Participation-Ratio Entropy and Critical Fluctuations in the Thermodynamics of Pancake Vortices

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Abstract

We report on a study of the thermodynamics of the Ginzburg-Landau model for two-dimensional type-II superconductors near the transition from the normal state to the Abrikosov-lattice state. We couch our analysis in terms of the participation-ratio entropy, $s(P)$, which expresses the volume in order-parameter-space with a given participation-ratio for the local superfluid density. $s(P)$ completely determines the thermodynamics of the system. We report on results for $s(P)$ obtained analytically using perturbation expansion methods and numerically using Monte Carlo simulation methods and discuss the weak first-order phase transition which occurs in this system in terms of the properties of $s(P)$.
The discovery of high-temperature superconductivity in materials with strong planar anisotropy has led to renewed experimental [1–4] and theoretical [5–9] interest in the properties of two-dimensional and strongly anisotropic three-dimensional type-II superconductors at fields near $H_{c2}(T)$ where thermal fluctuations are important. Phase transitions of type-II superconductors in a magnetic field are unusual because of the Landau level degeneracy of Cooper-pair states in a magnetic field $[[10]]$. In mean-field-theory continuous phase transitions occur simultaneously in a number of channels equal to the Landau level degeneracy and the low-temperature Abrikosov lattice state has both superconducting and positional order. The Cooper-pair Landau level degeneracy also increases the importance of fluctuations and as a result the phase transition is considerably rounded. It is well established experimentally and theoretically that the Abrikosov vortex lattice state in $D = 3$ dimension melts into a vortex liquid state through a weakly first order phase transition, $[[3,4,6,11,12]]$. A consensus $[[8,13–15]]$ has emerged from recent work that a weak first-order phase transition with a latent heat which is $\sim 2\%$ of the mean-field condensation energy at the depressed transition temperature also survives in $D = 2$, although this view is not universally held $[[16]]$. We have previously $[[14]]$ introduced a formulation of the thermodynamics of this system in terms of a quantity, $s(P)$, which we refer to here as the participation-ratio entropy and which measures the volume in order-parameter space associated with a given participation ratio for the local superfluid density. In this Letter we report on evaluations of $s(P)$ based on high-temperature and low-temperature expansions and on Monte-Carlo simulations of the Ginzburg-Landau (GL) model.

For fields sufficiently close to $H_{c2}$ the order parameter is confined to the lowest Cooper-pair Landau-level $[[17]]$. The free energy density of the lowest-Landau-level GL (LLL-GL) model is

$$f[\Psi] = (\alpha(T) + \hbar e H/m^* c)|\Psi|^2 + \frac{\beta}{2}|\Psi|^4$$

(1)

where $\alpha(T) = \alpha'(T - T_{c0})$, $T_{c0}$ is the zero-field transition temperature, $m^*$ parameterizes the energy cost of spatial variation of the order parameter and $\beta$ is taken to be independent of
The mean-field theory transition temperature satisfies $\alpha_H(T_{c2}) \equiv \alpha(T_{c2}) + \hbar e H / m^* c = 0$. The LLL-GL model free energy is $F_{GL} \equiv \int d\vec{r} f[\Psi(\vec{r})]$. For $T < T_{c2}$ the quadratic term in Eq. (1) lowers $F_{GL}$ while the quartic term always makes a positive contribution. Our approach to the thermodynamics of this system is based on the observation that for a given magnitude of the quadratic term in $F_{GL}[\Psi]$ the quartic term is larger when the order parameter has a smaller participation ratio $\beta_A[\Psi]$.

$$P[\Psi] = \frac{\left(\int d^2 \vec{r} |\Psi|^2\right)^2}{A \int d^2 \vec{r} |\Psi|^4},$$

(2)

$P[\Psi]$ is roughly the fraction of the area $A$ of the sample over which the local superfluid density $|\Psi|^2$ is spread. (In LLL-GL theory $P^{-1}[\Psi]$ is known as the Abrikosov ratio, $\beta_A[\Psi]$.) For a given participation ratio the minimum of $F_{GL}/A$ is $-\alpha_H^2 P/2$. Any order parameter in the LLL has one zero (vortex) for each magnetic flux quantum through the system and therefore cannot have the constant value required to obtain $P = 1$. The mean-field-theory order parameter of the LLL-GL model is the LLL order parameter with the maximum value of $P$; $P$ is maximized by placing the vortices on a triangular lattice; $P_\Delta = 1/\beta_A \Delta = 0.862370 \cdots$. At finite temperatures the properties of the LLL-GL model are determined by a competition between the thermal weighting factor $\exp(-F_{GL}[\Psi]/k_B T)$ which favors large values of $P[\Psi]$ and the distribution function of $P[\Psi]$ which is peaked at smaller values of $P$ as we discuss below.

We choose to work in the Landau gauge ($\vec{A} = (0, B x, 0)$). The order parameter $\Psi(\vec{r})$ can then be expanded in the form, [14]

$$\Psi(\vec{r}) = \left(\frac{|\alpha_H| \pi \ell^2}{\beta}\right)^{1/2} \sum_k C_k (\pi^{1/2} L_y \ell)^{-1/2} \exp(i k y) \exp(-(x - k \ell^2)^2 / 2 \ell^2)$$

(3)

where the number of terms in the sum over $k$ is $N_\phi = L_x L_y / 2 \pi \ell^2$ and $\ell^2 = \hbar / 2 e B$. We define the following intensive thermodynamic variables, which will be used to describe the system. A dimensionless average local superfluid density is defined by

$$\Delta_0[C_k] = \frac{1}{N_\phi} \left(\frac{|\alpha_H| \pi \ell^2}{\beta}\right)^{-1} \int d\vec{r} |\Psi(\vec{r})|^2 = \frac{1}{N_\phi} \sum_k |C_k|^2.$$

(4)
The participation ratio, defined by Eq. (2) is

\[ P[C_k] = \frac{\left( \sum_k |C_k|^2 \right)^2}{\sum_{k_1k_2k_3k_4} \bar{C}_{k_1} \bar{C}_{k_2} C_{k_3} C_{k_4} \delta_{k_1+k_2+k_3+k_4} \Theta(k_1, k_2, k_3, k_4)} \] (5)

where \( \Theta(k_1, k_2, k_3, k_4) = (N_\phi L_x/L_y)^{1/2} \exp\left\{ -\frac{\ell^2}{2} \left[ \sum_1^4 k_i^2 - \frac{1}{4} \left( \sum_1^4 k_i \right)^2 \right] \right\} \). In terms of \( \Delta_0 \) and \( P \), the LLL-GL free energy has the following form:

\[ \frac{F_{GL}[C_k]}{N_\phi k_B T} = g^2 (\text{sgn}(\alpha_H) \Delta_0[C_k] + \frac{(\Delta_0[C_k])^2}{4P[C_k]}). \] (6)

Temperature and field enter only through \( g \equiv \alpha_H(\pi\ell^2/\beta k_B T)^{1/2} \propto (T - T_{c2})/(TH)^{1/2} \).

The partition function for the LLL-GL model is

\[ Z = (\frac{\alpha_H|\pi\ell^2/\beta}{C_k})N_\phi \prod_k d\bar{C}_k dC_k \exp\{-F_{GL}[C_k]/k_B T\}, \] (7)

and can be rewritten as the following form: \[ Z = \int d\Delta_0 dP \exp\{-N_\phi f(\Delta_0, P, g^2)\} \] (8)

where

\[ f(\Delta_0, P, g^2) = g^2 (\text{sgn}(\alpha_H) \Delta_0^2 + \frac{\Delta_0^2}{4P}) - s(\Delta_0, P) - \ln(|\alpha_H|\pi\ell^2/\beta) \] (9)

and

\[ s(\Delta_0, P) = \frac{1}{N_\phi} \ln \prod_k \int d\bar{C}_k dC_k \delta(P - P[C_k]) \delta(\Delta_0 - \Delta_0[C_k]). \] (10)

Because \( P[C_k] \) is invariant under a scale change of \( |\Psi(\vec{r})|^2 \), it follows that

\[ s(\Delta_0, P) = \ln \Delta_0 + s(P). \] (11)

The participation-ratio entropy, \( s(P) \equiv s(1, P) \), expresses the portion of volume in the phase space with a given participation ratio.

In the thermodynamic limit fluctuations in \( \Delta_0[C_k] \) and \( P[C_k] \) are negligible so that the free energy of the system at a given temperature \( (g) \) can be obtained by simply minimizing
\( f(\Delta_0, P, g^2) \) with respect to \( \Delta_0 \) and \( P \). It follows that the equilibrium values of \( \Delta_0 \) and \( P \) satisfy

\[
g^2(\text{sgn}(\alpha_H)) + \frac{1}{2P}\Delta_0 - \frac{1}{\Delta_0} = 0 \tag{12}
\]

and

\[
s'(P) = -\frac{1}{4P^2}g^2\Delta_0^2. \tag{13}
\]

Eq. (12) establishes a functional relationship between \( \Delta_0 \) and \( P \) which originates in the fact that the properties of the system do not depend on \( \alpha_H \) and \( \beta \) independently but only on \( g \propto \alpha_H/\beta^{1/2} \). Note that for \( g >> 1 \) \( \Delta_0 = g^{-2} \) while for \( g << 1 \) \( \Delta_0 = 2P \). Eq. (13) then fixes the equilibrium values of \( P \) and \( \Delta_0 \) and hence the free energy. This equation reflects the balance between the rate of increase of volume in order-parameter-space and the rate of decrease of condensation energy which fixes the equilibrium participation ratio. Note that the right hand side of Eq. (13) vanishes for \( g >> 1 \); the equilibrium value of \( P \) in the high temperature limit is the value of \( P \) where \( s(P) \) is maximized, i.e. the most probable value of \( P \) in order parameter space. We remark a stable equilibrium can occur at any temperature at participation-ratio \( P \) only if

\[
s''(P) < 0. \tag{14}
\]

We now turn to the evaluation of \( s(P) \). Since \( P \) is positive definite this function is defined on the interval \((0, P_\Delta)\) and we can evaluate it analytically near both end points of the interval. For \( P \) near \( P_\Delta \) we can approximate \( P[C_k] \) by a Taylor series expansion to second order around an Abrikosov vortex lattice state. Since the Abrikosov lattice states occur at an extremum of \( P[C_k] \) linear terms are absent and by formally diagonalizing the resulting quadratic form we find that the volume in order-parameter-space with a given value of \( P \) is proportional to the surface area of a sphere in \( \sim 2N_\phi \) dimensions with radius proportional to \((P_\Delta - P)^{1/2}\). It follows that for \( P \) near \( P_\Delta \)

\[
s(P) \approx \ln(P_\Delta - P). \tag{15}
\]
The participation-ratio entropy for small $P$ is most easily evaluated by using the symmetric gauge expansion of the order parameter $\tilde{\alpha}_x/\pi k_B T$ in terms of eigenfunctions with definite angular momentum, $m$. In this case order parameters which are confined to an area $\sim k/N_\phi A$ centered on the origin, must be expanded in terms of the eigenfunctions with $m < k$. It follows that the order-parameter-space volume with $P < k/N_\phi$ at $\Delta_0 = 1$ is given by the surface area of a sphere in $k$ dimensions with radius $N_\phi^{1/2}$ and hence that for $P$ going to zero

$$s(P) \approx -P \ln P.$$  

(16)

We can also obtain analytic results for the expansion of $s(P)$ about its maximum by using the high-temperature expansion of the free-energy of the GL-LLL model [20]:

$$F = N_\phi k_B T (\ln(\tilde{\alpha}_x/\pi k_B T) + f_{2D}(x))$$  

(17)

where $\alpha_H = \tilde{\alpha}_x(1 - 4x)$, $x \equiv (\beta k_B T)/(4\pi\ell^2\tilde{\alpha}_x^2)$ and $g = (1 - 4x)/\sqrt{4x}$. ($x$ is non-negative, $x = 1/4$ at $T_{c2}$, $x \to 0$ for $g \to +\infty$ and $x \to \infty$ for $g \to -\infty$.) Coefficients in the power series expansion of $f_{2D}(x)$ may be evaluated using a diagrammatic perturbation expansion in terms of self-consistent Hartree correlation functions. The six leading coefficients were obtained by Ruggeri and Thouless [20] and the expansion was later extended to eleventh order by Brézin, Fujita and Hikami [21] and recently to thirteenth order by us. [22]. The equilibrium values of $\Delta_0$ and $P$ may be expressed in terms of $f_{2D}(x)$ by differentiating the free energy with respect to $\alpha_H$ and $\beta$. [22]:

$$P(x) = \frac{(1 - 2x f'_{2D}(x))^2}{(4 + (1 - 4x)f_{2D}(x))(1 + 4x)}$$

$$= \frac{1}{2} + x - \frac{8}{3} x^2 + \frac{452}{15} x^3 - 431.59018759018753 x^4 + 7170.5968205856756 x^5$$

$$- 134096.68933891651 x^6 + 2772357.9400791259 x^7 - 62615750.77811569 x^8$$

$$+ 1532019484.1067800 x^9 - 40349691260.478735 x^{10} + 1138241888638.9989 x^{11}$$

$$- 3424789174798.4099 x^{12} + \cdots.$$  

(18)

Using Eq. (13) and the high temperature expansion of $\Delta_0(x)$ we obtain the following expansion for the parametric dependence of $s'(P)$ on $x$:
\[ s'(P(x)) = - \frac{(4 + (1 - 4x)f'_{2D}(x))^2 x}{(1 - 2xf'_{2D}(x))^2} \]
\[ = -4x + 8x^2 - \frac{260}{3} x^3 + 1020.800000000000 x^4 - 14012.376334776334 x^5 \]
\[ + 219842.58347280514 x^6 - 3870523.5408992074 x^7 + 75492832.18250102 x^8 \]
\[ - 1615943686.2025482 x^9 + 37680981633.278216 x^{10} - 951344015946.40479 x^{11} \]
\[ + 25869507417290.368 x^{12} + \cdots \] (19)

Eq. (18) can be inverted to expand \( x \) in terms of \( \tilde{P} \equiv P - 1/2 \). Inserting this series in Eq. (19) gives \( s'(P) \) as a series in \( \tilde{P} \). Integrating this series and determining \( s(P = 1/2) \) by direct evaluation we find

\[ S(P) = 1 + \ln \pi + 0 \tilde{P} - 4 \tilde{P}^2 - \frac{160}{9} \tilde{P}^3 + \frac{1096}{45} \tilde{P}^4 - 802.2613949013954 \tilde{P}^5 \]
\[ + 16926.259949713371 \tilde{P}^6 - 499062.26189198034 \tilde{P}^7 + 17336002.792339820 \tilde{P}^8 \]
\[ - 688621672.74816198 \tilde{P}^9 + 30506759410.693500 \tilde{P}^{10} - 1483164272081.5901 \tilde{P}^{11} \]
\[ + 78249334359919.989 \tilde{P}^{12} - 4439326835886646.1 \tilde{P}^{13} + \cdots \] (20)

Directly evaluating the low-temperature expansion of the LLL-GL model has proven to be an arduous task [23–25] and has led to discordant results. In contrast, using Eq. (15) we can obtain a result for the leading low-temperature correction to the mean-field free energy of the LLL-GL model in a very simple way. We find immediately, in agreement with Ref. [25], that for large \( x \) \((g << 1)\)

\[ f_{2D}(x) = -\frac{(1 - 4x)^2 P_\Delta}{4x} + \ln x. \] (21)

The first term here is the mean-field-theory energy and the correction comes from the low-temperature equilibrium participation-ratio entropy.

It is interesting to observe that equilibrium values of \( P \) vary through a relatively narrow range between the largest possible value for \( P[\Psi] \) \((P_\Delta)\) and the most probable value for \( P[\Psi] \) \((1/2)\) from low temperature to high temperature limits. Useful approximate expressions for the free energy, the magnetization, and the specific heat of the GL-LLL system have been proposed by Tešanović and collaborators [26,27] motivated by this property.
The high-temperature expansion of $s(P)$ around $P = 1/2$ can be extrapolated with the use of Padé approximants for $s'(P)$. The Padé approximants were chosen to satisfy $s'(P) = 1/(P - P_\Delta)$ for $P \to P_\Delta$, and $s(P)$ was obtained by integration. Results are shown in Fig. 1. Poles appear in the approximants for $\bar{P} \sim -0.2$ and the extrapolation to negative values of $\bar{P}$ is not very successful. Nevertheless, we believe that $s(P)$ is a smooth function over the entire interval $(0, P_\Delta)$. This expectation is consistent with numerical results for $s(P)$ obtained by Monte Carlo methods which are also shown in Fig. 1. The Monte Carlo results were extracted from distribution functions for participation-ratio values, $A_\lambda(P)$, calculated using $\exp(-N_\phi(\lambda P + \Delta_0))$ as the sampling function. Since $A_\lambda(P) \propto \exp(N_\phi(s(P) - \lambda P))$, extrema of the distribution occur where $s'(P) = \lambda$. By performing calculations at a series of $\lambda$ values we were able to map out the function $s'(P)$; the results shown in Fig. 1 were obtained by numerical quadrature from the Monte-Carlo results for $s'(P)$. The overall agreement between the analytic and numerical results for the participation-ratio entropy is excellent. The inset in Fig. 1 shows Monte-Carlo results for $s'(P)$ in the narrow range of equilibrium participation-ratio values which occur near the first-order melting transition. We see that in the Monte-Carlo simulations (but not in the analytic results) $s''(P) > 0$ for $P$ in the interval $(0.832, 0.837)$. Equilibrium $P$ values cannot occur in this interval and must therefore have a discontinuity in their temperature dependence. It is this property of the participation-ratio entropy which leads to the weakly first order phase transition in the LLL-GL model.

Our description of the thermodynamics of the LLL-GL model is summarized in Fig. 2 in terms of three contour plots for $f(\Delta_0, P, g^2) + \ln(|\alpha_H|\pi\ell^2/\beta)$. At each $g$ the equilibrium $(\Delta_0, P)$ minimizes $f(\Delta_0, P, g^2)$. The top panel is for a temperature at which the system is in the vortex liquid state, the middle panel is for a temperature close to the phase transition and the bottom panel is for a temperature at which the system is in the vortex lattice state. The trend to decreasing participation ratios at higher temperatures is driven by the increase in the relative importance of the entropy. The first order phase transition occurs because of the occurrence of an interval over which $s''(P)$ is positive. When the optimal $P$ values are close to this interval two local minima appear in the free energy contours and the global
minimum switches from the local minimum at larger $P$ to the local minimum at smaller $P$ as the temperature increases. In the high temperature limit of the model, thermal fluctuations are Gaussian and $P$ approaches $1/2$.

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FIGURES

FIG. 1. Analytic and numerical data for $s(P)$. The inset shows Monte Carlo results for $s'(P)$.

FIG. 2. Contour plots for $f(\Delta_0, P, g^2) + \ln(|\alpha_H|\pi\ell^2/\beta)$ at $g = -5.5$ (top panel, vortex liquid state), $g = -6.6$ (middle panel, at phase transition) and $g = -7.1$ (bottom panel, vortex solid state).