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The Order Parameter Length Scale of a Vortex Line in a Type II Superconductor
—— *Variation with Temperature* ——

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In this paper, we show that the scale of spatial variation of the order parameter ξ in extreme type II superconductors has a temperature dependence other than that of the temperature dependent Ginzburg Landau coherence length $\xi_0(T)$. Furthermore for temperatures in the vicinity of the critical temperature T_c our results indicate that $\xi/\xi_0(T)$ decreases with decreasing temperature.

When an external magnetic field is applied to a type II superconductor, vortex lines form provided that the magnetic field is below the upper critical field H_{c2}.[1] For temperatures just below the superconducting transition temperature T_c, or for a magnetic field just below H_{c2}, such vortices can be analysed within the Ginzburg Landau (GL) framework.[2] For temperatures further below T_c the Eilenberger and Bogoliubov equations have been investigated, through interative or variational methods.[3)~5)] Kramer et al.[3] and Gygi et al.[4] find that the scale of spatial variation of the order parameter divided by the GL temperature dependent coherence length decreases with decreasing temperature. On the other hand Dorsey et al.[5] claim that there is no appreciable temperature dependence in this quantity.

Instead of formulating the problem in terms of Green's functions and the order parameter we adopt a path integral approach. Here the fermion fields associated with the electrons are integrated out, resulting in a formal expression for the free energy in terms of a functional determinant. The order parameter configuration is then given by minimisation of the free energy.

In this paper we will be concerned with the quantity $\lambda=\xi/\pi\xi_0(T)$, where ξ is the scale of spatial variation of the order parameter and $\xi_0(T)$ is the GL temperature dependent coherence length. Any temperature dependence of λ indicates that ξ has a temperature dependence that is different from the GL variation. This work aims to determine whether λ has any temperature dependence.

The vortex free energy, relative to that of the uniform configuration, at finite temperature, $T=1/\beta$, can be written as a ratio of two path integrals over Grassmann fields[6]

$$e^{-\beta(F-F_0)}=\frac{\int[d\bar{\Psi}][d\psi]e^{-S}}{\int[d\bar{\Psi}][d\psi]e^{-S_0}} \tag{1}$$

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with

$$S=\int_0^\beta d\tau L+\frac{\beta}{g}\int d^3x|\Delta(x)|^2+S_B\,, \tag{2}$$

where $L=\int d^3x\bar{\psi}(\partial_\tau+H)\psi$, g is the coupling constant defining the system and S_B arises purely from magnetic field contributions. The Hamiltonians are given by

$$H=\sigma_3\varepsilon(\hat{\boldsymbol{p}}+e\boldsymbol{A}\sigma_3)+V\,,$$

$$H_0=\sigma_3\varepsilon(\hat{\boldsymbol{p}})+V_0 \tag{3}$$

in which

$$V=\begin{pmatrix}0 & \Delta\\ \Delta^* & 0\end{pmatrix},\quad V_0=\begin{pmatrix}0 & \Delta_0\\ \Delta_0 & 0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{4}$$

Also, $\varepsilon(\hat{\boldsymbol{p}})=(\hat{\boldsymbol{p}}^2/2m)-\mu$, where μ is the chemical potential, Δ is the order parameter, Δ_0 the uniform gap and $\boldsymbol{A}$ the vector potential. For a vortex of unit quantised flux along the z-axis, $\Delta=\Delta_0 f(r/\xi)e^{-i\varphi}$, where $f(0)=0$ and $f(\infty)=1$, $r=\sqrt{x^2+y^2}$ and $\varphi=\arctan(y/x)$. We assume that, with regard to the minimisation of the free energy, it is adequate to approximate the functional variation of f by a single scale parameter ξ. Below we take $f=\tanh(r/\xi)$. This assumption has been questioned for very low temperatures by Gygi et al.;[4] they found that two scales are required. We will investigate this possibility in a later work. The vector potential is given by $\boldsymbol{A}=-\hat{\varphi}/r\ \alpha(r/\xi_B)$, with $\alpha(0)=0$ and $\alpha(\infty)=1$. We have assumed, as for the order parameter, that only a single length scale need be considered in the variation of $\boldsymbol{A}$ and have taken this to be ξ_B.

Integrating over the Fermi fields we obtain

$$F-F_0=-\frac{1}{2\beta}\sum_n \mathrm{Tr}\ln\left(\frac{\omega_n^2+H^2}{\omega_n^2+H_0^2}\right)+\frac{1}{g}\int d^3x(|\Delta|^2-\Delta_0^2)+F_B\,, \tag{5}$$

where $\omega_n=(\pi/\beta)(2n+1)$ are the Matsubara frequencies and the trace is to be understood in the functional sense. That is, $\mathrm{Tr}(\cdots)=\mathrm{tr}\int d^3x\langle x|(\cdots)|x\rangle$ and tr is the trace over the internal matrix space. In deriving Eq. (5) we have made the replacement

$$\ln \mathrm{Det}(\partial_\tau+H)=\frac{1}{2}\ln[\mathrm{Det}(\partial_\tau+H)(\partial_\tau+H)^\dagger]=\frac{1}{2}\ln \mathrm{Det}(-\partial_\tau^2+H^2)\,,$$

which holds for real positive determinants. We have also used the standard identity $\ln \mathrm{Det}(\cdots)=\mathrm{Tr}\ln(\cdots)$. The gap equation is given by minimising F_0 with respect to Δ_0, that is,

$$\frac{1}{2\beta}\sum_n \mathrm{Tr}\frac{\Delta_0}{\omega_n^2+H_0^2}=\frac{1}{g}\int d^3x\Delta_0\,. \tag{6}$$

Using this the order parameter contribution to Eq. (5) can be absorbed into the trace

$$F-F_0=-\frac{1}{2\beta}\sum_n \mathrm{Tr}\left[\ln\left(\frac{\omega_n^2+H^2}{\omega_n^2+H_0^2}\right)-\frac{H^2-H_0^2}{\omega_n^2+H_0^2}\right]+F_B\,. \tag{7}$$

The argument of the trace can be represented as an integral over the "proper time", s. We find, in a similar way to Ref. 7),

$$F-F_0=\frac{1}{2\beta}\sum_n^{\infty}\int_0^{\infty}\frac{ds}{s}e^{-s(\omega_n^2+\Delta_0^2)}K(s)+F_B\,, \tag{8}$$

where $K(s)$ is a modified heat kernel, given by

$$K(s)=\mathrm{Tr}\,e^{-s(H_0^2-\Delta_0^2)}(e^{sH_0^2}e^{-sH^2}-1+s(H^2-H_0^2))\,. \tag{9}$$

The modified kernel $K(s)$ can be expanded in powers of the proper time s. The expansion of $K(s)$, when substituted into Eq. (8), does not result in any infinities because there are no $s^{-1/2}$ or $s^{1/2}$ terms in the expansion. Moreover, this expansion has a well-defined zero temperature limit.[8)] This is because the large s part of the integrand of Eq. (8) is exponentially damped by the factor $\exp(-s\Delta_0^2)$. Let us write the series as

$$K(s)=\sum_{n=2}^{\infty}A_n s^{n-1/2}\,. \tag{10}$$

In evaluating the expansion it is convenient to drop the vector potential and introduce it later by gauging the A_n's. Of course some terms will be missed by this procedure; these are either pure magnetic terms or combinations of the magnetic field with covariant derivatives of the order parameter. As we are concerned with extreme type II systems, where the vector potential varies over a much larger scale than the order parameter, such terms will make a negligible contribution. Evaluating the trace in Eq. (9), we obtain (see Appendix 3 of Ref. 9) for additional steps leading to this equation)

$$K(s)=\mathrm{tr}\int\frac{d^3k}{(2\pi)^3}d^3x e^{-s\varepsilon^2(k)}[e^{-s(H^2(\boldsymbol{p}\to\boldsymbol{k}-i\boldsymbol{\partial})-\varepsilon^2(k)-\Delta_0^2)}-1+s(V^2-\Delta_0^2)]\,, \tag{11}$$

where $\boldsymbol{\partial}$ acts on everything to its right. The problem can be substantially simplified by linearising the spectrum.[10)] This is a good approximation as all the integrals are peaked about the Fermi surface. Linearising we make the replacement

$$\int\frac{d^3k}{(2\pi)^3}f(k)\simeq N(0)\int\frac{d\hat{\boldsymbol{k}}}{4\pi}\int_{-\infty}^{\infty}d\varepsilon f(\hat{\boldsymbol{k}}p_F)\,, \tag{12}$$

where $\hat{\boldsymbol{k}}$ is a unit vector (and not an operator) and $N(0)=mp_F/2\pi^2$ is the density of states at the Fermi surface. Also, neglecting derivatives of the order parameter in favour of powers of the Fermi momentum, we have

$$\begin{aligned}H^2(\boldsymbol{p}\to\boldsymbol{k}-i\boldsymbol{\partial})-\varepsilon^2(\boldsymbol{k})-\Delta_0^2\cong&-2i\varepsilon v_F\hat{\boldsymbol{k}}\cdot\boldsymbol{\partial}-v_F^2(\hat{\boldsymbol{k}}\cdot\boldsymbol{\partial})^2\\&-i\sigma_3 v_F\hat{\boldsymbol{k}}\cdot(\boldsymbol{\partial}V)+V^2-\Delta_0^2\,.\end{aligned} \tag{13}$$

Now let us convert to dimensionless variables: $s\to s/\Delta^2$, $\boldsymbol{x}\to\boldsymbol{x}/\xi$, $\varepsilon\to\varepsilon\Delta_0^2$, $V\to V\Delta_0^2$. So that the modified heat kernel becomes

$$K=\frac{LN(0)v_F^2}{\Delta_0}\lambda^2\int d^2x\int\frac{d\hat{\boldsymbol{k}}}{4\pi}\int d\varepsilon e^{-s\varepsilon^2}\mathrm{tr}(e^{-s\mathcal{O}}-1+s(V^2-1))\,, \tag{14}$$

where L is the length of the vortex and the operator $\mathcal{O}$ is given by

$$\mathcal{O}=-\frac{2i\varepsilon}{\lambda}\hat{\boldsymbol{k}}\cdot\boldsymbol{\partial}-\frac{1}{\lambda^2}(\hat{\boldsymbol{k}}\cdot\boldsymbol{\partial}^2)-\frac{1}{\lambda}i\sigma_3\hat{\boldsymbol{k}}\cdot(\boldsymbol{\partial}V)+V^2-1 \tag{15}$$

with $\lambda=\Delta_0\xi/v_F=\xi/\pi\xi_0(T)$ and $\xi_0(T)$ the temperature dependent GL coherence length. This enables us to define the dimensionless coefficients $\bar{A}_n$, given by

$$\bar{A}_n=\frac{A_n}{LN(0){v_F}^2}{\Delta_0}^{-2(n-1)} \tag{16}$$

with

$$K=\frac{LN(0){v_F}^2}{\Delta_0}\sum_{n=2}\bar{A}_n s^{(n-1/2)}. \tag{17}$$

From the nature of $\mathcal{O}$, Eq. (15), it follows that $\bar{A}_n$'s are functions only of λ. When they are gauged they will have an additional contribution, which will be a function of λ/λ_B, where $\lambda_B=\xi_B/\pi\xi_0(T)$. So that the free energy takes the following form:

$$F-F_0=\frac{LN(0){v_F}^2}{2\beta\Delta_0}\sum_m\int_0^\infty\frac{ds}{s}e^{-s[(\omega_m/\Delta_0)^2+1]}\sum_{n=2}\bar{A}_n(\lambda,\lambda_B)s^{n-1/2}+F_B. \tag{18}$$

If, therefore, the value of λ that minimises $F-F_0$ is independent of temperature it implies that the same λ minimises each of the coefficients $\bar{A}_n$ individually. This follows since changing the temperature changes ω_m/Δ_0 and hence the weighting of the different $\bar{A}_n$'s within the proper time integral of Eq. (8). Thus the logic is: given

$$\left.\frac{\partial(F-F_0)}{\partial\lambda}\right|_{\lambda=\lambda_e}=0,$$

$$\text{then}\qquad \lambda_e\neq\lambda_e(T)\Rightarrow\left.\frac{\partial\bar{A}_n}{\partial\lambda}\right|_{\lambda=\lambda_e}=0,\ ^\forall n. \tag{19}$$

We are now in a position to determine whether λ_e is a function of temperature. First we note that in the GL region only $\bar{A}_2$ has an appreciable contribution to the free energy since higher order terms are down by powers of Δ_0. Thus the GL value for λ_e is obtained by extremising $\bar{A}_2$. In fact we can construct an expansion in powers of $\Delta_0(T)/T$, from Eq. (18), which is valid for temperatures just below T_c. It takes the form

$$\begin{aligned}F-F_0=\frac{LN(0){v_F}^2}{2\beta\Delta_0}&\left[\left(\frac{\Delta_0}{T}\right)^3\frac{7\zeta(3)}{4\pi}\Gamma\left(\frac{3}{2}\right)\bar{A}_2\right.\\&\left.+\left(\frac{\Delta_0}{T}\right)^5\frac{31\zeta(5)}{32\pi}\left(-\frac{3}{2}\Gamma\left(\frac{3}{2}\right)\bar{A}_2+\Gamma\left(\frac{5}{2}\right)\bar{A}_3\right)\right]+\mathcal{O}\left(\frac{\Delta_0}{T}\right)^7.\end{aligned} \tag{20}$$

After a lengthy calculation we find

$$\bar{A}_2=\frac{\sqrt{\pi}}{2}\int d^2x\left[\lambda^2(V^2-1)^2-\frac{1}{3}(\sigma_3(\boldsymbol{\partial}V))^2\right],$$

$$\bar{A}_3=-\frac{\sqrt{\pi}}{6}\int d^2x\left[\lambda^2(V^2-1)^3-(\sigma_3(\boldsymbol{\partial}V))^2V^2+\frac{1}{6}(\boldsymbol{\partial}V^2)^2-\frac{1}{10\lambda^2}(\sigma_3\boldsymbol{\partial}^2V)^2\right]. \tag{21}$$

The above are gauged by making the replacement $\partial \to \partial + 2ie\sigma_3 A$ and remembering that $A = -(\hat{\varphi}/r)\alpha(r\lambda/\lambda_B)$. Note that we have twice the electric charge since the order parameter is bilinear in the Fermi fields. Gauging the $\bar{A}_n$'s and substituting for the order parameter profile, $f(r) = \tanh(r)$, we find

$$\bar{A}_2 = \pi^{3/2}\left[\lambda^2\left(\frac{2}{3}(\ln 2) - \frac{1}{6}\right) + \frac{1}{3}I_1\left(\frac{\lambda}{\lambda_B}\right)\right],$$

$$\bar{A}_3 = \frac{\pi^{3/2}}{3}\left[\lambda^2\left(\frac{8}{15}(\ln 2) - \frac{11}{60}\right) - I_2\left(\frac{\lambda}{\lambda_B}\right) - \frac{1}{10\lambda^2}I_3\left(\frac{\lambda}{\lambda_B}\right)\right], \tag{22}$$

where the integrals I_n are given by

$$I_1 = \int_0^\infty drr\left[\mathrm{sech}^4 r + (1 - \alpha(r\lambda/\lambda_B))^2 \frac{\tanh^2 r}{r^2}\right],$$

$$I_2 = \int_0^\infty drr\left[\frac{5}{3}\tanh^2 r\,\mathrm{sech}^4 r + (1 - \alpha(r\lambda/\lambda_B))^2 \frac{\tanh^4 r}{r^2}\right],$$

$$I_3 = \int_0^\infty drr\left[2\sinh r\,\mathrm{sech}^3 r - \frac{\mathrm{sech}^2 r}{r} + (1 - \alpha(r\lambda/\lambda_B))^2 \frac{\tanh^2 r}{r^2}\right]^2. \tag{23}$$

For extreme type II systems $\lambda/\lambda_B \ll 1$ and we find, independently of profile choice for α, that

$$\frac{\partial I_{1,2}}{\partial \lambda} = -\frac{1}{\lambda} + \mathcal{O}(1/\lambda_B),$$

$$\frac{\partial I_3}{\partial \lambda} = \mathcal{O}(1/\lambda_B). \tag{24}$$

This means that for an extreme type II system the vector potential can be neglected in I_3. We find that $I_3 = 1.246\cdots$. Extremising $\bar{A}_2$ with respect to λ, we find $\lambda_e = 1/\sqrt{(4\ln 2 - 1)} = 0.75\cdots$, which is the temperature independent GL result for λ. On the other hand $\bar{A}_3$ has no extremum value of λ. This allows us to conclude that λ_e depends on the temperature. This is in contrast to the extremum size of kinks in polyacetylene.[8] Thus decreasing the temperature in the vicinity of T_c results in corrections to the leading term in $F - F_0$ (which is the GL contribution). From Eq. (20) we see that this includes the $\bar{A}_3$ term. Since $\partial\bar{A}_3/\partial\lambda$ is positive we can infer that decreasing the temperature in the vicinity of T_c results in the decrease of λ_e.

In conclusion we make the following statements:

(i) The ratio ξ/ξ_0 is generally temperature dependent implying that the vortex scale ξ has additional temperature dependence beyond that of Ginzburg Landau theory.

(ii) At temperatures close to the transition temperature T_c, the dimensionless vortex scale λ_e is smaller than the Ginzburg Landau value $1/\sqrt{(4\ln 2 - 1)} = 0.75\cdots$.

What happens for very low temperatures has to be answered using a different approximation,[11] since the expansion for the free energy, Eq. (18) has been tested on an exactly solvable system and yielded errors in the analogue of λ_e of approximately 50 %. This inability of the method is not surprising since at $T = 0$ there is no small expansion parameter.

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