Vortex Entanglement and Broken Symmetry

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Based on the London approximation, we investigate numerically the stability of the elementary configurations of entanglement, the twisted-pair and the twisted-triplet, in the vortex-lattice and -liquid phases. We find that, except for the dilute limit, the twisted-pair is unstable and hence irrelevant in the discussion of entanglement. In the lattice phase the twisted-triplet constitutes a metastable, confined configuration of high energy. Loss of lattice symmetry upon melting leads to deconfinement and the twisted-triplet turns into a low-energy helical configuration.

The combination of the soft elastic moduli and the large temperatures attainable in the vortex system of the high-$T_c$ superconductors boosts the importance of fluctuations and leads to interesting phenomena such as vortex-lattice melting and the appearance of vortex-liquid phases. In this context, topological excitations in the vortex system leading to entanglement of the flux lines play an important role, both with respect to statistical mechanics as well as dynamical properties of the vortex-solid and -liquid phases. In this letter, we present a detailed analysis of the stability and recombination properties of the elementary entangled configurations, the twisted-pair and the twisted-triplet (see Fig. 1), for both the vortex-solid and for a model vortex-liquid phase.

Topological excitations of the vortex-lattice in the form of edge- and screw-dislocations are long time known objects \cite{1}. Recently, interest has concentrated on more exotic configurations such as interstitials and vacancies \cite{2}. The latter are relevant in the discussion of a novel super-conductor, namely the vortex-liquid \cite{5}, where the entanglement of the elementary entangled configurations, the twisted-pair (TP) and the twisted-triplet (TT). The analysis is done for an isotropic superconductor (penetration depth $\lambda$, coherence length $\xi$) within the framework of the lowest Landau level approximation valid close to $H_{c2}$.

A metastable twisted-pair configuration does exist in a model vortex-liquid, where the pressure of the surrounding vortices acting on the pair is modelled by a circular potential. This situation has been investigated by Carraro and Fisher \cite{13}, who calculated the reswicthing barrier in the limiting case of an infinitely extended twist using quite ingenious symmetry arguments. Below we will argue that in a realistic description of the vortex-fluid the pressure exerted on a vortex pair by its surroundings destroys the metastable twist in the same way as in a vortex lattice and hence entanglements involving three or more vortices have to be considered.

Vortex entanglement is equally relevant for the dynamical properties of the vortex-liquid: the prohibitively long relaxation times via reptation \cite{8} make the barriers for vortex reswicthing the limiting factor in the vortex dynamics. The reswicthing barriers then determine the inner viscosity of the liquid and hence its pinning, creep, and flow properties \cite{8}.

Previous work on vortex cutting \cite{9,10} has produced first estimates for the reswicthing barrier of two isolated vortices; however, as we will show below the relevance of these results for the entanglement problem in vortex-solids and -liquids is rather limited. Wilkin and Moore \cite{11} have determined the excitation energy of the crossing configuration of a vortex pair in a vortex-lattice, assuming this configuration to constitute a saddle for vortex reswicthing. However, as we will show below, there is no metastable state for the twisted-pair configuration in a vortex-solid and hence there exists no saddle for reswicthing (a similar result has recently been obtained by Dodgson and Moore \cite{12} within the framework of the lowest Landau level approximation valid close to $H_{c2}$). The role played by such basic loops of entanglement on the statistical mechanics of vortex-liquids is the following \cite{1}: If the equilibrium state of the vortex-liquid contains loops of all scales with a finite density, the liquid exhibits a normal (dissipative) response under application of a longitudinal current density $j \parallel B$, and the entangled vortex-liquid is equivalent to the normal metallic phase \cite{1}. If, on the other hand, the vortex-liquid remains disentangled, longitudinal superconducting response survives the melting transition and we obtain a new intermediate liquid phase distinct from the normal metallic one \cite{1}.
simple rescaling \( \mathbb{1} \), at least for \( B > H_{c_1} \). We start out with the vortex-lattice and show that no metastable twisted-pair configuration exists for fields \( B > H_{c_1} \). The TP state can be rendered metastable either by artificially enhancing the vortex core energy or by going over to the dilute limit \( B < H_{c_1} \), where the interaction between vortices becomes short range. Next, we consider the twisted-triplet in the vortex-solid and find a metastable state. The twist is restricted to a finite length along the field axis and we call this a “confined” excitation. The confinement is a consequence of the discrete lattice symmetry and leads to a high excitation energy when compared to the rectilinear groundstate. In comparison, the barrier stabilizing the TT state against reswitching is small and one concludes that the lattice phase shows only little entanglement. In the model vortex-liquid the situation remains essentially unchanged as regards the twisted-pair — the pressure of the neighboring vortices destroys the metastable state in the same manner as in the vortex-solid phase. For the twisted-triplet the assumption of a circular effective potential mimicking the liquid environment is realistic. The restoration of planar rotational symmetry upon melting leads to deconfine-ment and the TT turns into a low-energy helical configuration stabilized by a high barrier against reswitting. As a consequence, one expects the liquid to become entangled, however, due to the large reswitching barrier, a non-entangled system only slowly transforms into an entangled state. Whether a thermodynamic vortex-fluid phase becomes entangled immediately upon melting is a complicated statistical mechanics problem \( \mathbb{1} \) and we will not go into this discussion here. In the following, we give a brief description of the (numerical) technique on which our analysis is based and then present the results for the twisted-pair and twisted-triplet configurations in the vortex-lattice and the model vortex-liquid.

We base our analysis on the London approximation valid for the important low and intermediate field range \( B < 0.2 H_{c_2} \). Choosing a set of \( n \) vortices (labelled by \( \mu, \nu = 1, \ldots n \)) involved in the excitation, the free energy functional takes the form (see Ref. \( \mathbb{1} \), \( r_\mu = (R_\mu, z) \))

\[
\mathcal{F}[r_\mu] = \sum_{\mu=1}^{n} \left( \mathcal{F}_{self}[r_\mu] + \mathcal{F}_{surr}[r_\mu] \right) + \frac{1}{2} \sum_{\mu \neq \nu=1}^{n} \mathcal{F}_{int}[r_\mu, r_\nu]
\]

with

\[
\mathcal{F}_{self}[r_\mu] = \frac{\varepsilon_0}{2} \int dr_\mu \cdot dr_\nu \frac{e^{-\sqrt{r_\mu^2 + r_\nu^2} + \xi^2/\lambda}}{\sqrt{r_\mu^2 + \xi^2}} + \varepsilon_0 \int |dr_\mu|, \nonumber
\]

\[
\mathcal{F}_{int}[r_\mu, r_\nu] = \varepsilon_0 \int dr_\mu \cdot dr_\nu \frac{e^{-\sqrt{r_\mu^2 + r_\nu^2} + \xi^2/\lambda}}{\sqrt{r_\mu^2 + \xi^2}}, \nonumber
\]

\[
\mathcal{F}_{surr}[r_\mu] = 2\varepsilon_0 \int dr_\mu \cdot \hat{z} V(R_\mu), \nonumber
\]

where \( r_\mu \) and \( r_\mu' \), \( (r_\mu = r_\mu - r_\mu') \) refer to separate points on the same line. Here, we treat the constant \( c \) describing the vortex core energy as a parameter; within the London model its physical value is \( c_0 \approx 0.5 \). Taking all nearest neighbors into account (see Fig. 1), we choose \( n = 10 \) and \( n = 12 \) for the TP and the TT, respectively. Twisted metastable configurations are obtained from a topologically correct initial state with subsequent application of a conventional conjugate gradient method to minimize the energy. In case a metastable state exists, the reswitting barrier is found by imposing a constraint dragging the configuration from the metastable minimum over the saddle towards the rectilinear groundstate. Within a constrained configuration the vortex pair/triplet is forced to have a prescribed distance \( d_0 \) in the \( z = 0 \) symmetry plane. With this constraint imposed, the metastable minimum is force-free, however, the saddle configuration in general remains forced and hence we obtain only an upper estimate for the energy of the true (force-free) saddle configuration. We point out that neglecting the contribution of the core to the self-energy \( \mathcal{F}_{self} \) produces severe instabilities leading to unphysical fluctuations upon relaxation. The origin of these short-range single-vortex fluctuations can be traced back to the dispersive nature of the line tension \( \varepsilon \ell(k_z) = \varepsilon_a \ln(1/k_z \xi) \). The functional containing a finite core energy \( (c_0 \approx 0.5) \) is not only physically correct but also stable with respect to such pathological fluctuations.

Before turning to the specific discussion we briefly mention the natural scales in the problem: For a confined excitation the natural length scale along the field axis is the lattice constant \( a_0 \), whereas the scale for the excitation energy is \( \varepsilon_0 a_0 \). For the (uniaxially) anisotropic situation these scales change to \( \varepsilon \ell a_0 \) for the length and \( \varepsilon \ell a_0 \) for the energy, where we have introduced the effective mass ratio \( \hat{\varepsilon}^2 = m/M \ll 1 \). The energy scale is conveniently expressed through the melting temperature \( \mathbb{1} \), \( \varepsilon \ell a_0 \approx T_m/2.7a_0^2 \approx 6T_m \), where we have used a Lindemann number \( a_L = 0.25 \) in the last equation.

**Vortex-lattice:** For the interaction with the surrounding vortices we choose the lattice potential

\[
V(R) = \sum_{m} K_0(|R - R_m|/\lambda) - \sum_{\mu} K_0(|R - R_\mu|/\lambda), \nonumber
\]

with \( R_m \) denoting the equilibrium lattice sites and \( K_0 \) is the zero-order modified Bessel function. For intermediate fields \( H_{c_1} < B < H_{c_2} \) we can use the limit \( \lambda \rightarrow \infty \) in \( V \), leading to a simple and rapidly convergent series upon resummation in Fourier space. We then proceed along the lines described above and first search for a metastable twisted-pair configuration. For fields \( B > H_{c_2} \) and using the correct core energy with \( c_0 \approx 0.5 \) no such metastable state exists; in fact, although such a state does exist for the isolated pair, it is squeezed away by the pressure of the surrounding vortices as the lattice
potential $V$ is switched on. Thereby the twisted vortices tend to align antiparallel in the crossing region and the resulting attractive force between the segments leads to their collapse and mutual annihilation. This tendency of antiparallel alignment can be suppressed by artificially increasing the vortex core energy: for large enough $c$ such that $c > c_0 \approx 4.9 - \ln(a_c/\xi)$ the metastable TP is recovered. Extrapolating this result (obtained for $a_c/\xi < 20$) to smaller fields, a metastable TP configuration is predicted for $a_c/\xi > \exp(4.9 - c_0) \approx 80$ even in the limit $\lambda \to \infty$, a result relevant for $^4$He and marginally relevant for the high-$T_c$ superconductors with $\kappa \approx 50 - 100$. A (more physical) alternative to stabilize the twisted-pair configuration is to decrease the surrounding pressure via reducing the vortex density. For fields $B \lesssim H_{c1}$ the interaction becomes short-range and we have to return to a finite screening length $\lambda \ll \infty$ in $V$. Indeed, in the dilute limit we find a metastable TP for fields $B < 1.65 H_{c1}$, i.e., $a_c > 1.8 \lambda$, where $\kappa = 10$ has been chosen.

Next we discuss the twisted-triplet state in the vortex-lattice (results for $a_c/\xi = 10$ are quoted in the text; see Table I for a summary). Following the scheme described above we find a metastable TT configuration well in the London regime, i.e., with a minimal separation $d_{\text{min}} \approx 0.8 a_c \gg \xi$ between the vortices. Due to the hexagonal symmetry of the surrounding lattice, the twist is constrained within a length $L_{\text{TT}} \approx 2.2 a_c$ and its energy is high as compared to the rectilinear groundstate, $E_{\text{TT}} - E_0 \approx 2.1 \varepsilon_c a_c$, see Fig. 2. On the other hand, the barrier stabilizing the metastable state is small, $E_s - E_{\text{TT}} \approx 0.32 \varepsilon_c a_c$. The saddle still is in the London regime with $d_{\text{min}} > 0.3 a_c$. The reswitching goes through a first collapse, leading to the creation of a small transverse loop which subsequently shrinks to zero, leaving behind three rectilinear vortices in their groundstate, see the inset of Fig. 2. Note the sharp drop in energy when crossing the saddle, a consequence of the sudden reswitching and an indication that the present constraint does not produce a force-free configuration at the saddle-point. We defer the detailed discussion of the various types of (re)switching saddles (loop creation, hysteresis effects) to a forthcoming paper.

**Model vortex-liquid:** Here we reduce the description to those vortices directly involved in the entanglement, i.e., $n = 2$ and $n = 3$ for the twisted-pair and twisted-triplet, respectively. We choose the surrounding potential mimicking the vortex-liquid to be of the form

$$V(R) = \frac{f}{2}(x^2 + s^2y^2),$$

with $f = 2/a_c^2$ ($f = 3/a_c^2$) for the TP (TT) configuration; $s$ denotes an asymmetry parameter. In their analysis of the TP problem, Carraro and Fisher [13] chose a circular symmetry with $s = 1$, where the metastable twisted state takes a helical shape (with a pitch $L_p$) and is degenerate with the rectilinear groundstate in the limit $L_p \to \infty$. In this limit, the reswitting barrier is characterized by a high degree of symmetry and using $a_c/\xi = 10$ we find $E_s - E_h \approx 1.0 \varepsilon_c a_c$, in agreement with previous work [13]. However, in a liquid phase one does not expect the potential acting on a vortex pair to have a circular symmetry; rather the pressure of the surrounding vortices produces an asymmetric potential with $s > 1$ (one expects $s \approx 2.7$ on simple geometrical grounds, assuming a similar pressure to act in the liquid phase as in the solid one). Increasing $s$ beyond the critical value $s_c \approx 1.3$ the entangled configuration becomes unstable and no metastable TP configuration is expected to exist in the liquid phase either. One could argue, that in a vortex liquid the asymmetric potential can accommodate itself and rotate along with the pair, however, such a configuration involves the twist of four lines at least. The approximation of a circular effective potential mimicking the pressure of the surrounding liquid is already quite reasonable for the triplet (and further improves for the configurations involving larger loops with 6 and more vortices). In fact, the main reason for studying the triplet as the elementary enangled configuration is the existence of a metastable twisted configuration in the solid, implying the existence of a similar metastable state in the liquid which still exhibits lattice order on short spatial and temporal scales; in a (viscous) liquid, the entanglement will first go through a confined high-energy twist, similar to the one in the lattice, which subsequently relaxes into a low-energy helical state due to the absence of shear forces in the liquid. The excitation energy of this relaxed state depends on the pitch $L_p$ of the helix and we have verified that for $L_p \gg a_c$ the tilt energy $E_h - E_0 \approx (2\pi^2/9)\ln(a_c/\xi) + 0.5\varepsilon_c a_c^2/L_p$ provides a good approximation within the London regime (note that here the vortices twist by the angle $2\pi/3$ on the length $L_p$). The saddle-point energy for (re)switching remains high, however; in the limit $L_p \to \infty$ an analysis based on symmetry arguments similar to those used by Carraro and Fisher [13] provides the result $E_s - E_h \approx 2.4 \varepsilon_c a_c$, where $a_c/\xi = 10$ and $\lambda \to \infty$ has been chosen. Results for other values of $a_c/\xi$ are summarized in Table I.

In conclusion, we have investigated the elementary enangled configurations, the twisted-pair and the twisted-triplet in a vortex-lattice and -liquid phase. Away from the dilute limit, we find that the twisted-pair is unstable and hence irrelevant for the discussion of entanglement. The basic loop of entanglement is the twisted-triplet which is metastable both in the vortex-lattice and -liquid phase. In the vortex-lattice, the TT is a high energy state stabilized by a comparatively small barrier and hence the vortex-lattice does not entangle. The high energy of the TT excitation is a consequence of the confinement produced by the lattice symmetry of the surrounding potential. Upon melting, the shear modulus disappears and the hexagonal lattice symmetry changes to a rotational one in the liquid. The high-energy twisted-
triplet dissolves into a low-energy helix with a pitch $L_p$ determined by the mutual entanglement in the liquid. It is the phenomenon of deconfinement and its associated drop in excitation energy which tends to bind the two (originally unrelated) transitions of melting (loss of translational lattice symmetry) and entanglement (loss of longitudinal superconductivity) together. Whereas melting immediately triggers entanglement in a system with short range interactions, it remains to be shown whether a disentangled liquid state can be stabilized in a system characterized by an interaction with long range.

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TABLE I. Numerical results obtained for the triplet configurations in the vortex-solid (s) and -liquid (l) phases.

| $a_0/\xi$ | $L_{TT, p}/a_0$ | $(E_{TT, h} - E_0)/\varepsilon a_0$ | $(E_s - E_{TT, h})/\varepsilon a_0$ |
|----------|-----------------|-------------------------------|-------------------------------|
| 5 (s)    | 1.7             | 1.62                          | 0.05                          |
| 5 (l)    | $\infty$        | 0                             | 1.6                           |

FIG. 1. Twisted-triplet configuration embedded within a vortex-lattice. The 9 nearest neighbors are allowed to relax when twisting the inner vortex triplet. A confined ($L_{TT} \approx 2.2 a_0$), high energy metastable state is found, with an excitation energy $E_{TT} - E_0 \approx 2.12 a_0$ and stabilized against reswitching by the small barrier $E_s - E_{TT} \approx 0.32 a_0$.

FIG. 2. Excitation energy $E_{TT}(d_0) - E_0$ versus distance $d_0$ for the clamped twisted-triplet configuration in a vortex-lattice. Inset shows top-view of the clamped configurations marked by the arrows, particularly the metastable state and the fast reswitching geometry close to the saddle. Note the small relaxation amplitude of the surrounding vortices. Upon melting, the confined high-energy twisted configuration turns into a low-energy helical state, whereas the saddle-point configuration for (re)switching stays confined and remains at high energy (see Table I).