Vortices and the Ginzburg-Landau phase transition

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Abstract

The methods for studying the role of vortex loops in the phase transition of the Ginzburg-Landau theory of superconductivity using lattice Monte Carlo simulations are discussed. Gauge-invariant observables that measure the properties of the vortex loop distribution are defined. The exact relations between the lattice and continuum quantities make it possible to extrapolate the results of the simulations to the continuum limit. The relationship between spontaneous symmetry breaking and phase transitions is also reviewed, with an emphasis on the fact that a local symmetry cannot be broken.

Key words: Superconductivity, Vortices, Lattice simulations

1 Introduction

Vortex lines result from the classical Ginzburg-Landau equations of motion, when the behavior of a Type II superconductor in the presence of an external magnetic field is calculated [1]. However, in the classical approximation the effect of thermal fluctuations is neglected, and near the critical temperature this is not justified anymore [2].

The inclusion of the fluctuations means moving from the Ginzburg-Landau equations to a three-dimensional field theory called the Ginzburg-Landau theory or the U(1)+Higgs model. One striking consequence of the fluctuations is

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that they restore the gauge symmetry at all temperatures [3]. Therefore, the phase transition cannot be understood to be a consequence of spontaneous symmetry breakdown. One property that is expected to distinguish between the phases is the behavior of the vortex loops created by the thermal fluctuations [4].

No reliable methods are available to study the behavior of the vortices directly from the continuum theory. Approximative approaches have been used both in analytical and in numerical calculations [4–6]. However, the only way to be able to systematically remove the error of the approximation is to perform Monte Carlo simulations with a discretized lattice version of the full theory and then extrapolate the results to zero lattice spacing. Such simulations have been performed and the results were reported in Ref. [7], from the point of view of particle physics. The purpose of this talk is to discuss the starting points and the ideas of these simulations and to make a link to condensed matter physics.

This talk is organized as follows. Section 2 contains the starting points of our analysis: the basic properties of the continuum Ginzburg-Landau theory. In Section 3, we review the phenomenon of spontaneous symmetry breaking and its absence in gauge theories. The definition of the lattice version of the Ginzburg-Landau theory is given in Section 4, and its vortex configurations are discussed in Section 5, where we also discuss the observables measured in Monte Carlo simulations.

2 Ginzburg-Landau theory of superconductivity

The Ginzburg-Landau theory contains two fields, a complex scalar field \( \psi \) and a real vector-valued gauge field \( A \). The action of the theory (the Ginzburg-Landau energy) is

\[
S = \int d^3x \left[ |(\nabla - iA)\psi|^2 + y|\psi|^2 + x|\psi|^4 + \frac{1}{2} (\nabla \times A)^2 \right].
\]  

(1)

The theory is parameterized by two dimensionless variables, \( x \) and \( y \). The fields and the coordinate \( x \) have been scaled to dimensionless quantities. The parameters \( x \) and \( y \) are uniquely fixed by the requirement that the gauge coupling constant is scaled to unity. It is a trivial matter to transform the results to physical dimensions, if desired. The values of the parameters \( x \) and \( y \) can be derived from the microscopical BCS theory of superconductivity:

\[
y = \frac{1}{q^4} \left( \frac{T}{T_0} - 1 \right), \quad x = \frac{g}{q^2},
\]  

(2)
where \( g \approx 111.084 \left( \frac{T_0}{T_F} \right)^2 \sim 10^{-6} \), and \( q \approx 0.730 \sqrt{\frac{e^2 v_F}{\hbar c^2}} \sim 10^{-2} \) [5, 8]. It can be seen that \( x = \kappa^2 \) depends on the material of the superconductor and is small in Type I superconductors and large in Type II superconductors. The parameter \( y \) depends on the temperature. Since the factor multiplying the temperature in \( y \) is so large, \( 1/q^4 \sim 10^8 \), the temperature range in which \( y \) is small is very narrow.

The Lagrangian (1) is invariant under (local) gauge transformations

\[
\psi(x) \rightarrow \exp(i\theta(x)) \psi(x), \quad A(x) \rightarrow A(x) - \nabla \theta(x),
\]

where \( \theta(x) \) is an arbitrary real-valued function. In more complicated theories, \( \theta(x) \) can be an element of some non-Abelian Lie group.

When \( T \) is far enough from the critical temperature, the fluctuations are often assumed to be negligible. Then one can use the mean-field approach and derive the Ginzburg-Landau equations as the Euler-Lagrange equations of motion from the action (1) and solve them to find out the lowest-energy field configuration \((\psi_{EL}(x), A_{EL}(x))\). When \( T > T_0 \), i.e. when \( y > 0 \), the solution is trivial and both fields vanish. At temperatures below \( T_0 \) the system appears to be in the broken phase, in which the field \( \psi \) has a non-zero value. Because of this, the Higgs mechanism [9] gives the photon a non-zero mass and explains the Meissner effect. Since the solution \((\psi_{EL}(x), A_{EL}(x))\) is not invariant under the gauge transformation (3), the state of the system seems to break the symmetry spontaneously. This is then interpreted to imply a second-order phase transition, analogously to ferromagnets. A second-order transition is indeed what seems to be observed in experiments, but there are still fundamental difficulties in this interpretation.

### 3 Spontaneous symmetry breaking

In statistical mechanics or quantum field theory, the state of the system is specified by the observables, i.e. the expectation values of different functions \( \langle f[\psi] \rangle \) [10]. In thermal equilibrium the state is given by the Gibbs measure:

\[
\langle f[\psi] \rangle = Z^{-1} \sum_{\psi} f[\psi] \exp \left( -\beta H[\psi] \right),
\]
where the sum is taken over all the possible configurations of the system\footnote{In quantum statistical mechanics one should take a trace in the Fock space instead of a sum, but the trace can be transformed to a similar form with \(d + 1\) dimensions \cite{[11]}, and therefore we will not consider it separately.} and \(Z\) is a constant defined by \(\langle 1 \rangle = 1\). The definition (4) can be extended to the infinite case by defining the system in a box of size \(L^d\), where \(d\) is the dimensionality of the system, and taking \(L\) to infinity. In the infinite-volume limit the analyticity of the observables is no longer guaranteed. The possible non-analyticities are called phase transitions.

Let us consider a model defined on an \(L^d\) lattice and given by a Hamiltonian \(H_{L,h}[\psi]\), where \(\psi\) denotes the fields of the theory and \(H_{L,h}\) is a linear function of the real variable \(h\) (typically an external field coupling to \(\psi\)). Suppose that when \(h = 0\) the Hamiltonian is invariant under some transformation \(\Lambda\) of the fields, i.e. \(H_{L,0}[\psi] \equiv H_{L,0}[\Lambda \psi] = H_{L,0}[\psi]\). Now let us choose some local function of the fields \(f[\psi]\), i.e. one that depends only on the values of \(\psi\) at finitely many points. For any values of \(h\) and \(L\), we will denote the expectation value of \(f[\psi]\) by

\[
\langle f[\psi] \rangle_{L,h} = Z_{L,h}^{-1} \sum f[\psi] \exp \left[ -\beta H_{L,h} \right].
\]

(5)

If, for any such \(f[\psi]\),

\[
\langle f[\psi] \rangle = \lim_{h \to 0^+} \lim_{L \to \infty} \langle f[\psi] \rangle_{L,h}
\]

(6)

is non-invariant, i.e. \(\langle f[\Lambda \psi] \rangle \neq \langle f[\psi] \rangle\) the symmetry is said to be spontaneously broken in the infinite-volume state. This implies that the equilibrium state is non-unique, since it is related by a symmetry transformation to another state, which can be obtained by using \(H^\Lambda_{L,h}\) instead of \(H_{L,h}\) in Eq. (5). Thus \(\langle f[\psi] \rangle\) is discontinuous at \(h = 0\), i.e. the system is at a first-order transition line. If the symmetry is broken only at low temperatures, there is some critical temperature \(T_c\), at which the first-order line terminates. At that point the system undergoes a first- or second-order transition to the symmetric phase.

In many models, e.g. in the Ising model \cite{[12]}, the phase transition occurs because the symmetry is broken at low temperatures. Nevertheless, one can show that one-dimensional systems with only local interactions cannot have spontaneous symmetry breakdown. A less trivial result is the Mermin-Wagner theorem \cite{[13]}, which states that in two dimensions a continuous symmetry cannot be broken. From our point of view the most interesting such result was proven by Elitzur \cite{[3]}: A local symmetry cannot be broken. This means that the equilibrium state of the theory is gauge invariant at all temperatures. There can certainly be phase transitions in the theory, but one needs more
complicated arguments than spontaneous symmetry breaking to explain them. For example in the confinement transition of gauge field theories topological properties of the theory are expected to play an important role. Similarly, in the two-dimensional XY model condensation of vortices causes a Korterlitz-Thouless transition although spontaneous symmetry breaking is forbidden by the Mermin-Wagner theorem. On the other hand in the SU(2)+Higgs theory the symmetry-breaking phase transition predicted by the mean-field theory disappears completely in the non-perturbative regime of the parameter space when fluctuations are taken into account [14].

Despite the Elitzur’s theorem, arguments based on broken symmetry in gauge theories work often very well. The reason is that one fixes the gauge to get rid of the unphysical degrees of freedom. Without gauge fixing, the expectation value of any non-invariant function coincides with the expectation value of its average on the gauge orbit. For example, the expectation value $\langle \psi \rangle$ of the order parameter field vanishes, since $\psi$ transforms covariantly under gauge transformations (3).

Gauge fixing breaks the gauge symmetry explicitly. Gauge-invariant quantities remain unchanged but non-invariant quantities can acquire non-trivial values. For example in the Landau gauge it is possible that $\langle \psi \rangle$ is non-zero, and it actually acts as an order parameter, obtaining non-zero values for some parameter values while vanishing for others [15]. However, it is not a local order parameter in the sense of Eq. (6). Namely, in the Landau gauge $\nabla \cdot A = 0$, and therefore

$$\psi(x) \exp \left[ \frac{i}{4\pi} \int d^3y \frac{A(y) \cdot (y - x)}{|y - x|^3} \right] = \psi(x). \quad (7)$$

Since the left-hand side of the equation is gauge invariant, it is really its expectation value we are calculating, but it is a non-local quantity. We can see from Eq. (7) that a non-zero expectation value of $\psi$ in the Landau gauge implies that the invariance under transformations (3) with $\theta$ constant in space is broken, since in that case the exponential is unchanged in the transformation while $\psi$ transforms as usual.

Since gauge-invariant quantities are unchanged in the gauge fixing, one can use perturbation theory in the gauge-fixed theory to calculate their expectation values, and the resulting expansion is the correct one [16]. This explains why the arguments based on symmetry breaking work so well: The order parameter may have a non-zero value in the particular gauge used in the calculation. Nevertheless, this does not guarantee a phase transition in the original theory without gauge fixing.
4 Lattice model

In our case the analogue of $\beta H$ is the action $S$ given in Eq. (1). However, it is non-trivial to define the sum in Eq. (4) in a continuum theory. In a perturbative approach it can be done with some standard renormalization method, and we interpret the action (1) as renormalized in the $\overline{\text{MS}}$ scheme. In Monte Carlo simulations the problem is solved by defining the theory on a lattice with lattice spacing $a$ and then taking the limit $a \to 0$. In our case this can be done consistently [17].

The lattice action is given by the Lagrangian

$$\mathcal{L} = \frac{1}{2a} \sum_{i<j} \alpha_{ij}^2(x) + \frac{1}{2} \sum_i |\psi(x) - U_i(x)\psi(x + \hat{i})|^2 + \lambda \left(|\psi(x)|^2 - v^2\right)^2,$$

where $\alpha_{ij}(x) = \alpha_i(x) + \alpha_j(x + \hat{i}) - \alpha_i(x + \hat{j}) - \alpha_j(x)$ and $U_i(x) = \exp[\alpha_i(x)]$. Now $\alpha_i(x)$ is a real number defined on each link between the lattice sites and corresponds to the continuum gauge field $A(x)$, and $\psi(x) = \rho(x) \exp[i\gamma(x)]$ is a complex field defined on the sites. The gauge transformation (3) becomes

$$\gamma(x) \to [\gamma(x) + \theta(x)]_\pi, \quad \alpha_i(x) \to \alpha_i(x) + \theta(x) - \theta(x + \hat{i}),$$

where $\theta(x)$ is a real valued function on the lattice, and the notation $[X]_\pi$ means $X + 2\pi n \in (-\pi, \pi]$ with $n \in \mathbb{Z}$.

The continuum Ginzburg-Landau theory is obtained by taking the limit $a \to 0$ in the lattice theory in such a way that the long-range properties remain unchanged. This means that we have to vary the values of the lattice couplings $v^2$ and $\lambda$ as functions of $a$ [18]. In our case the leading terms in $a$ can be obtained in perturbation theory by calculating some physical correlator both in lattice and in continuum perturbation theory and requiring that they coincide. The required two-loop calculation was performed in Ref. [19] and it gives us the lattice parameters $\lambda, v^2$ as functions of $x, y$ and $a$:

$$\lambda = \frac{1}{4}xa,$$

$$v^2 = -\frac{a}{x} \left[ y - \frac{3.1759115(1 + 2x)}{2\pi a} \right]$$

We use the non-compact formulation, i.e. the actual gauge group is $\mathbb{R}$. In the compact formulation, the phases are analytically connected and the vortex lines are not closed loops. Both formulations are expected to have the same continuum limit, Eq. (1).
\[-\frac{(-4 + 8x - 8x^2)(\log(6/a) + 0.09) - 1.1 + 4.6x}{16\pi^2}\]. \hspace{1cm} (10)

The result is exact in the limit $a \to 0$. Clearly, $\lambda$ vanishes in the continuum limit. Furthermore, the coefficient of the term $\alpha^2_{ij}$ diverges yielding $\alpha_{ij} = 0$. Therefore the short-range properties of the theory in the continuum limit are given by a massless free-field theory. However, at large distances the behavior is different, since then also higher corrections in $a$ yield a non-vanishing contribution.

The phase structure of the lattice $U(1)+$Higgs model is relatively well understood [20]. There are two phases, the normal phase with a massless photon and the superconducting phase with a massive photon, i.e. the Meissner effect. The system has been rigorously proven to be in the normal phase if $a$ is larger than some constant $a_0 > 0$, or if $v^2$ is smaller than some $a$-independent value $v_0^2(\lambda) \geq 0$. However, at values of $a$ smaller than some constant $a_1 > 0$ and $\lambda$ larger than some $\lambda_1 > 0$, the system is in the superconducting phase provided $av^2 > a_1v_1^2$ with some constant $v_1^2$. Also, if $\lambda v^2$ and $av^2$ are positive, the system will be in the superconducting phase for small enough $\lambda$. However, the values of the constants appearing in these statements are not known, and therefore the rigorous results do not tell much about the continuum limit $a \to 0$ of the theory.

Results of numerical Monte Carlo simulations (see Ref. [8] and references therein) can be extrapolated to the continuum limit using the renormalization equations (10), and in this way both phases have been found also in the continuum theory. The phase diagram is shown in Fig. 1. There is a first-order transition at small $x$, as expected from the perturbative approximation [21]. At large $x$, the transition seems to be continuous and its order is not known. In any case, the latent heat of the first-order transition is too small to be observed experimentally in superconductors.

## 5 Vortices

The two-dimensional XY model is a well-known example of a theory that displays a phase transition without a symmetry breaking [22]. In the low-temperature phase, the dominating excitations are the spin waves, and the correlation length of the system is infinite. Fluctuations create small vortex-antivortex pairs, but they do not have much effect on any large-scale properties. At high enough temperature, nevertheless, the fluctuations are capable of creating vortices and antivortices arbitrarily far apart from each other and therefore they become the dominating excitations. This makes the correlation length finite. Therefore, there must be a phase transition point at which the
correlation length diverges.

The Ginzburg-Landau theory (1) has similar properties. It has two phases, one of which has an infinite correlation length. It also contains vortices, in the form of closed loops [1]. To see this, consider a field configuration \((\psi(\mathbf{x}), \mathbf{A}(\mathbf{x}))\). Let us write \(\psi(\mathbf{x}) = \rho(\mathbf{x}) \exp[i\gamma(\mathbf{x})]\), where \(\gamma\) is only defined modulo \(2\pi\) and has singularities when \(\psi(\mathbf{x}) = 0\). If we require that \(\gamma\) is continuous when \(\psi(\mathbf{x}) \neq 0\), it becomes a multi-valued function. Therefore it is possible that the contour integral around a closed curve \(C\)

\[
\oint_C \mathbf{d}\mathbf{x} \cdot \nabla \gamma(\mathbf{x}) \equiv 2\pi n_C
\]  

(11)

can have non-zero values. The winding number \(n_C\) is a gauge-invariant integer and can be non-zero if there is a singularity, a vortex line, going through the curve. These vortex lines cost energy and they can be removed only by shrinking them to a point. Therefore they are classically stable objects. It is natural to think that in the superconducting phase, the fluctuations can create only small vortex loops, but in the normal phase, they can be arbitrarily large. However, the problem is how to calculate their distribution, or the expectation

Fig. 1. The phase diagram of the continuum theory [8]. The diamonds show the parameter values at which the vortex simulations have been performed.
value of $|n_C|$, to confirm this idea.

The effects of the vortices have been studied intensively in the London limit $\lambda \to \infty$ of the lattice theory [6]. In this limit, the length of $\psi$ is fixed and the theory can be further simplified by replacing the Lagrangian with the Villain version [23]. One can then construct a dual theory [4] in which the vortex loops are the fundamental objects. The phase transition takes place because of condensation of vortices. It still remains to be seen, to what extent the same is true in the realistic case, i.e. when $a \to 0$ together with $\lambda \to 0$.

To answer this question, Monte Carlo simulations must be performed in the original lattice theory (8). Then the relations (10) make the continuum extrapolation of physical quantities possible. To study the properties of the vortices, the winding number (11) must be also defined on the lattice, but the most straightforward choice, i.e. replacing the gradient by its lattice counterpart

$$\partial_i \gamma(x) \to \frac{1}{a} [\gamma(x + \hat{i}) - \gamma(x)]_\pi$$

leads to problems. The resulting winding number would not be gauge invariant, since one can, for example, choose $\theta(x) = -\gamma(x)$ in Eq. (9), in which case there would be no vortices. One solution would be to fix the gauge, but then the result would depend on the gauge chosen and would be difficult to interpret. Therefore a gauge-invariant lattice analogue for Eq. (11) is needed.

For each positively directed link $l = (x, x + \hat{i})$, let us define

$$Y_l = [\alpha_i(x) + \gamma(x + \hat{i}) - \gamma(x)]_\pi - \alpha_i(x).$$

This is clearly nothing but

$$Y_l = \gamma(x + \hat{i}) - \gamma(x) + 2\pi n_i(x),$$

where $n_i(x)$ is such an integer that $Y_l \in (-\pi - \alpha_i(x), \pi - \alpha_i(x))$. For links with negative direction, $l' = (x + \hat{i}, x)$, we define the sign to be the opposite: $Y_{l'} = -Y_l$. Then, for each closed loop $C$, we can define the winding number $n_C$ as

$$Y_C = \sum_{l \in C} Y_l \equiv 2\pi n_C.$$  

This definition of the winding number coincides with that given in Ref. [4] for the $\lambda = \infty$ case.
From Eq. (14), it is easy to see that $n_C$ is an integer, since in the sum every $\gamma$ appears twice with opposite signs and only $n_i$ give a non-vanishing contribution. It is also gauge invariant, since the part of Eq. (13) in the brackets is invariant by itself, and the contribution from the last term $-\alpha_i(x)$ to Eq. (15) gives only the magnetic flux through the curve $C$, which is a gauge-invariant quantity. The winding number has also the correct continuum limit (11) in the sense that $\alpha_i$ in Eq. (13) is proportional to the lattice spacing and what remains is exactly the gradient of the phase $\gamma$.

The winding number $n_C$ is additive in the sense that if $C$ is composed of two curves $A$ and $B$, $n_C = n_A + n_B$. This is of course necessary for it to be meaningful to think of $n_C$ as the number of vortices going through $C$. It also means that vortices do not end, but form closed loops. Therefore Eq. (15) is a valid definition for the existence of a vortex on a lattice.

Let us then consider the Monte Carlo simulations [7]. The simplest quantity to measure is the expectation value of number of vortices through a single plaquette, $\langle |n_{1\times1}| \rangle$. The absolute value has to be taken since otherwise the contribution of vortices going through the plaquette in opposite directions would cancel each other and the result would be zero. This is a non-trivial quantity at finite lattice spacing and it behaves as is expected for the vortex density of the system: It is large in the normal and small in the superconducting phase (See Fig. 2). Nevertheless, it is not a true order parameter since it does not vanish in the superconducting phase.

To find an observable that really can distinguish between the two phases, we have to consider non-local ones. One qualitative difference in the vortex distributions above and below the critical temperature is expected to be the presence of percolating vortices in the high-temperature phase. There is percolation in the system if a vortex that extends through the whole lattice is found with a non-zero probability even in the infinite-volume limit. To observe this, one has to trace the individual vortices on the lattice. Of course, it is possible that the percolation and the true critical point do not coincide, and numerical simulations cannot exclude this possibility, but they can still give much insight to the problem.

Although the lattice Ginzburg-Landau model (8) has interesting and non-trivial properties even at non-zero $a$, the continuum limit $a \to 0$ has more physical significance. Therefore one should ask, which quantities have a finite continuum limit. Unlike in four-dimensional field theories, there is no problem with the renormalization of the theory, since the relations (10) allow one to express everything in terms of renormalized continuum quantities. Since $\langle |n_{1\times1}| \rangle$ depends only on the values of the fields in a finite-size region in lattice units, it measures only the ultraviolet properties. Actually, at the continuum limit its value coincides with the analogous quantity in the massless free-field theory.
Fig. 2. The values of $N_{1 \times 1} \equiv \langle n_{1 \times 1} \rangle$ at various lattice spacings $a = 1/\beta_G$ measured at the points shown in Fig. 1 [7]. Far from the continuum limit, a discontinuity is found at small $x$, but not at large $x$. Note, however, that the values converge to the same point on the continuum limit, and no dependence on the parameters or the phase of the system remains.

and is independent of the parameters $x$ and $y$ and the phase of the system (See Fig. 2). Therefore it is not an interesting quantity from our point of view.

To find non-trivial quantities we need to consider observables that measure the physics at finite distances in physical units. The choice of Ref. [7] was to increase the size of the curve $C$ in $\langle |n_C| \rangle$ accordingly in such a way that for each value of $a$ it is of the same size in physical units. An example is a square of $(c/a) \times (c/a)$ plaquettes. However, one has to remove the contribution of the ultraviolet effects to get physically meaningful results. It is not clear whether there is a way to do this for $\langle |n_C| \rangle$ itself, but in Ref. [7] evidence was given for its discontinuity at the phase transition line to be independent of the ultraviolet details.

In subsequent studies the emphasis should be on the spatial distribution of the vortices. Suitable observables for that purpose are correlation lengths of the vortex density. If we denote by $n_{ij}(x)$ the winding number of the plaquette $(x, x+i, x+i+j, x+j)$, the correlation lengths are given by the exponential
decay of the correlators

\[ G_{ij,kl}(x - y) = \langle n_{ij}(x)n_{kl}(y) \rangle. \] (16)

Percolation can also be studied on the continuum limit but it may be numerically demanding, since at small \( a \) there will be many vortices present also in the superconducting phase.

## 6 Conclusions

We have discussed the properties of the phase transition of the Ginzburg-Landau theory. To stress the importance of the fluctuations in this problem, we gave a brief review of the phenomenon of spontaneous symmetry breakdown and Elitzur’s theorem. We pointed out that, like in the XY model, vortices may have an important role in the transition. The only systematic way to study the behavior of the vortices are lattice simulations, but the naive discretization of the continuum winding number does not give a valid lattice observable since it is not gauge-invariant and leads to trivial results. Therefore we defined a gauge-invariant criterion for the existence of vortices. We also suggested some vortex-related quantities that would give interesting information on the phase transition. The full details and the analysis of the results of the Monte Carlo simulations are given in Ref. [7].

In the studies of vortices in the superconductors, one is usually interested in their behavior in an external magnetic field. The formalism discussed here can also be extended to that case. In cosmology, the interesting question is the nature and the subsequent evolution of the vortex network created in a phase transition. Our approach can be used for that purpose by calculating the properties of the network at the instant when the strings fall out of equilibrium. This gives the initial conditions for the time evolution of the strings. As opposed to the mean-field approach, any value of the parameter \( x \) can be used.

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