The effect of topological fluctuations on the heat capacity of superconductor

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Abstract. The effect of topological excitations in the form of small size $(r \ll \xi(T))$ vortex rings on thermodynamics of a bulk superconductor is considered. These specific short wavelength fluctuations of the order parameter are analogous to small vortex-antivortex pairs in superconducting film which were recently studied in Y.N. Ovchinnikov, A.A. Varlamov, Phys. Rev. Lett. **94**, 107007 (2004). The corresponding contribution to the free energy below T_c is calculated. It is shown that fluctuations of this type give the main temperature dependent contribution to the heat capacity of the superconductor in the sufficiently large interval of temperatures below the transition point. Important, that the sign of this contribution is opposite to that one appearing due to the usual long wavelength fluctuation, leading to smearing of the BCS jump of heat capacity.

PACS. 05.70.Fh Phase transitions: general studies – 74.25.Qt Vortex lattices, flux pinning, flux creep

1 Introduction

Temperature behavior of the physical characteristics of a superconductor in the vicinity of the transition, but beyond the critical region, is usually supposed to be governed by the long wavelength fluctuations of the order parameter [2]. Nevertheless, recently it was demonstrated [1], that in the case of 2D superconductor parametrically large interval of temperatures below critical temperature exists, where the essential role belongs to some specific short wavelength fluctuations (small vortex-antivortex pairs). This is due to the fact that the energy of such pairs tends to zero when the distance between vortex centers becomes less than $\xi(T)$ [3,4]. As a consequence, such "cheap" pairs become "affordable" for thermal fluctuations along with the long wavelength fluctuations of the order parameter. In this article we will demonstrate that the analogous situation takes place also in a bulk superconductor, but the role of vortex-antivortex pairs here play topological vortex rings.

In the mean field approximation the heat capacity of superconductor at the transition temperature undergoes the jump [5]

$$C_{\rm S} - C_{\rm N} = \frac{8\pi^2 \nu T_c}{7\zeta(3)}, \qquad C_{\rm N} = \frac{1}{3}mp_F T,$$
 (1)

where $C_{S,N}$ is the heat capacity of superconductor correspondingly in superconducting and normal states, $\nu = mp_F/2\pi^2$ is the density of states, $\zeta(x)$ is Riemann zeta-function. At least two reasons exist which result in smearing of the heat capacity jump. These are structure inhomogeneities of the sample [6] and thermal fluctuations [1]. The contribution of long wavelength fluctuations to heat capacity is usually assumed to be principal below T_c both in bulk superconductor and thin superconducting film [1]. We will show that the process of the vortex rings proliferation in bulk superconductor, similarly to the vortex-antivortex pairs formation in superconducting film, can successively compete with it in a wide interval of temperatures below the transition. As the temperature decreases the characteristic size of such vortex rings also decreases. At some temperature this size reaches the interatomic distance and has to be cut off. At this point the crossover in the temperature dependence of heat capacity takes place.

2 Vortex rings in bulk superconductor

As the first step of the vortex ring description we will neglect its spheric asymmetry. In this approximation the energy of a small vortex ring of radius $r \ll \xi(T)$ can be majorized by the energy of the formation in the bulk

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of superconductor of a normal sphere of radius r. Our assumption lies in the equivalence of these two energies with the accuracy to $O(r/\xi(T))$. Below we will see that the main contribution to the partition function comes from the pairs with characteristic size $r_{\text{eff}} \ll \xi(T)$, where the coherence length $\xi(T)$ in the vicinity of transition has the form:

$$\xi^2\left(T\right) = \frac{\pi \mathcal{D}}{16T_c\tau}.$$

Here $\tau = 1 - T/T_c$ is the reduced temperature, $\mathcal{D} = \eta(T) \mathcal{D}_{\text{dif}}, \mathcal{D}_{\text{dif}} = v_F l_{\text{tr}}/3$ is the diffusion coefficient, v_F is the Fermi velocity and l_{tr} is the electron transport mean free path. The function $\eta(T)$ was found by Gor'kov in [7]

$$\eta(T) = 1 - \frac{8T\tau_{\rm tr}}{\pi} \left[\psi\left(\frac{1}{2} + \frac{1}{4\pi T\tau_{\rm tr}}\right) - \psi\left(\frac{1}{2}\right) \right], \quad (2)$$

where $\psi(x)$ is the Euler psi-function. It must be stressed that such definition of ξ differs by a factor of two from the standard Ginzburg-Landau expression.

In order to calculate the contribution to heat capacity related with the formation of the small vortex rings let us start from the Ginzburg-Landau functional for the free energy of superconductor

$$\mathcal{F}_{\mathrm{S}}\left[\Delta_{\mathrm{v.r.}}\left(\mathbf{r}\right),\Delta_{\mathrm{v.r.}}^{*}\left(\mathbf{r}\right)\right]-\mathcal{F}_{\mathrm{N}}= \\ \nu\int d^{3}\mathbf{r}\left[-\tau|\Delta_{\mathrm{v.r.}}\left(\mathbf{r}\right)|^{2}+\frac{\pi\mathcal{D}}{8T_{c}}|\partial_{-}\Delta_{\mathrm{v.r.}}\left(\mathbf{r}\right)|^{2} \\ +\frac{7\zeta\left(3\right)}{16\pi^{2}T_{c}^{2}}|\Delta_{\mathrm{v.r.}}\left(\mathbf{r}\right)|^{4}\right]+\frac{1}{8\pi}\int d^{3}\mathbf{r}\left[\operatorname{rot}\mathbf{A}-\mathbf{H}_{0}\right]^{2}.$$
(3)

Here $\partial_{-} = \partial/\partial \mathbf{r} - 2ie\mathbf{A}$, **A** is the vector potential and $\Delta_{v.r.}(\mathbf{r})$ is the superconducting order parameter corresponding to the configuration with one vortex ring. Our goal is to find the minimal energy $F_{v.r.}$ necessary for formation of such ring.

In accordance with the above assumption in practice we will look for the free energy necessary for formation of the normal phase sphere of the radius $a \ll \xi(T)$ in superconductor. This can be done finding the corresponding order parameter profile $\Delta_{\rm sp}(r)$. Formally one has to solve the Ginzburg-Landau equation

$$\frac{\pi \mathcal{D}}{8T_c} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \Delta_{\rm sp} \left(r \right) + \tau \Delta_{\rm sp} \left(r \right) \\ - \frac{7\zeta \left(3 \right)}{16\pi^2 T_c^2} \Delta_{\rm sp}^3 \left(r \right) = 0 \quad (4)$$

with the boundary condition

$$\Delta_{\rm sp}\left(a\right) = 0.\tag{5}$$

Passing to the dimensionless variables

$$\rho = r/\xi(T), \quad \widetilde{\Delta}(\rho) = \Delta_{\rm sp} \left[\xi\left(T\right)\rho\right]/\Delta_0, \quad \widetilde{a} = a/\xi(T)$$
(6)

where

$$\Delta_{0}^{2}(T) = 8\pi^{2}T_{c}^{2}\tau / \left[7\zeta(3)\right],$$

we reduce the equation (4) and its boundary condition (5) to the form

$$\frac{2}{\rho^2}\frac{\partial}{\partial\rho}\left(\rho^2\frac{\partial}{\partial\rho}\right)\widetilde{\Delta}\left(\rho\right) + \widetilde{\Delta}\left(\rho\right) - \widetilde{\Delta}^3\left(\rho\right) = 0, \quad (7)$$

$$\widetilde{\Delta}\left(\widetilde{a}\right) = 0. \tag{8}$$

In the region $\rho \ll 1$ one can find

$$\widetilde{\Delta}(\rho) = A_1 \left(1 - \frac{\widetilde{a}}{\rho} \right) \tag{9}$$

where A_1 is some numerical factor. In the region $\rho \gg 1$ the order parameter $\widetilde{\Delta}(\rho)$ can be presented in the form

$$\widetilde{\Delta}(\rho) = 1 - f(\rho), \qquad (10)$$

where the function $f(\rho)$ satisfies the equation

$$\frac{1}{\rho^2} \frac{\partial}{\partial \rho} \left(\rho^2 \frac{\partial}{\partial \rho} \right) f(\rho) - f(\rho) = 0.$$
 (11)

The solution of this equation which decays at infinity is

$$f(\rho) = \frac{A_2}{\rho} \exp\left(-\rho\right). \tag{12}$$

Matching solutions (9) and (10), (12) in the region $\rho \sim \tilde{a}$ one can find the values of the order parameter in all domain $\rho > 0$:

$$\widetilde{\Delta}(\rho) = 1 - \frac{a}{\rho} \exp\left(-\rho\right).$$
(13)

Substituting expression (13) in formula (3) one can find the value of free energy necessary to create the normal sphere of the radius a:

$$F_{\rm sp}\left(\widetilde{a},T\right) = \frac{7\zeta\left(3\right)\Delta_0^4}{\pi T_c^2}\nu\xi^3\left(T\right)\int_0^\infty d\rho\rho^2\frac{\widetilde{a}}{\rho}\exp\left(-\rho\right).$$
 (14)

In accordance with our assumption this value with the accuracy to $O\left(\tilde{a}/\xi\left(T\right)\right)$ coincides with the energy cost of corresponding vortex ring:

$$F_{\text{v.r.}}\left(\widetilde{a}\right) = B\left(T\right)\widetilde{a}\tag{15}$$

with

$$B(T) = \frac{7\zeta(3)\Delta_0^4}{\pi T_c^2} \nu \xi^3(T).$$
 (16)

3 Vortex rings thermodynamics

In order to take into account the specifics of the fluctuation processes under consideration let us start from the general expression for the partition function in the vicinity of T_c

$$Z = \int \mathfrak{D}\Delta(\mathbf{r}) \int \mathfrak{D}\Delta^{*}(\mathbf{r}) \exp\left\{-\frac{\mathcal{F}_{\mathrm{S}}\left[\Delta\left(\mathbf{r}\right), \Delta^{*}\left(\mathbf{r}\right)\right]}{T}\right\}$$
(17)

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with $\mathcal{F}_{\rm S}\left[\Delta\left(\mathbf{r}\right), \Delta^{*}\left(\mathbf{r}\right)\right]$ being the Ginzburg-Landau functional. In contrast to the usual Ginzburg-Landau approximation, where the simple long wavelength fluctuations are considered, the calculation of the functional integral in (17) now has to take into account the vast variety of the order parameter functions $\Delta_{\rm v.r.}\left(\mathbf{r}\right)$, which correspond to specific realizations of vortex rings.

First, let us separate the partition function Z_0 of the bulk superconductor without fluctuations:

$$Z = Z_0 \cdot Z_{\text{(fl)}}.$$

We will calculate the partition function $Z_{(ff)}$ in the gas approximation. Namely, we will assume that the main contribution comes from small vortex rings and neglect their overlap. Hence

$$Z_{\rm (fl)} = Z_{\rm v.r.}^{V/\left[\frac{4}{3}\pi\alpha^{3}\xi^{3}(T)\right]},$$
(18)

where V is the sample volume. The power $V/[\frac{4}{3}\pi\alpha^3\xi^3(T)]$ in equation (18) takes into account the combinatorial factor corresponding to the independent formation of vortex rings. Since $\xi(T)$ is the only parameter with the dimensionality of length in the Ginzburg-Landau functional it is clear that the coefficient $\alpha \sim 1$. The choice of its form is dictated by the fact that as we have seen above even a small vortex ring disturbs the order parameter on the scale $\xi(T)$, so the maximum density of non-interacting rings is indeed of the order of $\xi^{-3}(T)$.

Taking into account formulas (15) and (16) one can find

$$Z_{\text{v.r.}} = \frac{1}{\left[\alpha p_F \xi\left(T\right)\right]^3} + 3 \int_{1/\left[\alpha p_F \xi\left(T\right)\right]}^{\alpha} \widetilde{a}^2 d\widetilde{a} \exp\left\{\frac{-F_{\text{sp}}\left(\widetilde{a},T\right)}{T}\right\}$$
$$= \frac{1}{\left[\alpha p_F \xi\left(T\right)\right]^3} + 3 \left[\frac{T}{\alpha B\left(T\right)}\right]^3$$
$$\times \left[\Gamma\left(3,\frac{B\left(T\right)}{\alpha T p_F \xi\left(T\right)}\right) - \Gamma\left(3,\frac{\alpha B\left(T\right)}{T}\right)\right]$$
(19)

where $\Gamma(\beta, x)$ is the incomplete Euler gamma-function. Formally the gas approximation means that

$$\alpha B\left(T\right) \gg T.\tag{20}$$

This condition is equivalent to the requirement

$$\tau \gg Gi_{(3)},\tag{21}$$

where the Ginzburg-Levanyuk parameter of a bulk superconductor is determined from the condition [2]

$$\nu Gi_{(3)} \Delta_0^2 \xi^3 (T) = \frac{T_c}{16\pi\sqrt{2}} \Rightarrow Gi_{(3)}$$
$$= \left[\frac{7\zeta(3)}{128\sqrt{2}\pi^3 T_c \nu} \left(\frac{16T_c}{\pi \mathcal{D}}\right)^{3/2}\right]^2. \quad (22)$$

For temperatures which satisfy the condition (21) one can use the asymptotic expression for incomplete gamma function and get

$$Z_{\text{v.r.}} = \frac{1}{\left[\alpha p_F \xi\left(T\right)\right]^3} + 6 \left[\frac{T}{\alpha B\left(T\right)}\right]^3 \exp\left[-\frac{B\left(T\right)}{\alpha T p_F \xi\left(T\right)}\right] \\ \times \left[1 + \frac{B\left(T\right)}{\alpha T p_F \xi\left(T\right)} + \frac{1}{2} \left(\frac{B\left(T\right)}{\alpha T p_F \xi\left(T\right)}\right)^2\right].$$

In result fluctuation generation of the small size vortex rings results in appearance of the correction to the free energy

$$F_{\rm v.r}(T) = -\frac{3TV}{4\pi\alpha^3\xi^3(T)}\ln Z_{\rm v.r.}.$$
 (23)

Corresponding correction to the heat capacity is

$$C_{\text{fl.r}}(T \to T_c) = -T\left(\frac{\partial^2 F_{\text{v.r}}(T)}{\partial T^2}\right).$$
 (24)

Looking at the formulas (22), (23) and (24) one can see that besides the narrow region of strong fluctuations $\tau \leq Gi_{(3)}$ other two regions of temperatures exist:

$$Gi_{(3)} \ll \tau \lesssim \tau_{\rm cross}$$
 (25)

and

$$\tau_{\rm cross} \lesssim \tau \ll 1,$$
 (26)

where

$$\tau_{\rm cross} = Gi_{(3)} \left[p_F \xi \left(T_{\rm cross} \right) \right]^2 = \frac{21\zeta(3)}{4\sqrt{2}\pi^2 \eta p_F l_{\rm tr}} = \frac{36}{\pi} Gi_{(2)}$$
(27)

is the value of crossover temperature. Let us stress that with the accuracy to the numerical factor it coincides with the 2D Ginzburg-Levanyuk number.

In the first region (see Eq. (25)) fluctuation correction to the heat capacity due to generation of small vortex rings is

$$C_{\rm fl.r}\left(\tau\right) = -\frac{9V}{4\pi\alpha^3} \frac{\partial^2}{\partial\tau^2} \left[\frac{1}{\xi^3\left(\tau\right)} \ln\left(\frac{\alpha B\left(T\right)}{6^{1/3}T}\right)\right]$$
(28)

$$= -C_{\rm N} \left(T_c\right) \frac{324\sqrt{2}}{7\zeta(3)\,\alpha^3} \sqrt{\frac{Gi_{(3)}}{\tau}} \times \left[\ln\left(\frac{\alpha}{2^{3/2} 6^{1/3}} \sqrt{\frac{\tau}{Gi_{(3)}}}\right) + 4/3\right].$$
(29)

In the second region (see Eq. (26)) corresponding correction is

$$C_{\rm fl.r}(\tau) = -C_{\rm N}(T_c) \frac{324\sqrt{2}}{7\zeta(3)\alpha^3} \sqrt{\frac{Gi_{(3)}}{\tau}} \{\ln[\alpha p_F \xi(\tau)] - 4/3\}.$$
(30)

Let us stress that in both regions the correction is negative and exceeds the fluctuation contribution related to the long wavelength fluctuations [1] by large parameter $\left\{ \ln \left(\tau/Gi_{(3)} \right), \ln \left[p_F \xi \left(\tau \right) \right] \right\}.$

4 Case of low temperatures

In the region of low temperatures $T \ll T_c$ the electronic contribution to heat capacity of superconductor, being proportional to $\exp(-\Delta(T)/T)$ is exponentially small. It turns out that the fluctuation corrections to the heat capacity in this region are also small by the same parameter. The latter circumstance is related with the weak temperature dependence of the parameters $\Delta(T)$ and $\xi(T)$ at temperatures $T \ll T_c$. In the BCS approximation temperature dependence of the order parameter is determined by the equation [8,9]:

$$\ln \frac{T}{T_c} = 2\pi T \sum_{\omega_n > 0} \left(\frac{1}{\omega_n} - \frac{1}{\sqrt{\omega_n^2 + \Delta_0^2(T)}} \right), \qquad (31)$$

where $\omega_n = 2\pi T (n + 1/2)$ is the fermionic Matsubara frequency. The correlation length $\xi(\tau)$ in the most general case can be determined from the position of the pole of the linear response operator to the modulus of order parameter [10]:

$$T \sum_{\omega_n > 0} \left(\frac{\omega_n^2}{[\omega_n^2 + \Delta_0^2(T)] \left[\sqrt{\omega_n^2 + \Delta_0^2(T)} - \mathcal{D}/2\xi^2(T) \right]} - \frac{1}{\sqrt{\omega_n^2 + \Delta_0^2(T)}} \right) = 0. \quad (32)$$

At low temperatures $(T \ll T_c)$ both functions $\Delta(T)$ and $\xi(T)$ tend to their values at zero temperature $\{\Delta(0), \xi(0)\}$ being only exponentially small different from them:

$$\Delta(T) - \Delta(0) \sim \exp(-\Delta(T)/T).$$
(33)

Analyzing equations (31) and (32) at T = 0 one finds

$$\Delta^2(0) \sim \left(\frac{\pi T_c}{\gamma}\right)^2, \qquad \xi^2(0) = \frac{\mathcal{D}}{2\theta \Delta(0)}. \tag{34}$$

Here $\gamma=\exp C, C=0.577$ is the Euler constant, while $\theta=0.76595$ is the solution of the transcendental equation

$$\frac{\pi}{4} = \sqrt{1 - \theta^2} \left[\frac{\pi}{2} - \arctan \sqrt{\frac{1 - \theta}{1 + \theta}} \right].$$
(35)

In low temperature region the exact expression for the free energy with the strong space dependence of the order parameter $\Delta(\mathbf{r})$ is unknown. It is why for the vortex rings contribution to the heat capacity in this region only the rough estimate basing in equations (31–33) can be done, which we do not present here.

5 Discussion

In conclusion, let us summarize the results. We have demonstrated that the proliferation of small vortex rings in a bulk superconductor, analogously to the small vortexantivortex pairs in the case of 2D superconducting film, results in appearance of the specific contribution to its heat capacity. This contribution dominates over the usual GL fluctuation correction in the wide interval of temperatures below T_c . We found that both in two and three dimensional cases full fluctuation correction to heat capacity in the vicinity of the superconducting transition has the opposite signs at the opposite sides of the region of strong fluctuations $(|\tau| \lesssim Gi_{(3)})$. This fact is related to the presence of the heat capacity jump at the transition point in the mean field approximation. Let us recall that the coherence length $\xi(T)$ in this approximation has the same singularity $|\tau|^{-1/2}$ with the coefficients which differ by factor $\sqrt{2}$ below and above the transition point.

One can expect that considered in this communication type of fluctuations contributes not only to the thermodynamic but also to the transport properties of superconducting films.

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