1/2} \right)^2 + \left( -a_h^r - \frac{b}{2} \right) \frac{1}{\sqrt{2\pi}} \Lambda^{1/2} - a_h^r u' \\
- \varepsilon u' + \omega (u')^2 + u. \quad (71)
\]

Thus the temperature \( T_c \) and vacuum energy will be renormalized. The first two terms in free energy are divergent and linear in fluctuation temperature \( \omega \), they will not contribute to any physical quantities like magnetization and specific heat. Minimizing the energy eq. (71), we get the gap equation:

\[
\varepsilon = -a_h^r + 2\omega u' \quad (72)
\]

Superscript "\( r \)" will be dropped later on. The function \( u(\varepsilon, b) \) can be written in the following form

\[
u(\varepsilon, b) = \frac{1}{\sqrt{2\pi}} b^{3/2} v \left( \frac{\varepsilon}{b} \right), \quad (73)
\]

where

\[
v(x) = \sum_{n=0}^{\infty} \left[ \sqrt{n + x} - \frac{2}{3} (x + n + \frac{1}{2})^{3/2} + \frac{2}{3} (x + n - \frac{1}{2})^{3/2} \right] - \frac{2}{3} (x - \frac{1}{2})^{3/2}. \quad (74)
\]

For the LLL model in the Gaussian approximation, \( v(x) = \sqrt{x} \). In the "Prange" limit \([66]\) \( G_i \to 0 \), the free energy is

\[
\frac{\omega H^2}{2\pi \kappa^2} \frac{1}{\sqrt{2\pi}} b^{3/2} v \left( -\frac{a_h}{b} \right). \quad (75)
\]
C. Integration of the HLL modes and the effective LLL model

A method for treating HLL modes is integrating them and obtaining an effective LLL model. The (effective) LLL model is applicable in a surprisingly wide range of fields and temperatures determined by the condition that the relevant excitation energy $\varepsilon$ is much smaller than the gap between Landau levels $b$. Within the mean field approximation in the liquid $\varepsilon$ is a solution of the gap equation of eq.(72). For the LLL dominance region, we take a conservative condition $\varepsilon/\varepsilon_c = 1/20$. One observes that, apart from the fields smaller than $H_{LLL} \approx 0.1 T$ for YBCO, the experimentally observed melting line and its neighborhood are well within the range of applicability of this approximation as shown in Fig.1.

The effective LLL energy (we will use unit of energy density $H_2^2c^2/2\pi\kappa$ in this subsection) functional is defined by:

$$g_{eff}[\psi_0] = -\frac{\omega}{vol} \log \int \prod_{i=1}^{\infty} D\psi_i D\psi_i^* \exp \{-f[\psi_0, \psi_0^*, \psi_i, \psi_i^*]\}, \quad (76)$$

where $\psi_0$ is the LLL $N = 0$ component field and the rest are denoted by $\psi_i$. Expanding the functional up to the fourth order in $\psi_0$ and to the second order in $\partial_z$ one obtains:

$$g_{eff}[\psi_0] = \Delta g + \frac{\Delta t}{2}\|\psi_0\|^2 + \omega f_{LLL}[\psi_0]. \quad (77)$$

$$f_{LLL}[\psi_0] = \frac{1}{\omega} \left[ \frac{1}{2}\|\partial_z \psi_{HLL}\|^2 - a_h\|\psi_{HLL}\|^2 + \frac{1}{2}\|\psi_{HLL}\|^4 \right]. \quad (79)$$

The direct (no $\psi_0$ dependence) renormalization of energy is:

$$\Delta g = -\frac{\omega}{vol} \log \int \prod_{i=1}^{\infty} D\psi_i D\psi_i^* \exp \{-f_{HLL}[\psi_i]\}, \quad (78)$$

where the HLL energy is

$$f_{HLL} = \frac{1}{\omega} \left[ \frac{1}{2}\|\partial_z \psi_{HLL}\|^2 - a_h\|\psi_{HLL}\|^2 + \frac{1}{2}\|\psi_{HLL}\|^4 \right], \quad (79)$$

where $\psi_{HLL} = \sum_{i=1}^{\infty} \psi_i$. To calculate $\Delta g$, we divide the $f_{HLL}$ into

$$K_{HLL} = \frac{1}{\omega} \left( \frac{1}{2} (|D\psi|^2 - b|\psi|^2) + \frac{1}{2} |\partial_z \psi|^2 + \varepsilon|\psi|^2 \right) \quad (80)$$

plus $f_{HLL} - K_{HLL}$. Taking $\varepsilon$ as the solution of the gap equation of eq.(72), $\Delta g$ takes a form:

$$\Delta g = g_{Gauss} - g_{LLL} + 2 \langle |\psi_0|^2 \rangle \left( \langle |\psi_0|^2 \rangle - \langle |\psi|^2 \rangle \right); \quad (81)$$

$$g_{LLL} = -\frac{\omega}{vol} \log \int D\psi_0 D\psi_0^* \exp \{-f_{LLL}[\psi_0]\}.$$
quantity $g_{\text{LLL}}$ is the effective free energy calculated with variational parameter $\varepsilon$ and $\langle |\psi_0|^2 \rangle$ is the expectation value in the LLL GL. The consistency (or matching) requirement is:

$$g_{\text{eff}} = -\frac{\omega}{\text{vol}} \log \int \mathcal{D}\psi_0 \overline{\mathcal{D}\psi_0} \exp \left\{ -\frac{1}{\omega} g_{\text{eff}}[\psi_0] \right\}. \quad (82)$$

This condition determines the value of $\Delta t$:

$$\Delta t = 4 \left( \langle |\psi|^2 \rangle - \langle |\psi_0|^2 \rangle \right) = 4\omega \left[ u'(\varepsilon, b) \right] - 4 \langle |\psi_0|^2 \rangle$$

$$= 4\omega \frac{1}{\sqrt{2\pi}} b^{1/2} \left[ v' \left(\frac{\varepsilon}{b}\right) - \frac{1}{2} \sqrt{\frac{b}{\varepsilon}} \right]. \quad (83)$$

For $YBCO$, the correction $\Delta t$ is small. The effective LLL GL approach achieves a simplification by starting from the LLL effective model with $T_c$ and other parameters renormalized to account for the contribution of the HLL modes. This is what we assumed in sections III and IV. In particular, this approach is very precise if we calculate the properties along the melting line. For example, the magnetization jump is mostly due to the fluctuation of the LLL modes, the background effective energy $\Delta g$ will not contribute anything since it is the same on both sides of the melting line.

**D. The HLL contribution to Magnetization**

Generally when $\kappa$ is quite large and magnetization can be approximated by

$$M = -\frac{\partial}{\partial H} G(T, H). \quad (84)$$

The HLL correction will be calculated as follows. We numerically solve the gap equation (72) from which $G(T, H)$ can be obtained. Then eq.(84) is used to calculate the magnetization of the full GL model in Gaussian approximation. The HLL correction is thus the magnetization of the full GL model in gaussian approximation minus the magnetization of the LLL contribution in gaussian approximation. We compare the experiments using following approximation. While the corrections due to HLL are calculated in gaussian approximation, the LLL contribution will be calculated nonperturbatively. The comparison of the theoretical predictions with the experiments for fully oxidized $YBa_2Cu_3O_7$ [6], is shown on Fig. 3 of ref. [18]. We used the experimental asymmetry value $\gamma = 4$ and values of $T_c$, $H_{c2}$ and $G_i$ from the fitting of the melting curve (see Table 2). The agreement is fair at intermediate magnetic fields, while at low magnetic fields is not good. It is expected that agreement is improved at higher fields. It is not clear whether magnetization (in contrast to magnetization jump at melting) will be strongly influenced by disorder, so at this time it is not possible to consider optimal doped $YBCO$ magnetization curved more quantitatively.

We comment that the theory of the full GL model (higher Landau levels included) beyond Gaussian approximation is required at low magnetic fields. Indeed experimentally it is often claimed that one can establish the LLL scaling for fields above 3 T for $YBCO$ (see, for example, ref. [35]) as at low magnetic fields, the HLL contribution will be significant.
VI. SUMMARY

The problem of calculating the fluctuations effects in the framework of the Ginzburg-Landau approach to vortex matter in type II superconductors is sufficiently precisely solved in the LLL approximation to allow quantitative description of the melting transition. We provided an evidence that metastable homogeneous state (the supercooled liquid state) exists down to zero fluctuation temperature by solving the large \( N \) Ginzburg-Landau model. Based on this understanding the supercooled liquid state is approached using methods of physics of critical phenomena (the Borel - Pade resummation technique). Applicability of the effective lowest Landau level model was subsequently discussed and corrections due to higher levels is calculated.

The theory is then applied to quantitatively describe a great variety of experiments (confined to a region not far from \( T_c \)) including melting curves of \( \textit{YBCO}, \textit{DyBCO}, (\textit{K,Ba})\textit{BiO}_3 \), magnetization curves, discontinuities of various quantities at melting.

We speculate that any system of repelling objects (examples include classical one component plasma, electron gas...) exhibits similar features. The supercooled metastable state extends down to zero temperature. At this limit there is a well defined Madelung energy of the "ideal liquid". This ideal liquid is a pseudo critical point which controls the supercooled state possibly up to the melting temperature and might have universal features.

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\[ \int dz \int dk \left( -\frac{1}{2} \frac{\partial^2}{\partial z^2} + \varepsilon \right) \psi_k^*(z) \psi_k(z) + c \left| \psi_k^*(z) \psi_k(z) \right|^2 \]. Different momenta in directions xy are decoupled, thus the fixed point is not related to second order melting. This also explains the appearance of unexpected critical exponents.
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Figure captions

Fig. 1
Comparison of the experimental melting line for fully oxidized YBa$_2$Cu$_3$O$_7$ with our theoretical fitting. Applicability of the LLL approximation is between two lines, the solid LLL applicability line and the (liquid) LLL dominance line. The GL model applicability line is also plotted.

Fig. 2
Free energy of solid (line) and liquid (dashed line) of the LargeN model as function of the fluctuation temperature $1/|a_T|^{3/2}$. The solid line ends at a point (dot) indicating the loss of metastability.

Fig. 3
Internal energy of the classical one component Coulomb plasma. The dashed line is the fit given by eq.(46) and the solid line is the fit given by eq.(44).

Fig. 4
The BP approximation for the free energy. BP3 and BP5 are the free energy results given by $h_3$ and $h_5$. The dashed line $Ti$ is the original perturbative expansion of order $i$ in ref. [14] and the the dot dashed line $i$ is the optimized expansion of order $i$. 
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Fig. 1
Scaled Free Energy

Fluctuation Temperature

Liquid
Solid
Instability Point
Melting Point

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Fig. 2
Li and Rosenstein

Fig. 3

\[ U + C_M \]
Fig. 4