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Vortex origin of tricritical point in Ginzburg-Landau theory

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Abstract. – Motivated by recent experimental progress in the critical regime of high-T_c superconductors, we show how the tricritical point in a superconductor can be derived from the Ginzburg-Landau theory as a consequence of vortex fluctuations. Our derivation explains why usual renormalization group arguments always produce a first-order transition, in contrast to experimental evidence and Monte Carlo simulations.

The critical regime of old-fashioned superconductors can be described extremely well by the Ginzburg-Landau theory [1] in mean-field approximation [2,3]. The reason is the smallness of the Ginzburg temperature interval $\Delta T_{\rm G}$ around the mean-field critical temperature $T_c^{\rm MF}$ where fluctuations become important [4]. A first discussion of the order of the superconductive phase transition by Halperin, Lubensky, and Ma in 1972 [5] appeared therefore somewhat academic.

The situation has changed with the advent of modern high-T_c superconductors. In these the Ginzburg temperature interval is large enough to observe violent field fluctuations and see critical properties beyond mean field. Several experiments have found a critical point of the XY universality class [6]. In addition, there seems to be recent evidence for an additional critical behavior associated with the so-called charged fixed point [7]. In view of future experiments, it is important to understand precisely the nature of critical fluctuations.

The Ginzburg-Landau theory [1] describes a superconductor with the help of an energy density

$$\mathcal{H}(\psi, \boldsymbol{\nabla}\psi, \boldsymbol{A}, \boldsymbol{\nabla}\boldsymbol{A}) = \frac{1}{2}\Big\{[(\boldsymbol{\nabla} - ie\boldsymbol{A})\psi]^2 + \tau|\psi|^2 + \frac{g}{2}|\psi|^4\Big\} + \frac{1}{2}\,(\boldsymbol{\nabla}\times\boldsymbol{A})^2\,, \tag{1}$$

where $\psi(x), \boldsymbol{A}(x)$ are pair field and vector potential, respectively, and e is the charge of the Cooper pairs. The parameter $\tau \equiv T/T_c^{\rm MF} - 1$ is a reduced temperature measuring the distance from the characteristic temperature $T_c^{\rm MF}$ at which the $|\psi|^2$-term changes sign. The theory needs gauge fixing, which is usually done by setting $\psi(x) = \rho(x)e^{i\theta(x)}$, rewriting the covariant derivative of ψ as

$$D\psi = [i(\boldsymbol{\nabla}\theta - e\boldsymbol{A})\rho + \boldsymbol{\nabla}\rho]e^{i\theta}, \tag{2}$$

and eliminating the phase variable $\theta(x)$ by a local gauge transformation $\boldsymbol{A} \to \boldsymbol{A} + \boldsymbol{\nabla}\theta/e$. This brings $\mathcal{H}(\psi, \boldsymbol{\nabla}\psi, \boldsymbol{A}, \boldsymbol{\nabla}\boldsymbol{A})$ to the form

$$\mathcal{H}_1 = \frac{1}{2}(\boldsymbol{\nabla}\rho)^2 + V(\rho) + \frac{1}{2}(\boldsymbol{\nabla} \times \boldsymbol{A})^2 + \frac{\rho^2 e^2}{2}\boldsymbol{A}^2, \tag{3}$$

where $V(\rho)$ is the potential of the ρ-field:

$$V(\rho) = \frac{\tau}{2}\rho^2 + \frac{g}{4}\rho^4. \tag{4}$$

The last term in (3) is the famous Meissner-Higgs mass $m_A = \rho e$ [2,3] of the vector potential $\boldsymbol{A}$. An analogous mass in the gauge theory of electroweak interactions explains why interactions are so much weaker than electromagnetic interactions.

At the mean-field level, the energy density (3) describes a second-order phase transition. It takes place if τ drops below zero where the pair field $\psi(x)$ acquires the nonzero expectation value $\langle\psi(x)\rangle = \rho_0 = \sqrt{-\tau/g}$, the order parameter of the system. The ρ-fluctuations around this value have a *coherence length* $\xi = 1/\sqrt{-2\tau}$. The Meissner-Higgs mass term in (3) gives rise to a finite *penetration depth* of the magnetic field $\lambda = 1/m_A = 1/\rho_0 e$. The ratio of the two length scales $\kappa \equiv \lambda/\sqrt{2}\xi$, which for historic reasons carries a factor $\sqrt{2}$, is the Ginzburg parameter whose mean-field value is $\kappa_{\rm MF} \equiv \sqrt{g/e^2}$. Type-I superconductors have small values of κ, type-II superconductors have large values. At the mean-field level, the dividing line is at $\kappa = 1/\sqrt{2}$.

In high-T_c superconductors, field fluctuations become important. These can be taken into account by calculating the partition function and field correlation functions from the functional integral

$$Z = \int \mathcal{D}\rho\, \rho\, \mathcal{D}\boldsymbol{A}\, e^{-\int {\rm d}^3x\, \mathcal{H}_1} \tag{5}$$

(in natural units with $k_B T = 1$). So far, all analytic approximations to Z pursued since the initial work [5] have had notorious difficulties in accounting for the order of the superconductive phase transition. In [5], simple renormalization group arguments [8] in $4 - \epsilon$ dimensions suggested that the transition should be of first order. The technical signal for this was the nonexistence of an infrared-stable fixed point in the renormalization group flow of the coupling constants e and g as a function of the renormalization scale. However, due to the smallness of the Ginzburg interval $\Delta T_{\rm G}$, the first order was never verified experimentally. Since then, there has been much work [9] trying to find an infrared-stable fixed point in higher loop orders or by different resummations of the divergent perturbations expansions, with little success.

Recall the simplest argument suggesting a first-order nature of the transition arises at the mean-field level of the pair field ρ as follows: The fluctuations of the vector potential are Gaussian and can be integrated out in (5). Assuming ρ to be smooth, this may be done in the Thomas-Fermi approximation [10], leading to an additional cubic term in the potential (4), changing it to

$$V(\rho) = \frac{\tau}{2}\rho^2 + \frac{g}{4}\rho^4 - \frac{c}{3}\rho^3, \qquad c \equiv \frac{e^3}{2\pi}. \tag{6}$$

The cubic term generates, for $\tau < c^2/4g$, a second minimum at

$$\tilde{\rho}_0 = \frac{c}{2g}\left(1 + \sqrt{1 - \frac{4\tau g}{c^2}}\right). \tag{7}$$

If τ decreases below

$$\tau_1 = 2c^2/9g, \tag{8}$$

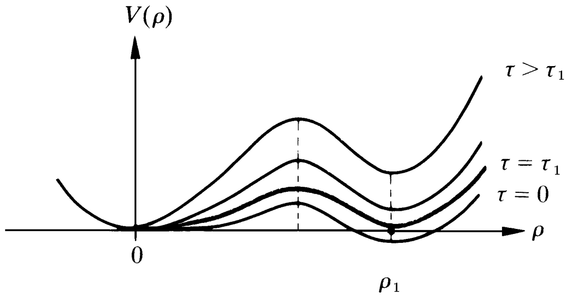

Fig. 1 – Potential for the order parameter ρ with cubic term. A new minimum develops around ρ_1 causing a first-order transition for $\tau = \tau_1$.

the new minimum lies *lower* than the one at the origin (see fig. 1), so that the order parameter jumps from zero to

$$\rho_1 = 2c/3g \tag{9}$$

in a phase transition. At this point, the coherence length of the ρ-fluctuations $\xi = 1/\sqrt{\tau + 3g\rho^2 - 2c\rho}$ has the finite value (the same as the fluctuations around $\rho = 0$)

$$\xi_1 = \frac{3}{c}\sqrt{\frac{g}{2}}. \tag{10}$$

The phase transition is therefore of first order.

This conclusion is reliable only if the jump of ρ_0 is sufficiently large. For small jumps, the mean-field discussion of the energy density (6) cannot be trusted. The place where the transition becomes second order has, so far, never been explained satisfactorily within the Ginzburg-Landau theory. This has been done only with the help of a dual disorder field theory derived from the Ginzburg-Landau theory in refs. [11,12]. This theory is constructed in such a way that its Feynman diagrams are direct pictures of the vortex lines of the superconductor. The dual disorder field theory shows that there is indeed a first-order transition if the Ginzburg parameter $\kappa \equiv \lambda/\sqrt{2}\xi$ is smaller than the tricritical value $\kappa^{\rm tric} \approx 0.8/\sqrt{2}$. This point is close to the mean-field value $\kappa = 1/\sqrt{2}$, where the superconductor changes from type II to type I, and the average short-range repulsion between vortex lines changes into an attraction.

In contrast to the Ginzburg-Landau theory, the vector potential of the disorder field theory is massive from the outset, so that its fluctuations do not generate a cubic term. Instead, they generate an additional negative *quartic* term [11], making the transition first order for $\kappa < \kappa^{\rm tric}$, while leaving it second order for $\kappa > \kappa^{\rm tric}$.

The purpose of this letter is to show how the tricritical point can be derived from the original Ginzburg-Landau theory by a proper inclusion of fluctuation corrections. The mistake in the above discussion of (1) lies in the neglect of vortex fluctuations. In fact, the transformation of the covariant derivative $D\psi$ to the ρ-θ expression in eq. (2) is false. Since $\theta(\boldsymbol{x})$ and $\theta(\boldsymbol{x}) + 2\pi$ are physically indistinguishable —the complex field $\psi(\boldsymbol{x})$ is the same for both— the correct substitution is

$$D\psi = [i(\boldsymbol{\nabla}\theta - 2\pi\boldsymbol{\theta}^v - e\boldsymbol{A})\rho + \boldsymbol{\nabla}\rho]e^{i\theta}. \tag{11}$$

The cyclic nature of the scalar field $\theta(\boldsymbol{x})$ requires the presence of a vector field $\boldsymbol{\theta}^v(\boldsymbol{x})$ called *vortex gauge field*. This field is a sum of δ-functions on Volterra surfaces across which $\theta(\boldsymbol{x})$ has jumps by 2π. The boundary lines of the surfaces are vortex lines. They are found from the vortex gauge field $\boldsymbol{\theta}^v(\boldsymbol{x})$ by forming the curl

$$\boldsymbol{\nabla}\times\boldsymbol{\theta}^v(\boldsymbol{x})=\boldsymbol{j}^v(\boldsymbol{x}), \tag{12}$$

where $\boldsymbol{j}^v(\boldsymbol{x})$ is the *vortex density*, a sum over δ-functions along the vortex lines $\boldsymbol{\delta}(L;\boldsymbol{x})\equiv\int_L \mathrm{d}\bar{\boldsymbol{x}}\,\delta(\boldsymbol{x}-\bar{\boldsymbol{x}})$. Vortex gauge transformations are deformations of the surfaces at fixed boundary lines which add to $\boldsymbol{\theta}^v(\boldsymbol{x})$ pure gradients of the form $\boldsymbol{\nabla}\delta(V;\boldsymbol{x})$, where $\delta(V;\boldsymbol{x})\equiv\int_V \mathrm{d}^3\bar{x}\,\delta(\boldsymbol{x}-\bar{\boldsymbol{x}})$ are δ-functions on the volumes V over which the surfaces have swept. The theory of these fields has been developed in the textbook [12] and the Cambridge lectures [13]. Being a gauge field, $\boldsymbol{\theta}^v(\boldsymbol{x})$ may be modified by a further gradient of a smooth function to make it purely transverse, $\boldsymbol{\nabla}\cdot\boldsymbol{\theta}^v_T(\boldsymbol{x})=0$, as indicated by the subscript T. Since the vortex gauge field is not a gradient, it cannot be absorbed into the vector potential by a gauge transformation. Hence it survives in the last term in eq. (3), and the correct partition function is

$$Z\approx\int\mathcal{D}\boldsymbol{\theta}^v_T\int\mathcal{D}\rho\rho\,\mathcal{D}\boldsymbol{A}\exp\left[-\frac{1}{2}(\boldsymbol{\nabla}\rho)^2-\frac{\tau}{2}\rho^2-\frac{g}{4}\rho^4-\frac{1}{2}(\boldsymbol{\nabla}\times\boldsymbol{A})^2-\frac{\rho^2e^2}{2}(\boldsymbol{A}-2\pi\boldsymbol{\theta}^v_T/e)^2\right]. \tag{13}$$

The symbol $\int\mathcal{D}\boldsymbol{\theta}^v_T$ does not denote an ordinary functional integral. It is defined as a sum over all numbers and shapes of Volterra surfaces S in $\boldsymbol{\theta}^v_T$, across which the phase jumps by 2π [13].

The important observation is now that the partial partition function of the $\boldsymbol{A}$-field contained in (13)

$$Z_1[\rho]\equiv\int\mathcal{D}\boldsymbol{\theta}^v_T\mathcal{D}\boldsymbol{A}\exp\left[-\frac{1}{2}\int\mathrm{d}^3x(\boldsymbol{\nabla}\times\boldsymbol{A})^2-\frac{\rho^2}{2}\int\mathrm{d}^3x[e\boldsymbol{A}-2\pi\boldsymbol{\theta}^v_T]^2\right] \tag{14}$$

can give rise to a second-order transition of the XY-model type if the Ginzburg parameter κ is sufficiently large. To see this we integrate out the $\boldsymbol{A}$-field and obtain

$$Z_1[\rho]=\exp\left[\int\mathrm{d}^3x\frac{e^3\rho^3}{6\pi}\right]\int\mathcal{D}\boldsymbol{\theta}^v_T\exp\left[\frac{4\pi^2\rho^2}{2}\int\mathrm{d}^3x\left(\frac{1}{2}\boldsymbol{\theta}^{v\,2}_T-\boldsymbol{\theta}^v_T\frac{\rho^2e^2}{-\boldsymbol{\nabla}^2+\rho^2e^2}\boldsymbol{\theta}^v_T\right)\right]. \tag{15}$$

The second integral can be simplified to

$$\frac{4\pi^2\rho^2}{2}\int\mathrm{d}^3x\left(\boldsymbol{\theta}^v_T\frac{-\boldsymbol{\nabla}^2}{-\boldsymbol{\nabla}^2+\rho^2e^2}\boldsymbol{\theta}^v_T\right). \tag{16}$$

Integrating this by parts, and replacing $\nabla_i\boldsymbol{\theta}^v_T\,\nabla_i\boldsymbol{\theta}^v_T$ by $(\boldsymbol{\nabla}\times\boldsymbol{\theta}^v_T)^2=\boldsymbol{j}^{v\,2}$, since $\boldsymbol{\nabla}\cdot\boldsymbol{\theta}^v_T=0$, the partition function (15) without the prefactor takes the form

$$Z_2[\rho]=\int\mathcal{D}\boldsymbol{\theta}^v_T\exp\left[-\frac{4\pi^2\rho^2}{2}\int\mathrm{d}^3x\left(\boldsymbol{j}^v\frac{1}{-\boldsymbol{\nabla}^2+\rho^2e^2}\boldsymbol{j}^v\right)\right]. \tag{17}$$

This is the partition function of a grand-canonical ensemble of closed fluctuating vortex lines. The interaction between them has a finite range equal to the penetration depth $\lambda=1/\rho e$.

It is well known how to compute pair and magnetic fields of the Ginzburg-Landau theory for a single straight vortex line from the extrema of the energy density [2]. In an external magnetic field, there exist triangular and various other regular arrays of vortex lattices and various phase transitions. In the core of each vortex line, the pair field ρ goes to zero over a distance ξ. If we want to sum over grand-canonical ensemble of fluctuating vortex lines of any shape in the partition function (13), the space dependence of ρ causes complications. These can be avoided by an approximation, in which the system is placed on a simple-cubic lattice of spacing $a = \alpha\,\xi$, with α of the order of unity, and a *fixed* value $\rho = \tilde{\rho}_0$ given by eq. (7). Thus we replace the partial partition function (17) approximately by

$$Z_2[\tilde{\rho}_0] = \sum_{\{\boldsymbol{l};\boldsymbol{\nabla}\cdot\boldsymbol{l}=0\}} \exp\left[-\frac{4\pi^2\tilde{\rho}_0^2 a}{2}\sum_{\boldsymbol{x}} \boldsymbol{l}(\boldsymbol{x}) v_{\tilde{\rho}_0 e}(\boldsymbol{x}-\boldsymbol{x}')\boldsymbol{l}(\boldsymbol{x}')\right]. \tag{18}$$

The sum runs over the discrete versions of the vortex density in (12). These are integer-valued vectors $\boldsymbol{l}(\boldsymbol{x}) = (l_1(\boldsymbol{x}), l_2(\boldsymbol{x}), l_3(\boldsymbol{x}))$ which satisfy $\boldsymbol{\nabla}\cdot\boldsymbol{l}(\boldsymbol{x}) = 0$, where $\boldsymbol{\nabla}$ denotes the lattice derivative. This condition restricts the sum over all $\boldsymbol{l}(\boldsymbol{x})$-configurations in (18) to all non–self-backtracking integer-valued closed loops. The function

$$v_m(\boldsymbol{x}) = \prod_{i=1}^{3}\int \frac{\mathrm{d}^3(ak_i)}{(2\pi)^3}\frac{e^{i(k_1x_1+k_2x_2+k_3x_3)}}{2\sum_{i=1}^{3}(1-\cos ak_i)+a^2m^2} = \int \mathrm{d}s e^{-(6+m^2)s} I_{x_1}(2s)I_{x_2}(2s)I_{x_3}(2s). \tag{19}$$

is the lattice Yukawa potential.

The lattice partition function (18) is known to have a second-oder phase transition in the universality class of the XY model. This can be seen by a comparison with the Villain approximation [14] to the XY model, whose partition function is a lattice version of

$$Z_V[\rho] = \int \mathcal{D}\theta \int \mathcal{D}\boldsymbol{\theta}_T^v \exp\left[-\frac{b}{2}\int \mathrm{d}^3x\ (\boldsymbol{\nabla}\theta - \boldsymbol{\theta}_T^v)^2\right].$$

After integrating out $\theta(\boldsymbol{x})$, this becomes

$$Z_V[\rho] = \mathrm{Det}^{-1/2}(-\boldsymbol{\nabla}^2)\int \mathcal{D}\boldsymbol{\theta}_T^v \exp\left[-\frac{b}{2}\int \mathrm{d}^3x\, \boldsymbol{\theta}_T^{v\;2}\right], \tag{20}$$

and we can replace $\boldsymbol{\theta}_T^{v\,2}$ by $(\boldsymbol{\nabla}\times\boldsymbol{\theta}_T^v)(-\boldsymbol{\nabla}^2)^{-1}(\boldsymbol{\nabla}\times\boldsymbol{\theta}_T^v) = \boldsymbol{j}^v(-\boldsymbol{\nabla}^2)^{-1}\boldsymbol{j}^v$. By taking this expression to a simple-cubic lattice we obtain the partition function (18), but with $\tilde{\rho}_0^2 a$ replaced by $\beta_V \equiv ba$, and the Yukawa potential $v_{\tilde{\rho}_0 e}(\boldsymbol{x})$ replaced by the Coulomb potential $v_0(\boldsymbol{x})$.

The partition function (18) has the same transition at roughly the same place as its local approximation

$$Z_2[\tilde{\rho}_0] \approx \sum_{\{\boldsymbol{l};\boldsymbol{\nabla}\cdot\boldsymbol{l}=0\}} \exp\left[-\frac{4\pi^2\tilde{\rho}_0^2 a}{2} v_{\tilde{\rho}_0 e}(\mathbf{0})\sum_{\boldsymbol{x}} \boldsymbol{l}^2(\boldsymbol{x})\right]. \tag{21}$$

A similar approximation holds for the Villain model with $v_0(\boldsymbol{x})$ instead of $v_{\tilde{\rho}_0 e}(\boldsymbol{x})$, and $\tilde{\rho}_0^2 a$ replaced by $\beta_V \equiv ba$.

The Villain model is known to undergo a second-order phase transition of the XY-model type at $\beta_V = r/3$ with $r \approx 1$, where the vortex lines become infinitely long [14]. Thus we conclude that also the partition function (21) has a second-order phase transition of the XY-model type at $\tilde{\rho}^2 v_{\tilde{\rho}_0 e}(\mathbf{0})a \approx v_0(\mathbf{0})/3$. The potential (19) at the origin has the hopping expansion [12]

$$v_m(\mathbf{0}) = \sum_{n=0,2,4} \frac{H_n}{(a^2m^2+6)^{n+1}}, \qquad H_0 = 1, \qquad H_2 = 6,\ \ldots\,. \tag{22}$$

To lowest order, this yields the ratio $v_m(\mathbf{0})/v_0(\mathbf{0}) \equiv 1/(m^2/6+1)$. A more accurate numerical fit to the ratio $v_m(\mathbf{0})/v_0(\mathbf{0})$ which is good up to $m^2 \approx 10$ (thus comprising all interesting κ-values since m^2 is of the order of $3/\kappa^2$) is $1/(\sigma\, m^2/6+1)$ with $\sigma \approx 1.38$. Hence the transition takes place at

$$\frac{\tilde{\rho}_0^2 a}{(\sigma\, a^2 \tilde{\rho}_0^2 e^2/6+1)} \approx \frac{r}{3} \quad \text{or} \quad \tilde{\rho}_0 \approx \frac{1}{\sqrt{3a}}\sqrt{\frac{r}{1-\sigma r a e^2/18}}. \tag{23}$$

The important point is now that this transition can only occur until $\tilde{\rho}_0$ reaches the value $\rho_1 = 2c/3g$ of eq. (9). From there on, the transition will no longer be of the XY-model type but occur discontinuously as a first-order transition.

Replacing in (23) a by $\alpha\xi_1$ of eq. (10), and $\tilde{\rho}_0$ by ρ_1, we find the equation for the mean-field Ginzburg parameter $\kappa_{\rm MF} = \sqrt{g/e^2}$:

$$\kappa_{\rm MF}^3 + \alpha^2\sigma\frac{\kappa_{\rm MF}}{3} - \frac{\sqrt{2}\alpha}{\pi r} = 0. \tag{24}$$

Inserting $\sigma \approx 1.38$ and choosing $\alpha \approx r \approx 1$, the solution of this equation yields the tricritical value

$$\kappa_{\rm MF}^{\rm tric} \approx 0.81/\sqrt{2}. \tag{25}$$

In spite of the roughness of the approximations, this result is very close to the value $0.8/\sqrt{2}$ derived from the dual theory in [11]. The approximation has three uncertainties. First, the identification of the effective lattice spacing $a = \alpha\xi$ with $\alpha \approx 1$; second, the associated neglect of the $\boldsymbol{x}$-dependence of ρ and its fluctuations; and third, the localization of the critical point of the XY-model–type transition in eq. (23).

Our goal has been achieved: We have shown the existence of a tricritical point in a superconductor directly within the fluctuating Ginzburg-Landau theory, by taking the vortex fluctuations into account. This became possible after correcting the covariant derivative (2) of $\psi = \rho e^{i\theta}$ to (11). For $\kappa > 0.81/\sqrt{2}$, vortex fluctuations give rise to an XY-model–type second-order transition before the cubic term becomes relevant. This happens for $\kappa < 0.81/\sqrt{2}$ where the cubic term causes a discontinuous transition.

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