Effect of Vortex-Antivortex Fluctuations on the Heat Capacity of a Type-II Superconducting Film

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The small size vortex-antivortex pairs proliferation in a type-II superconducting film is considered below T_c. The corresponding contribution to the free energy is calculated. It is shown that these fluctuations give the main temperature dependent contribution to the heat capacity of the superconducting film in the sufficiently large interval of temperatures below the transition point.

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The special role of fluctuations in the 2D superconductor is well-known [1]. For example, the phase fluctuations of the order parameter invalidate the mean field picture of the phase transition destroying the long range order [2]. On the contrary, the fluctuations of the vortex-antivortex-type restore the phenomenon of superconductivity: slightly below the mean field transition temperature T_{c0}, vortex-antivortex pairing becomes energetically favorable and the Berezinskii-Kosterlitz-Thouless (BKT) transition to the state characterized by finite stiffness (nonzero elastic modulus) takes place. The corresponding transition temperature, $T_{\rm BKT}$, almost coincides with the temperature of the superconducting transition for the film of thickness d, calculated considering the order parameter fluctuations [3]:

$$T_c = T_{c0}(1 - 2Gi_{(2D)} \ln Gi_{(2D)}^{-1}),$$

where

$$Gi_{(2D)} = \frac{21\zeta(3)}{\pi^2} \frac{1}{p_F^2 d l_{\rm tr}} \ll 1 \qquad (1)$$

is the Ginzburg-Levanyuk number [1]. Here $\zeta(x)$ is the Riemann zeta function, p_F is the electron Fermi momentum, and $l_{\rm tr}$ is the electron transport mean free path.

It is important to remind the reader that the BKT transition is determined by the formation of large vortex-antivortex pairs. These large pairs also determine thermodynamic and transport properties of 2D superconductors in the critical region of the BKT transition. The 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 [1]. In this Letter, at the example of a heat capacity, we demonstrate that, contrary to current opinion, there is a sufficiently large interval of temperatures below $T_{\rm BKT}$ where the essential role in thermodynamics of the 2D superconductor belongs to some specific short wavelength fluctuations (small vortex-antivortex pairs).

For simplicity we consider the case of a dirty superconducting film of thickness $d \ll \xi(T)$. The coherence length $\xi(T)$ in the vicinity of transition has the form

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

Here $\tau = 1 - T/T_c$ is the reduced temperature and $\mathcal{D} = v_F l_{\rm tr}/3$ is the diffusion coefficient [it must be stressed that this definition differs by a factor of 2 from the standard Ginzburg-Landau (GL) expression]. The standard description of the BKT transition is based on the logarithmic expression for free energy corresponding to large [$R \gg \xi(T)$] vortex-antivortex pairs [2]

$$F_{\rm BKT} = \left[\frac{\pi n_{s2}(T)}{2m} - 2T\right] \ln \frac{R}{\xi(T)}, \qquad (2)$$

with $n_{s2}(T)$ being the superfluid density. The cornerstone of the presented theory is the fact that the energy of the vortex-antivortex pairs tends to zero when the distance between their centers is less than $\xi(T)$ [4,5]. As a consequence, such "cheap" pairs become "affordable" for thermal fluctuations along with the long wavelength fluctuations of the order parameter. Moreover, their proliferation gives the main contribution to the heat capacity due to fluctuations in the interval of temperatures

$$Gi_{(2D)} \ll \tau \lesssim Gi_{(2D)} \ln^2[p_F \xi(T)] \qquad (3)$$

below the transition.

As the temperature decreases the characteristic size of the small vortex-antivortex pairs also decreases. At the upper limit of the interval (3) this size reaches the interatomic distance and has to be cut off. At this point the crossover in the temperature dependence of the heat capacity takes place: at temperatures below it both the small vortex-antivortex pairs and the long wavelength fluctuations contribute to the heat capacity with the same intensity.

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

$$Z = \int \mathfrak{D}\Delta(\mathbf{r}) \int \mathfrak{D}\Delta^*(\mathbf{r}) \exp\left\{-\frac{F(\Delta(\mathbf{r}), \Delta^*(\mathbf{r}))}{T}\right\},$$

with $F(\Delta(\mathbf{r}), \Delta(\mathbf{r})^*)$ being the Ginzburg-Landau functional. In contrast to the usual GL-type long wavelength approximation, the calculation of the functional integral now has to take into account the vast variety of the order parameter functions $\Delta_p(\mathbf{r})$, which correspond to specific realizations of vortex-antivortex pairs in the film. In other words, in addition to the usual GL order parameter fluctuations we take into account some specific short wavelength fluctuations.

First, let us separate the partition function Z_0 of the superconducting film without fluctuations:

$$Z = Z_0 Z_{(fl)}.$$

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

$$Z_{(fl)} = Z_p^{S/[\pi\xi^2(T)]}, \tag{4}$$

where S is the area of the film and

$$Z_p = \int d\Delta_\delta(\mathbf{r}) \int d\Delta_\delta^*(\mathbf{r}) \exp\left\{-\frac{F_p(\Delta_\delta(\mathbf{r}), \Delta_\delta^*(\mathbf{r}))}{T}\right\} \tag{5}$$

is the contribution of isolated single pairs of all possible sizes $\delta \cdot \xi(T)$, with $0 \le \delta \lesssim 1$, to the partition function. The power $S/[\pi\xi^2(T)]$ in Eq. (5) takes into account the combinatorial factor corresponding to the independent formation of such pairs. The choice of its form is dictated by the fact that, as we demonstrate later [see Eqs. (10) and (11)], even a small pair disturbs the order parameter on the scale $\xi(T)$, so the maximum sheet density of noninteracting pairs is indeed of order ξ^{-2}. Let us stress that this factor is written with the accuracy up to an independent of temperature coefficient of the order of 1.

The order parameter $\Delta_\delta(\mathbf{r})$ must have two zeros of the opposite vorticity at the distance $2\delta\xi(T)$ (i.e., the total vorticity calculated along a contour enveloping the two zeros must vanish).

As the next step we neglect the axial asymmetry of the vortex-antivortex pair. Later we see that the main contribution to the partition function comes from pairs with characteristic size $r_{\text{eff}} \ll \xi(T)$. This justifies our gas approximation ($\delta \ll 1$). The free energy functional corresponding to Eq. (5) is

$$F_p = \nu d \int d^2\mathbf{r}\left\{\left[-\tau|\Delta_\delta(\mathbf{r})|^2 + \frac{\pi\mathcal{D}}{8T_c}|\partial_-\Delta_\delta(\mathbf{r})|^2 + \frac{7\zeta(3)}{16\pi^2T_c^2}|\Delta_\delta(\mathbf{r})|^4\right] + \frac{\tau}{2}|\Delta_0(T)|^2\right\}. \tag{6}$$

Here $\nu = mp_F/2\pi^2$ is the density of states, $\partial_- = \partial/\partial\mathbf{r} - 2ie\mathbf{A}$, and $\Delta_0^2(T) = 8\pi^2T_c^2\tau/[7\zeta(3)]$. The last term in Eq. (6) is related to the fact that F_p is the difference in the free energy of the state with one vortex-antivortex pair [the order parameter is $\Delta_\delta(\mathbf{r})$] and the ground state with the homogeneous order parameter $\Delta_0(T)$.

In the GL approach the contribution of all possible vortex-antivortex pairs to the partition function (5) is taken into account by minimization of the functional (6) over the class of functions $\Delta_\delta(\mathbf{r})$ with two zeros of opposite vorticity located at distance $2\delta\xi(T)$. In order to get rid of this constraint one should represent the order parameter as

$$\Delta_\delta(\mathbf{r}) = |\Delta_\delta(\mathbf{r})|e^{i\chi(\mathbf{r})} \tag{7}$$

and choose the phase in the form

$$\chi(\mathbf{r}) = \varphi_1(\mathbf{r}) - \varphi_2(\mathbf{r}) + \tilde{\chi}(\mathbf{r}). \tag{8}$$

Here the phases $\varphi_1(\mathbf{r}), \varphi_2(\mathbf{r})$ are the rotation angles with respect to the zeros. Hence they are multivalued functions of the coordinate, whereas $\tilde{\chi}(\mathbf{r})$ is a single value function. After this parametrization the variation over the functions $\Delta_\delta(\mathbf{r})$ and $\tilde{\chi}(\mathbf{r})$ can be performed in the standard way [6]. After some cumbersome calculations one can find that the proposed minimization procedure gives the same result for the free energy as one would get using in (6) the solution of the 2D Ginzburg-Landau equation with zero boundary condition, $\Delta_\delta(\mathbf{r}) = 0$, at the circle $|\mathbf{r}| = \delta\xi(T)$. It is worth mentioning that the same procedure is valid also for large vortex-antivortex pairs, and it gives not only the famous logarithmic dependence of energy on distance (2) but also the next order corrections.

In accordance with the above statement we write the order parameter in the form

$$\Delta_\delta(\rho) = \Delta_0(T)f(\rho)$$

and obtain the dimensionless GL equation

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)f + \frac{1}{2}f - \frac{1}{2}f^3 = 0. \tag{9}$$

Here $\rho = r/\xi(T)$ is the dimensionless radius.

Let us investigate the solutions of Eq. (9) in two limiting cases: small $\rho \sim \delta \ll 1$ and large $\rho \to \infty$. In the region of small $\rho \sim \delta \ll 1$ the function $f(\rho) \to 0$. This function can be found as the solution of the linearized Eq. (9):

$$f(\rho) = C_1J_0(\rho/\sqrt{2}) + C_2N_0(\rho/\sqrt{2}), \tag{10}$$

where J_0 and N_0 are the Bessel and Neumann functions, respectively.

When $\rho \gtrsim 1$, the solution of Eq. (9) takes the form $f(\rho) = 1 - f_1(\rho)$. Substituting this into Eq. (9) one finds

$$f(\rho) = 1 - f_1(\rho) = 1 - C_3K_0(\rho), \tag{11}$$

where K_0 is the modified Bessel function. The constant term corresponds to the usual contribution of long wavelength order parameter fluctuations that appear in the result of our analysis together with the contribution of small vortex-antivortex pairs.

One can see that the asymptotic expression (11), despite being calculated at $\rho \gtrsim 1$, extends to the region of small ρ. Therefore we can match solutions (10) and (11) at $\rho \sim \delta \ll 1$. In order to do this let us use an approximate expression for the Bessel functions J_0, N_0, and K_0 calculated for small arguments [7]. The comparison of constants and coefficients in logarithmic terms gives two equations for coefficients $C_{1,2,3}$. The third equation is determined by the boundary condition $f(\delta) = 0$ which corresponds to our disk model of the vortex-antivortex pair. Finally

$$C_i = \delta_{i1} + \frac{1}{2\ln\frac{2}{\gamma\delta}} \left\{ \begin{array}{c} \ln 2 \\ \pi \\ 2 \end{array} \right. .$$

Here $\gamma = \exp(C)$, where $C = 0.577\,215\cdots$ is the Euler constant.

Now we can find the energy of disk (vortex-antivortex pair) $F_p(\delta, T)$ as the function of its dimensionless radius δ. In order to do this one can use the general expression (6) and the fact that $\Delta = \Delta_0(T) f$ satisfies the nonlinear equation (9). As a result

$$F_p(\delta, T) = \frac{b(T)}{\ln\frac{2}{\gamma\delta}} \int_0^\infty x K_0(x) dx = \frac{b(T)}{\ln\frac{2}{\gamma\delta}}, \qquad (12)$$

with

$$b(T) = \frac{\pi^2 \nu d \mathcal{D} \Delta_0^2(T)}{4T_c}. \qquad (13)$$

Let us stress that the presence of the large logarithm in the denominator makes these localized vortex-antivortex-type fluctuations of the order parameter more energetically favorable than the almost homogeneous (long wavelength) Ginzburg-Landau ones.

Now let us perform the functional integration in Eq. (5). Vortex-antivortex pairs proliferate below T_c in a fluctuation way. In our model this is equivalent to taking into account disks of different radii. Cutting off their sizes at interatomic distances ($\sim p_F^{-1}$) one can rewrite Eq. (5) in the form

$$Z_p = \frac{1}{[p_F \xi(T)]^2} + 2 \int_{1/[p_F \xi(T)]}^{1} \delta d\delta \exp\left\{ -\frac{F_p(\delta, T)}{T} \right\}. \qquad (14)$$

One can see that in the considered range of temperatures (3) the integration in Eq. (14) may be carried out by the steepest descent method. That gives

$$Z_p = \frac{4 \cdot 2^{1/4} \pi^{1/2}}{\gamma^2} \left(\frac{b(T)}{T} \right)^{1/4} \exp\left\{ -2\sqrt{\frac{2b(T)}{T}} \right\}.$$

Finally, the corresponding contribution to the free energy is

$$\tilde{F}_p(T) = -T \ln Z_p^{S/\pi\xi^2} = -\frac{TS}{\pi\xi^2(T)} \left[-2\sqrt{\frac{2b(T)}{T}} + \frac{1}{4} \ln\frac{b(T)}{T} \right]. \qquad (15)$$

.

This expression is valid provided that $b(T) \gg T$, which justifies the use of the steepest descent method. Looking at Eq. (13) and recalling the definition of the 2D Ginzburg-Levanyuk number (1) one can see that the requirement $b(T) \gg T$ is equivalent to $\tau \gg Gi_{(2D)}$; i.e., our consideration is valid for the temperature interval defined by (3). This range still belongs to the GL region ($Gi_{(2D)} \ll \tau \ll 1$) and the main temperature dependence of Eq. (15) originates from functions $\xi(T)$ and $\Delta_0(T)$. The corresponding vortex-antivortex pair contribution to the heat capacity is

$$C_p(T \to T_c) = -\frac{48ST_c}{v_F l_{\mathrm{tr}}} \left(\frac{\partial^2}{\partial\tau^2} \right) \left[4\sqrt{\frac{\nu d \mathcal{D}}{7\zeta(3)}} \tau^{3/2} - \frac{\tau}{4\pi^2} \times \ln\frac{2\pi^4 \nu d \mathcal{D} \tau}{7\zeta(3)} \right]. \qquad (16)$$

One can see that the differentiation of the second term in the square brackets of Eq. (16) reproduces the well-known contribution of the GL long wavelength order parameter fluctuations to the heat capacity [1]:

$$C_{(fl)}^{(2)}(\tau) = \frac{8\pi^2 Sd}{7\zeta(3)} \nu T_c \left(\frac{Gi_{(2D)}}{\tau} \right). \qquad (17)$$

Nevertheless, the main fluctuation contribution to the heat capacity of 2D superconducting films [$d \ll \xi(T)$] results from the first term of Eq. (16). It corresponds to the short wavelength vortex-antivortex-type order parameter fluctuations:

$$C_p(\tau) = -\frac{48\pi^2 Sd}{7\zeta(3)} \nu T_c \left(\frac{2Gi_{(2D)}}{\tau} \right)^{1/2}. \qquad (18)$$

The contribution (18) dominates over (17) in the entire region (3).

At temperatures below $\tau_{\mathrm{cr}} \sim Gi_{(2D)} \ln^2 p_F \xi(T_{\mathrm{cr}})$ the second term of Eq. (14) is exponentially small and the vortex-antivortex contribution to the partition function is reduced to the first term:

$$Z_p = \frac{1}{[p_F \xi(T)]^2}. \qquad (19)$$

The corresponding contribution to the free energy,

$$\tilde{F}_p(T) = \frac{TS}{\pi\xi^2(T)} \ln[p_F \xi(T)]^2, \qquad (20)$$

results in the positive vortex-antivortex pair correction to heat capacity similarly to the usual long wavelength fluctuations of the order parameter Eq. (17). Let us stress that the correction $C_p(\tau)$ around the crossover point changes its sign, as it is expected to match at this temperature the positive $C_{(fl)}^{(2)}(\tau)$. Let us note that the negative sign of the vortex-antivortex fluctuation correction in the immediate vicinity of the transition temperature means that the mean field heat capacity jump overestimates the true value and the vortex-antivortex pairs contribution smears it out.

In conclusion, let us summarize the results. We have demonstrated that the proliferation of small vortex-antivortex pairs in 2D superconducting films results in the appearance of the specific contribution to its heat capacity. This contribution dominates over the usual GL fluctuation correction in the wide enough interval of temperatures below T_c. One can expect that this type of fluctuation contributes not only to the thermodynamic but also to the transport properties of superconducting films.

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