Heat Capacity of Mesoscopic Superconducting Disks

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We study the heat capacity of isolated giant vortex states, which are good angular momentum (L) states, in a mesoscopic superconducting disk using the Ginzburg-Landau (GL) theory. At small magnetic fields the L=0 state qualitatively behaves like the bulk sample characterized by a discontinuity in heat capacity at $T_c$. As the field is increased the discontinuity slowly turns into a continuous change which is a finite size effect. The higher L states show a continuous change in heat capacity at $T_c$ at all fields. We also show that for these higher L states, the behavior of the peak position with change in field is related to the paramagnetic Meissner effect (irreversible) and can lead to an unambiguous observation of positive magnetization in mesoscopic superconductors.

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Superconducting state in mesoscopic samples can have strikingly different properties as compared to the corresponding bulk samples because by definition [1-10], the intrinsic length scales in them, like the penetration depth and the coherence length are of the order of the sample dimensions. Essentially, in a magnetic field a bulk type II superconductor can exist either in the Meissner state (macroscopic condensation of the Cooper pairs to the zero momentum state) or it can exist in a mixed state of higher momenta with infinite components (when there are vortices in the sample). In the presence of a boundary there can be another state called the giant vortex state wherein a very thin region near the surface is superconducting. This edge state in bulk samples affects resistivity measurements because contacts applied at the edges of the superconductor are shorted by it. Therefore, resistivity measurements are useful to determine the magnetic field to nucleate the giant vortex states. Otherwise these edge states are not capable of affecting the thermodynamic properties of the sample inside the phase boundary. Besides, in a large sample it is not possible to isolate the individual giant vortex states because the sample encloses a large amount of flux and a large number of different giant vortex states are equally well formed at the same applied field.

Recent developments in nano-fabrication techniques now allow us to reach the limit of isolating these individual giant vortex states in mesoscopic samples. We expect the thermodynamic properties of these isolated giant vortex states (that can be designated an angular momentum quantum number L) to be completely different from each other and also from the bulk state. Recently, the phase boundary and magnetization of these isolated L states have received some attention. Magnetization in superconductors is due to a gauge dependent equilibrium current and thus it is different in origin from magnetization of magnetic materials where the ordering of individual dipole moments, their dynamics and their internal energy scale determine the magnetization. Heat capacity in superconductors is determined by the thermal excitations of quasiparticles and therefore, it can eventually lead to a better understanding of the microscopic dynamics. For the first time we present a quantitative study of the heat capacity of the isolated giant vortex states, a quantity which is accessible in an experiment. We show that at small fields there is a discontinuous jump in the heat capacity for L=0 state at the transition temperature, a typical feature of second order phase transition, but at higher fields this turns into a continuous change. The line shape shows drastic changes during this crossover which can be interpreted as a crossover from bulk-like to true mesoscopic behavior. On the other hand the higher L states show no discontinuity in heat capacity at all fields. Quantitative calculations strongly suggest that these features can be observed with present day experimental set-ups. Besides, we show that the paramagnetic Meissner effect (irreversible) can be indirectly but unambiguously observed through the heat capacity measurements.

In bulk samples Ginzburg-Landau (GL) theory is valid only close to the normal-superconductor transition when the gap at the Fermi surface approaches zero. So the jump in the specific heat of bulk samples at $T_c$ agrees with the GL theory with high accuracy for some metals. Well below the transition the observed specific heat scales, however, exponentially with temperature, signifying a unique energy scale associated with excitations and dynamics of quasiparticles in the system that originates from the presence of a gap at the Fermi surface, and this does not come out in the GL theory. In the giant vortex state, the GL theory gives the correct magnetization down to 0.33$T_c$ and very small fields. The giant vortex states are current carrying edge states because of which they are sometimes referred to as “gapless superconducting states” (for details we refer to [1]). In the absence of a gap the heat capacity will have a power law behavior below $T_c$ according to the predictions made here based on the GL theory. The absence of gap can also be the reason why the GL theory correctly describes the magnetization at low temperatures.

We consider superconducting disks with radius $R$ and thickness $d$ immersed in an insulating medium. Taking the axis of the disk to be parallel to the $z$ direction and keeping in mind the boundary condition at $z = \pm d/2$, 

one can expand the order parameter as a Fourier series
\( \psi(z, r) = \sum_{k} \cos(\frac{2\pi k}{d} z) \psi_k(r) \). Unlike in bulk samples \( \psi \) is coordinate dependent in the x-y plane. Substituting in the GL equations one can check that for \((\pi \xi / d)^2 >> 1\), the dominant contribution comes from \( \psi_{k=0} \), which naturally means that if the thickness of the disk is less than the coherence length then the order parameter cannot vary in the z direction. Therefore we may assume a uniform order parameter in the z direction and as a consequence the order parameter and currents become two dimensional with an effective penetration length that increases with thickness as \( \lambda_{eff} = \lambda^2 / d \) \( \square \). The flux expulsion from the disk becomes negligible when \( \lambda_{eff} \approx R \). In that case the system is quantitatively described by the GL equation \( \square \) which is generally accepted \( \square \) as a Schrödinger like quantum mechanical equation
\[
(-i \nabla - \vec{A})^2 \psi = (1 - T) \psi (1 - |\psi|^2),
\]
that correctly describes the center of mass of the Cooper pairs. Here \( T \) is temperature in units of \( T_c(0) \) of bulk samples. Distance is measured in units of \( \xi(0) \), the coherence length at zero temperature for bulk samples. The order parameter is measured in \( \Psi(0) \), the finite temperature order parameter of the bulk sample. The vector potential is measured in \( ch / 2e \xi(0) \) and the magnetic field in \( H_{z2} = ch / e \xi^2(0) \). Our choice of units is the same as that in Ref. \( \square \). On the disk surface we require that the normal component of the current density is zero, which gives
\[
(-i \nabla - \vec{A})_n \psi = 0.
\]
Rescaling the lengths \( (R \rightarrow R \sqrt{(1 - T)}) \) and fields \( (H \rightarrow H / (1 - T)) \) we rewrite equation (1) in the following form:
\[
(-i \nabla - \vec{A})^2 \psi = \Psi (1 - |\Psi|^2).
\]
For the bulk samples the gradient term can be neglected \( \square \) and in mesoscopic samples close to the normal superconductor transition the \( |\Psi|^2 \) term can be neglected \( \square \). We show that in the regime of our interest both the terms can be solved exactly in a semi-analytical way.

The difference of the free energy \( G \) between the superconducting and the normal state, measured in \( H^2(0) V / 8 \pi \), can be expressed through the integral
\[
G = \int \left( 2(1 - T)(\vec{A} - \vec{A}_0) \cdot \vec{j} - (1 - T)^2 |\Psi|^4 \right) d^2 r / V,
\]
over the disk volume \( V = \pi R^2 d \), where \( \vec{A}_0 = H r / 2 e \phi \) is the external vector potential, and \( \vec{j} = (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) / 2i - |\Psi|^2 \vec{A} \) is the dimensionless supercurrent. The heat capacity difference between the superconducting and normal states in units of \( C_0 = H_c(0) V / (8 \pi T_c) \) is defined as \( C = - \frac{T \partial G}{\partial T} \). The bulk limit of equation (3) is \( G = H_c(T)^2 V / 8 \pi T_c \) which yields a specific heat jump of 2 in units of \( C_0 \), whereas it can be accurately measured to an order of magnitude smaller values at lower temperatures. As explained before for \( d < \xi \) equation (1) becomes two dimensional \( \square \) i.e.,
\[
\left(-i \nabla - \vec{A}_{2D} \right)^2 \Psi = \Psi (1 - |\Psi|^2).
\]

We write the general solution as a truncated series in the solutions of the Linearized Ginzburg-Landau (LGL) equation (which is basically omitting the \( |\Psi|^2 \) term in (4)) i.e.,
\[
\Psi = A_0^{1/2} \Gamma_l(\vec{r}) + A_1^{1/2} \Gamma_L(\vec{r}) \exp(iL \theta).
\]
Here \( \Gamma_l(\vec{r}) \) and \( \Gamma_L(\vec{r}) \) are solutions of the LGL equation with eigen energies \( \lambda_0 \) and \( \lambda_L \), \( L \) being any non-zero integer giving the angular momentum quantum number. Hence,
\[
\lambda_L = (1 + 2 \nu) \frac{\phi}{R^2} - 1,
\]
where \( \nu \) is to be determined from the solution of the following equation.
\[
\left( L - \frac{\phi}{2} \right) F(-\nu, L + 1, 1 - \frac{\phi}{2}) - \frac{\nu \phi}{L + 1} F(-\nu + 1, L + 2, 1 - \frac{\phi}{2}) = 0,
\]
where \( \phi = HR^2 \) is the flux through the disk in units of flux quantum \( hc/e \). \( F(a, c, y) \) is the Kummer function, and finally
\[
\Gamma_L(\vec{r}) = r^L \exp(-\frac{H r^2}{4}) F(-\nu, L + 1, \frac{H r^2}{2}).
\]

Although we retain only two terms in the series we will show that this is not an approximation in the regime of our interest. Now substituting \( \Psi \) in equation (4) and simplifying we obtain
\[
\lambda_0 A_0 = a_{11} A_0^2 + a_{12} A_0 A_L \]
\[
\lambda_L A_L = a_{22} A_L^2 + a_{12} A_0 A_L \]
where \( V_{a_{11}} = \int \Gamma_l^2 dV \), \( V_{a_{22}} = \int \Gamma_L^2 dV \) and \( V_{a_{12}} = \int \Gamma_l \Gamma_L dV \). We have to solve equations (8) and (9) to evaluate \( A_0 \) and \( A_L \). Three possible solutions are
\[
(A_0 = \lambda_0 / a_{11}, \ A_L = 0),
\]
\[
(A_0 = 0, \ A_L = \lambda_L / a_{22})
\]
and
\[
(A_0 = \frac{\lambda_0 a_{22} - \lambda_L a_{12}}{a_{11} a_{22} - a_{12}^2}, \ A_L = \frac{\lambda_L a_{11} - \lambda_0 a_{12}}{a_{11} a_{22} - a_{12}^2}).
\]

The solution in (10) corresponds to \( L=0 \), the solution in (11) corresponds to \( L \neq 0 \) giant vortex states and the solution in (12) corresponds to a general mixed state solution. In (10) and (11), \( a_{ii} \) contains all the correction due to the non-linear term, \( \lambda_i \) being eigenvalue of
the LGL equation. The mixed state solutions were discussed earlier [14]. As we increase the number of terms in the expansion for $\Psi$ the solution (12) becomes more and more complicated and realistic but solutions (10) and (11) remain unchanged and exact. There is a definite parameter regime where the giant vortex states have a lower free energy than the mixed vortex states and in this regime equations (10) and (11) give the same results as the general numerical solutions [14]. The stability analysis of these giant vortex states has been done analytically from the GL differential equations [14] and numerically from the saddle point analysis of GL free energy [18], essentially proving their stability. Although the basic predictions of our work can be tested with just $L=0$ and the $L=1$ states which are under all conditions completely symmetric states the higher angular momentum giant vortex states have been detected experimentally [13]. Also numerical calculations [1] with a larger number of terms in the expansion, substituted into the GL free energy expression showed that numerically minimized free energy corresponds to only one term in the expansion and the rest are identically zero in certain parameter regimes. This parameter phase diagram is given in Ref. [21] and is the regime of our interest where the solutions (10) and (11) are valid.

In Fig. 1 (a), (b), and (c) we plot $C/C_0$ vs $T/T_c(0)$ at $\phi/\phi_0=0.1, 1.0$ and 1.5 respectively, for all possible $L$ states for a disk of $R = 4.0\ell_0(0)$. Figs. (b) and (c) are displaced by 3 and 6, respectively, in the $y$-direction. The $L=0$ state is the ground state (shown in Fig. 2) but in decreasing fields it is possible to trap the system in the higher $L$ states down to almost zero field due to the Bean-Livingston barrier [21], when fluxoids are trapped at the center of the sample and it can carry a large current [22]. In Fig. 1 (a) the $L=0$ state shows a discontinuity at $T_c$ (we refer to this as bulk-like behavior), while the higher $L$ states show a continuous change at their corresponding $T_c$s. As the flux is increased in Fig. 1 (b) and (c), the discontinuity in the heat capacity for the $L=0$ state slowly changes to a continuous change, although there is a striking difference in the line shapes of the $L=0$ state from those of the $L \neq 0$ states. For high enough fields the line shape of the $L=0$ state will be the same as that of the $L \neq 0$ states as will be shown in Fig. 3. A discontinuity in heat capacity is a characteristic feature of second order phase transition that can be observed in bulk samples. In finite samples the discontinuity is replaced by a continuous change. Symmetry breaking transitions, like solid-liquid melting transition, that are, however, first order transitions associated with a divergence in specific heat in the bulk, give a Gaussian curve in clusters [13]. So the $L=0$ state in Fig. 1 (b) and (c) exhibits mesoscopic effect but not in Fig. 1 (a). In the $L=0$ state the Cooper pairs condense into a zero momentum state ($L$ being its angular momentum) just as bulk superconductivity is macroscopic condensation to the zero momentum state. Then in the absence of fields the boundary condition (2) for the currents at the bound-

ary becomes irrelevant. Thus we get bulk-like behavior which persists at small but finite fields even though for infinitesimally small fields the effect of the boundary conditions set in. The higher $L$ states show no discontinuity in the heat capacity at all fields. This line shape for the $L=0$ state in Figs. 1 (b) and (c) is intermediate between mesoscopic and macroscopic limits and would be an interesting feature to observe experimentally.

In Fig. 2 we plot $G/G_0$ ($G_0 = 0.4H_0^2V/(8\pi)$ vs $\phi/\phi_0$ for a disk of $R = 4.0\ell_0(T)$ in dotted lines for different $L$ values. The solid lines show $(C/C_0)_{peak}$, the magnitude of the peak value in $C/C_0$ curves at corresponding fields for the different $L$ states. The dashed curve would be $(C/C_0)_{peak}$ for a bulk sample at zero field. The solid curves for any $L$ appear approximately as a mirror reflection of the dotted curves at the $x$-axis. The proportions of the solid and dashed curves are different in the $y$-direction because of which the crossings between the $L$ states in the solid curves occur at the slightly different fields compared to that in the dotted curves. But the minimum in the dotted curve for a particular $L$ is exactly at the same field of the maximum in the solid curve for the same $L$. This can be also argued from equation (3). Normally magnetic field in a bulk superconductor decreases the Cooper pair density and increases the free energy due to loss in the condensation energy associated with the breaking of Cooper pairs. But mesoscopic samples have a regime for each $L$ state where the free energy decreases with increase in field (this is nothing but paramagnetic Meissner effect [10] because magnetization is related to the flux derivative of free energy) as can be seen from the dotted curves in Fig. 2. In this regime the Cooper pair density $|\Psi|^2$ also increase with increase in magnetic field unlike that in bulk samples. For example in the inset to Fig. 2, we consider the $L=2$ state in a regime where it shows the paramagnetic Meissner effect. The solid curve gives the Cooper pair density profile along a line starting from the center of the disk and ending at the boundary of it at an applied flux of $2\phi_0$. The dotted curve gives the same at $4\phi_0$. Hence the density at every point can be enhanced by increasing the field and as a consequence free energy decreases with increase in field. In this regime heat capacity as well as the peak value of the heat capacity, at a fixed temperature increases with increase in magnetic field. Each $L$ state shows the paramagnetic Meissner effect at low fields when the field density in the disk exceeds the applied field. Field density decreases linearly with the applied field [24] and at higher fields in the diamagnetic regime the field density inside the disk is less than the applied field. In this monotonous field dependence the magnetic energy is proportional to the square of the field expelled (being always positive) and hence the free energy minimizes when Cooper pair density maximizes and field density is the same outside as well as inside the sample. In fact any observable quantity (like heat capacity) that depends on the density can identify the minima of the free energy and hence the regime where it decreases with in-
crease in field or the regime of paramagnetic Meissner effect. Hence at any fixed temperature, if the heat capacity of a mesoscopic sample shows enhancement with increasing field, it can be taken as an indirect but unambiguous observation of the paramagnetic Meissner effect (irreversible). Such an unambiguous observation is not possible by a direct magnetization measurement as has been clearly shown in Fig. 11 in Ref. [22]: while the sample is always diamagnetic the observed magnetization is increasing field, it can be taken as an indirect but unambiguous observation of the paramagnetic Meissner effect. Hence at any fixed temperature, if the heat capacity shows enhancement with increasing field or the regime of paramagnetic Meissner effect (irreversible) in mesoscopic samples. Besides, we show that the GL theory can be sufficiently simplified to incorporate mesoscopic corrections to heat capacity because it retains accurately the spatial variations of order parameter that is determined by the coherence length and quiet independent of the penetration length for $\lambda_{eff} > R$.

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Figure captions

Fig. 1 (a) \( C/C_0 \) versus \( T/T_c(0) \) for a disk of radius \( R = 4\xi(0) \) at a flux \( \phi/\phi_0 = 0.1 \) for all possible \( L \) states. (b) The same as (a) but \( \phi/\phi_0 = 1.0 \). (c) \( \phi/\phi_0 = 1.5 \).

Fig. 2. The solid curves show \((C/C_0)_{\text{peak}}\) versus \( \phi/\phi_0 \) for all possible \( L \) states. The dotted curves show \((G/G_0)\) versus \( \phi/\phi_0 \) for all possible \( L \) states. The first few \( L \) states are labeled with their corresponding \( L \) values. Radius \( R \) of the disk = 4.0\( \xi(T) \). The dashed curve gives \((C/C_0)_{\text{peak}}\) for a bulk sample at zero field having the same coherence length. The inset shows the density profile along a radial line of the disk at two different fields. \( C_0 \) and \( G_0 \), defined in text, contains all sample parameters. Thus the figure holds for all samples and at any temperature, the radius being four times the coherence length at that temperature. The radius in microns has to be thus properly chosen using the equations defined immediately below equation 2.

Fig. 3. \( C/C_0 \) versus \( T/T_c(0) \) for a disk of radius \( R = 4\xi(0) \) at a flux \( \phi/\phi_0 = 11.4 \) for all possible \( L \) states.
\[ \frac{C}{C_0} R = 4.0 \xi(0) \]

| \( L = 0 \) | \( L = 1 \) | \( L = 2 \) |
|-------------|-------------|-------------|
| \( \phi = 1.5 \phi_0 \) | \( \phi = 1.0 \phi_0 \) | \( \phi = 0.1 \phi_0 \) |

\[ \frac{T}{T_c(0)} \]
$R = 4.0 \xi(T)$

$\frac{C}{C_0}_{\text{peak}}$

$L=0$

$L=1$

$L=2$

$G / G_0$

$L=0$

$L=1$

$L=2$

$\frac{\rho}{\rho_0(T)}$

$0.0 \quad 0.5 \quad 1.0 \quad 1.5 \quad 2.0 \quad 2.5 \quad 3.0 \quad 3.5 \quad 4.0$

$0.0 \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1.0$

$0 \quad 4 \quad 8 \quad 12 \quad 16 \quad 20 \quad 24 \quad 28$

$-2 \quad -1 \quad 0 \quad 1 \quad 2$

$\phi / \phi_0$
R = 4.0 \xi(0)
\phi = 11.4 \phi_0

\frac{C}{C_0}

\frac{T}{T_c(0)}