Vortex nucleation barriers in superconductors revisited

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The knowledge of energetic barriers and free energy landscape is crucial for applications of superconductors. Examples include barriers for vortex nucleation and pinning in transmission lines, superconducting magnets, superconducting single-photon detectors, and superconductor-based qubits. Contrarily to the problem of finding energy minima and critical magnetic fields, currently, there are no controllable methods to explore the free energy landscape, identify saddle-points, and compute associated barriers. These barriers depend on coherence length, which makes the London-model-based approach by Bean and Livingston in general not reliable. Here we present a generalization of the string method to gauge field theories, which allows the calculation of free energy barriers in superconductors. We apply the technique to solve the full nonlinear problem of vortex nucleation in complicated geometries that previously were not amenable to analytical and numerical treatment. Then, we study the case of rough surfaces and the presence of pinning.

INTRODUCTION

In type-II superconductors, the Meissner state, characterized by the total magnetic field expulsion in the bulk, is stable up to the lower critical field \( H_{c1} \). Above it, quantum vortices appear. However, the Meissner state can survive as a metastable state causing the phenomenon known as magnetic superheating [1; 2]. The presence of fluctuations can trigger the spontaneous decay of the metastable Meissner state through vortex formation. This phenomenon is the effect of a surface barrier, which hinders the vortices nucleation from the sample boundaries [1; 2]. The barrier disappears when the applied magnetic field exceeds a critical value, the nucleation field. In contrast to the potential barrier, determining the nucleation field is amenable to analytical treatment and has been extensively addressed in [3–7]. However, the full problem of the vortex entry barrier is not solved even for the simplest case of a semi-infinite superconductor with an ideal surface. The existing Bean-Livingston estimate relies on the London model, but the result depends on the choice of cutoff, as emphasised by the authors themselves. Therefore the problem requires a solution of the full nonlinear model. Fundamentally, the problem of a vortex entry barrier consists of finding the sphaleron, i.e., the saddle point, which separates two stable states in a gauge theory [8]. In the case of vortex nucleation, it is an energy maximum of the minimum energy path between two states with different phase windings. Since it is a saddle point, the standard energy minimization techniques are not applicable. Related saddle point problems are of importance widely beyond superconductivity.

The knowledge of potential barriers for vortex nucleation is crucial for superconductor applications. The classical application is current transmission and superconducting magnets, where the dissipationless state is lost if free vortices form. Recently, the problems of vortex entry barriers appeared in quantum technologies. In superconducting single-photon detectors, it is believed that the principle of operation consists in the creation of a current-carrying state with a small potential barrier for vortex entry, so that a single photon creates a vortex, hence a detectable signal [9; 10]. However, small barriers yield spontaneous vortex nucleation caused by fluctuations resulting in dark counts. The ability to calculate potential barriers would allow to design devices with significantly improved performances. Likewise, the knowledge of vortex entry barriers is crucial to design superconducting topological qubits [11–13]. The latter case is especially challenging due to the complicated device geometry and presence of heterostructures, where there is no analytical or numerical tool to investigate the free energy landscape.

Here we generalize to gauge theories the simplified string method [14]. This allows us to perform surface barriers calculation in type-II superconductors for vortex nucleation (\( \Delta F_n \)) and escape (\( \Delta F_e \)), by computing the minimum energy path of the transition in the Ginzburg-Landau theory. The results differ from the Bean-Livingston theory [2], which neglects the vortex core and nonlinear effects. More importantly, the method allows computing the effect of a complicated geometry, surface roughness and presence of pinning on the vortex entry barrier and superheating field.

MODEL

The Ginzburg-Landau free energy functional describing the superconductor in dimensionless units is written
as follows:

\[
f[a, \psi] = \int_{\Omega} \frac{1}{2} \left| \left( -i \frac{\partial}{\partial s} \nabla + a \right) \psi \right|^2 + \frac{1}{2} \left( 1 - |\psi|^2 \right)^2 + \frac{1}{2} (\nabla \times a - \mathbf{h})^2.
\]

The complex field \( \psi = |\psi|e^{i\theta} \) describes the state of the superconductor. The vector potential \( \mathbf{a} \) is related to the magnetic field by \( \mathbf{b} = \nabla \times \mathbf{a} \). The coefficient \( \kappa \) is the Ginzburg-Landau parameter \( \kappa = \frac{\lambda}{\xi} \), which is the ratio of the magnetic field penetration depth \( \lambda \) and the coherence length \( \xi \) [15]. The external magnetic field \( \mathbf{H} \) is expressed in units of the thermodynamic critical field \( H_c \), i.e. \( h = H/H_c \). The free energy \( f = F/F_0 \) is expressed in units of \( F_0 \), which in SI units is \( F_0 = \mu_0 H_c^2 \lambda^2 d \) where \( d \) represents the thickness of the sample and \( \mu_0 \) is the vacuum permeability. Quantities in capital letters are intended in SI units, while variables in lower case are dimensionless. For an infinite system, when \( H < H_{c1} \) the system is in the Meissner phase, no vortices are present in the bulk, and thus the magnetic field is completely screened by the superconducting current at surface. For \( H > H_{c1} \), the system is in the Shubnikov phase in which vortices are present. In a finite system, the Meissner state can survive in a meta-stable way for higher fields than \( H_{c1} \), i.e. up to the spontaneous nucleation field \( H_n \). In the absence of fluctuations, only when this field is exceeded, vortices nucleate from the boundaries. Moreover, if the applied external field is higher than the spontaneous escape field \( H_e \) vortices cannot spontaneously escape from the sample without overcoming the surface barrier. This means that in the region \( H_e < H < H_n \) Shubnikov states are metastable as the presence of the surface energy barrier prevents changes in the number of vortices.

\section*{RESULTS}

To introduce a vortex in the system, in the presence of an external magnetic field \( H < H_n \), we need to overcome an energy barrier due to the formation of surface currents. The calculation of the energy barriers for superconductors is a nonlinear problem which is not in general amenable to analytical treatment. In this work, we adopt a numerical approach developed in other fields to study transitions between two metastable states through identification of Minimum Energy Path. The path is considered in the phase space (configuration space) of the system, and it is convenient to introduce a transition coordinate \( s \in [0, 1] \) to parametrize it. If one denotes by \( \mathbf{q} \) the state of the system, \( \mathbf{q}(s) = (a(s, r), \psi(s, r)) \), then \( \mathbf{q}(0) \) and \( \mathbf{q}(1) \) are two equilibrium solutions corresponding to the minima of the Hamiltonian in Eq. (1). By varying \( s \) from 0 to 1, we assist the transition of the system from the initial state to the final state. One can assume that a potential force \( \mathbf{g} = -\nabla f = -\left( \frac{\partial f}{\partial \mathbf{a}} - \left( \frac{\delta f}{\delta \psi} \right) \psi \right) \) acts on each point of the curve \( \mathbf{q}(s) \). The Minimum Energy Path is a trajectory in which the force \( \mathbf{f} \) acting on each point is uniquely directed along the tangent vector \( \frac{\partial \mathbf{q}}{\partial s} \), i.e.:

\[
\nabla f \cdot \frac{\partial \mathbf{q}}{\partial s} = \| \nabla f \| \frac{\partial \mathbf{q}}{\partial s}, \quad \forall s \in [0, 1].
\]

We emphasize that the optimal path defined by Eq. (2) does not correspond to the real time dynamics. It describes the most energetically favorable transformation undertaken by the system for the transition between the initial and the final state. To identify the minimum energy path, we have generalized to gauge field theories the simplified string method [14], which is an algorithm that evolves an initial guessed path in the configuration space, towards the minimal energy one. The application of the string method to sphalerons identification in gauge theories is associated with several technical challenges, mainly related to metric definition for a Hilbert space and gauge invariance preservation. For this reason, we have developed a variant that we called gauged string method, which we describe in detail in the supplementary material. The iterative procedure of the method we use consists of alternating steps of minimization and gauge-independent reparametrization. The role of the latter is to nullify the component of the displacement tangential to the path, with the effect of ”freezing” the system in different configurations. The minimization part, performed trough gradient flow, guarantees that the path we find is a minimal energy one. Consider a situation where we start from a Meissner state and end in the one-vortex state. To construct the initial guess, we used ansatz for the single wined vortex state. In the initial state, for \( s = 0 \), the vortex is outside of the domain and Ar the final state, for \( s = 1 \), it lies in the origin. The coordinate \( s \) parameterizes the minimum free energy path, i.e., each value of \( s \) corresponds to a particular configuration of the system. Hence, \( s \) is not equivalent to the position of the center of the vortex because static vortex deformations correspond, in general, to different values of \( s \). This method allows us to solve the full nonlinear problem in contrast to previous approaches. A previous study of the vortex entry barrier, based on the London model, was carried out by Bean-Livingston [2]. However, this introduced the uncontrollable approximation of considering the vortex core as a rigid cylinder of radius \( \xi \), which completely neglects the physics of the core and the nonlinear effects. The energy dependence \( F(s) \) is a function with one or more maxima. At the summit of the potential barrier, the configuration of the system is a saddle point of the free energy functional, which in the context of gauge theories is called sphaleron. The sphalerons are unstable stationary points of the effective Hamiltonian in Eq. (1).
Once the minimum energy path is computed, we can define the nucleation barriers \( \Delta F_n = F_{\text{sphaleron}} - F_{\text{Meissner}} \) for a given magnitude of the external magnetic field, \( H \). Consequently, the nucleation field \( H_n \) is the external field needed to nullify the nucleation barrier, i.e., \( \Delta F_n(H_n) = 0 \). Analogous definitions can be used for the escape barrier, i.e., the energy needed to expel one vortex from the superconductor. We include in the supplementary material the results regarding escape barriers. The minimum energy path contains more information than the height of the energy barrier as those paths are most likely to be followed in the nucleation process. By studying it, we can understand in detail how transitions between metastable states occur. In our framework, we can calculate the energy barrier free from any approximations, except fully controlled numerical errors. Let us begin by considering a vortex entry in a 2D superconductor with flat surfaces. We find that the vortex always enters, following the minimum energy path, from the sides of the superconductor and never from the corners. Figure 1 shows the free energy profile of the process. The barrier presents a single maximum corresponding to the sphaleron. The substantial core deformation confirms that this kind of problem is not in general treatable with controlled accuracy in the London limit. Figure 2 denotes how the maximal height of the energy barrier varies as a function of the applied field, for selected values of \( \kappa \). The data perfectly align with an exponentially decreasing profile. The barrier gets smaller when \( \kappa \) increases. The knowledge of \( \Delta F_n(\kappa, H) \) allows us to calculate the value of the nucleation field \( H_n \), which corresponds to the external field at which the Meissner state loses its (meta)stability and becomes unstable. The method allows studying how the barrier is affected by the sample geometry and by the presence of impurities or surface roughness. We consider illustrative cases in which we study the energy barrier for different sample geometries and impurity profiles, showing how the barrier changes in these situations. Figure 3 a displays the sphaleron field configuration for vortex entry in an L-shaped superconductor. The L-shaped geometry is a well-studied benchmark for the numerical finding of critical fields [17]. The problem of sphaleron and energy barrier for this case is still unsolved. Differently from Figure 1, in this situation, the vortex always enters from the concave corner. To gain further insight into the dependence of the barrier on the sample geometry, we continuously deform the L-shaped geometry by varying the curvature radius of the concave corner, as shown in Figure 3 b. For instance, curvature with a radius equal to zero corresponds to a sharp \( \pi/2 \) angle as in Figure 3 a, while \( r \gg 1 \) eliminates concave corner and thus should yield results similar to square geometry. The vortex entry barrier strongly depends on the geometry of the sample for high external magnetic fields Figure 3 c. In general, for \( H \geq H_c \), our numerical study shows that the vortex nucleation barrier decreases with the curvature radius. For complex materials, the surface can have different roughness, doping and oxidation, requiring taking into account the presence of impurities in the vortex entry problem. The knowledge of how impurities influence vortex physics is crucial for applications. Let us consider randomly distributed impurities, with a decreasing density as we enter the sample, as shown in Figure 4. To introduce the impurities in the
superconductor, we follow a procedure similar to the one outlined in [18; 19], where we modify the quadratic term in Eq. 1 accordingly:

\[
\frac{1}{2}(1 - |\psi(r)|^2)^2 \rightarrow \frac{1}{2}(1 + \sigma(r) - |\psi(r)|^2)^2, \quad (3)
\]

where \(\sigma(r)\) is normally distributed and linearly decreasing from the edge towards the bulk. As Figure 4 shows, in this situation, there can be multiple sphalerons with a minimum in between them. In this case, as depicted by the free energy profile, the global minimum lies in between the sphalerons acting as a vortex trap. This method can also be employed to predict how a vortex trapped near a surface affects the entrance of other vortices.

It is empirically known that in the presence of rough surfaces, the vortex entry barrier is altered [1]. However, there are no calculations able to predict their effect. Figure 5 compares the nucleation barriers \(\Delta F_n/F_0\), associated to different roughness profiles with characteristic size \(d\), as function of the external field \(H\). The green line reports the height of the barrier for \(d \sim \xi\). We can notice the complete overlap with the red-dashed line, depicting the energy barrier for a perfectly flat surface. Hence, up to the size of the coherence length, the effect of surface roughness on the vortex nucleation process is small. As the characteristic size of roughness increases, the energy barrier begins to decrease. The cyan line displays the case for \(d \sim \lambda\) yielding a moderate barrier reduction. In the case \(d > \lambda\) (orange line), we assist to a stronger barrier suppression, comparable with the L-shaped sam-
that previously developed models to estimate the vortex nucleation barrier, based on London approximation, are in general inadequate to describe the process even for a perfectly flat surface. We show that the method allows to calculate vortex entry barriers for complicated geometries and that in general the barriers depend non-trivially on the geometry, the presence of other pinned vortices and coherence and penetration lengths. The vortex entry barriers are of key importance in applications of superconductors and the method can be used to geometrically optimize design of quantum devices such as single-photon detectors and qubits, as well as superconducting transmission lines and magnets. The approach can be applied to microscopic models and to the problem of sphalerons in high energy physics problems.

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AUTHORS CONTRIBUTIONS

E.B. and F.N.R. conceived and supervised the project. A.M. developed the method and the numerical framework used to produce the results and co-wrote the paper. A.B. provided guidance to A.M. and had the leading role in writing the paper. A.M. and A.B. provided equal contribution to the realization of this work.

APPENDIX

The Ginzburg-Landau Model

The effective free energy Ginzburg-Landau functional describing a superconductors reads:

$$F[A, \Psi] = d \int_\Omega dxdy \left( \frac{1}{2m} \left| (-i\hbar \nabla + qA) \Psi \right|^2 + \alpha |\Psi|^2 + \frac{\beta}{2} |\Psi|^4 + \frac{(\nabla \times A - \mu_0 H)^2}{2\mu_0} \right),$$

(4)

The complex order field \( \psi \) is the superconducting order parameter, coupled to the electromagnetic field through

CONCLUSIONS

We formulated a method to compute the Minimum Energy Path of vortex nucleation in superconductors described by a Ginzburg-Landau energy functional. This is to the best of our knowledge the first solution of the full non-linear problem of vortex entry barrier. We showed
the vector potential $\mathbf{A}$. Here $d$ is the effective thickness of the sample with a cross-section denoted by $\Omega$, $m$ is the mass of a superconductive carrier (i.e., the Cooper pair), $g$ is the coupling constant with the gauge field, $\alpha$ and $\beta$ are two temperature-dependent parameters, $H$ is the uniform applied field while $\hbar$ and $\mu_0$ are, respectively, the Planck constant and the vacuum permeability. We consider the case $H \parallel \hat{z}_2$.

To make the model dimensionless we replaced the variables as follows:

$$F = F_0 f,$$
$$\mathbf{A} = \mu_0 H_\epsilon \lambda \mathbf{a},$$
$$\psi = \psi_0 \psi,$$

and the spatial coordinates become $x \to \lambda x$ and $y \to \lambda y$. $\psi_0 = \sqrt{\frac{-\nu}{\pi}}$ is the uniform state order parameter,

$$\lambda = \sqrt{\frac{m}{\rho_0 \mu_0}}$$

is the penetration depth, $H_\epsilon = \sqrt{\frac{1}{\rho_0} \frac{\alpha^2}{\beta^2}}$ is the thermodynamic critical field, $F_0 = \mu_0 H_\epsilon^2 \lambda^2 \beta$ is the characteristic energy value. We also introduce the Ginzburg-Landau parameter $\kappa = \frac{\lambda}{\xi}$ where $\xi = \frac{\hbar}{2 \sqrt{-\lambda \mu_0}}$ is the coherence length. With this choice of notation for the coherence length [15], the critical coupling which separate type-I and type-II superconductors corresponds to $\kappa = 1$.

The resulting dimensionless Ginzburg-Landau model is expressed, up to constant terms, by the following free energy functional:

$$f[a, \psi] = \int d \mathbf{x} \frac{1}{2} \left| \left( -i \frac{2}{\kappa} \nabla + \mathbf{a} \right) \psi \right|^2 + \frac{1}{2} \left( 1 - \left| \psi \right|^2 \right)^2 + \frac{\left( \nabla \times \mathbf{a} - \mathbf{h} \right)^2}{2},$$

where $\mathbf{h} = \mathbf{H}/H_\epsilon$. Quantities in capital letters are intended in SI units, while variables in lower case are dimensionless. The complex Ginzburg-Landau model features local $U(1)$ gauge symmetry. This means that $\mathbf{a}$ and the phase of $\psi$ do not represent physical quantities. Instead, the observable fields of the system are the magnetic field $\mathbf{b} = \nabla \times \mathbf{a}$ and the superconductive current density $j = -\frac{2}{\kappa} \text{Im} \{ \psi^* \left( -i \frac{2}{\kappa} \nabla + \mathbf{a} \right) \psi \}$, which are invariant to the local gauge transformation:

$$\psi' = e^{i \frac{2}{\kappa} x_\perp} \psi,$$
$$\mathbf{a}' = \mathbf{a} - \nabla \chi.$$

Minimum Energy Paths

Vortices nucleation in a magnetically superheated superconductor is an example of metastable state decay. Various approaches to the study of metastable decay have been proposed [20; 21], and they identify the transition rate as $\tau^{-1} = A \exp \left( -\frac{\Delta E}{k_B T} \right)$, where $A$ is a prefactor whose precise definition depends on the employed theory. $\Delta E$ is the energy barrier that has to be crossed for the transition to occur. In a system whose phase space is multidimensional, the barrier corresponds to a saddle point of the energy landscape, while in field theory, the infinite-dimensional saddle point is called sphaleron. Since the energy barrier appears as the argument of the exponential, the first step in the study of rare events is the sphaleron identification. A way to achieve this is the computation of the Minimum Energy Path (MEP) between two states. The MEP is a path in the configuration space such that it crosses the minimum in the cotangent space of the path point by point. Considering a mechanical system described by a potential energy $V(q)$, the mathematical definition can be written like

$$q(s) = \arg \min \{ V(q(s)) \}, \quad \forall s \in [0, 1],$$

where the transition coordinate $s$ has been introduced. The meaning of $V(q)$ is that the potential $V$ has been restricted to the cotangent space of the trajectory in the point $q(s)$. For a more intuitive way to understand the definition see Figs. 6 and 7.

![MEP of Müller-Brown potential](image)

**FIG. 6.** In dotted white, the Minimum Energy Path for the Müller-Brown potential which is a common example in the study of rare events. The two metastable states are $A$ and $B$, the saddle point with $S$, the tangent space with dashed blue, and the cotangent with dashed orange. The behavior of potential energy along the tangent and cotangent space of the saddle point is plotted in the small chart on the top left. As can be seen, the MEP always crosses the minimum in the cotangent space.

**Numerical methods for the computation of MEPs**

The most common family of methods to compute minimum energy paths are the so-called *chain-of-states* methods. These methods are based on the optimization of a collection of systems $\{q_n\}$, called frames, in to the same potential $V(q)$ but subjected to a different fictitious force. In this way, it is possible to capture the
dynamics of a transition without involving real-time dynamics [22; 23]. These methods can be summarized as variants of the widely known Nudged Elastic Band method [24; 25]. However, nudged elastic band techniques require an additional undefined constant (string elasticity) for introducing fictitious forces. Besides, the chain can miss the saddle point and trying to prevent this requires additional considerations [26].

The approach we use belongs to the string method family [27], generalized to a gauge field theory. Instead of evolving a finite set of frames, we evolve the entire path \( q(s) \) in the configurations space towards the minimal energy one. The variable \( s \) continuously parametrizes the path which connects the initial state \( q(0) \) to the final state \( q(1) \). It is crucial to notice that, when talking of evolution, we intend a pseudo-dynamics of the system and not real-time dynamics. To evolve the initial path to the minimal energy one, we apply a gradient descent algorithm according to:

\[
\frac{\partial q}{\partial \tau} = -\nabla f_\perp + \lambda(q, s) \frac{\partial q}{\partial s}.
\]

(8)

\( \nabla f_\perp \) is the gradient component directed along the cotangent space of the trajectory, while the term \( \lambda(q, s) \frac{\partial q}{\partial s} \) is used to enforce the parametrization on the path. In fact, since \( \partial q/\partial s \) is uniquely directed along the tangent direction, \( \lambda \) does not affect the trajectory of the string. Here \( \tau \) is the pseudo-time describing the evolution of the string towards the MEP. The quantity \( f(a, \psi) \) is defined in Eq. (5), \( q(s) = (a(r, s), \psi(r, s)) \) and \( \nabla f = \frac{\partial f}{\partial a} \frac{\partial a}{\partial s} + \frac{\partial f}{\partial \psi} \frac{\partial \psi}{\partial s} \).

A more efficient way of calculating Eq. (8) consists of writing the cotangent projection of the gradient as \( \nabla f_\perp = \nabla f - \nabla f_\parallel \), where \( \nabla f_\parallel \) is the gradient of the free energy along the tangent to the path trajectory, defined as follows:

\[
\nabla f_\parallel = (\nabla f \cdot \hat{t})\hat{t}
\]

(9)

where \( \hat{t} \) is the tangent vector to \( q(s) \):

\[
\hat{t} = \frac{\partial q}{\partial s} \left| \frac{\partial q}{\partial s} \right|^{-1},
\]

with the vector norm

\[
\left\| \frac{\partial q}{\partial s} \right\| = \sqrt{\left( \int d^2x \frac{\partial \psi}{\partial s} \right)^2 + \sum_i \left( \int d^2x \frac{\partial a_i}{\partial s} \right)^2}.
\]

(11)

The functional scalar product used in Eq. (9) \( \nabla f \cdot \hat{t} \) therefore reads:

\[
f_\parallel = \nabla f \cdot \frac{\partial q}{\partial s} \left| \frac{\partial q}{\partial s} \right|^{-1} = \int d^2x \left( \frac{\delta f}{\delta \psi} \frac{\partial \psi}{\partial s} + \frac{\delta f}{\lambda \partial A_j} \frac{\partial A_j}{\partial s} \right) \left| \frac{\partial q}{\partial s} \right|^{-1}.
\]

(12)

Let us consider Eq. (8) with the identity \( \nabla f_\perp = \nabla f - \nabla f_\parallel \); we modify the descent process by removing the tangential gradient \( \nabla f_\parallel \) from the total gradient. The force components directed along the tangent to the path \( q(s) \) do not affect the pseudo-evolution of the string but only its parametrization. To enforce the desired parametrization in the tangential subspace we introduce the term \( \lambda(q, s) \frac{\partial q}{\partial s} \). Using the results in Eq.(9) and (12) we obtain:

\[
\frac{\partial q}{\partial \tau} = -\nabla f + \left( f_\parallel \left| \frac{\partial q}{\partial s} \right|^{-1} + \lambda(q, s) \right) \frac{\partial q}{\partial s}.
\]

(13)

The term \( \lambda'(q, s) \frac{\partial q}{\partial s} \) still has uniquely the function of maintaining a certain parametrization of the path \( q(s) \). When working with Eq. (14) instead of the explicit form in Eq.(13), we utilize the variant of the string method called simplified string method [14].

In the numerical implementation the path is discretized in a collection \( \{q_n\} \) of \( N \) frames such that \( q_n = q \left( \frac{n}{N-1} \right) \). At each iteration, the algorithm performs a minimization procedure and a reparametrization. In the minimization phase, a certain number of gradient descend steps are performed. In the reparametrization phase, the displaced frames are used to compute a new path by an interpolation method. Usually, the cubic spline interpolation is employed as it guarantees a smooth curve. The interpolation function is then used to generate a new collection of frames that are chosen to be equidistant with respect to the selected metric. There is a certain freedom in the choice of the metric, which we analyze in the following section. To describe more in detail how the string method works, let us define \( q_{n,k}^{i,k} \) as the frame number \( n \) at iteration \( i \), while \( k \) is the index of minimization steps. The simplified string method iteration works in the following way:

![FIG. 7. The potential energy along the Minimum Energy Path for the Müller-Brown potential. The two metastable states are indicated with A and B, the saddle point with S.](image-url)
1. Minimization phase

Perform $M$ minimization steps using a gradient descent method:

$$q_n^{i,k+1} = q_n^{i,k} + \alpha_n^{i,k} d_n^{i,k}$$  \hspace{1cm} (15)

where $d_n^{i,k}$ is the descent direction and $\alpha_n^{i,k}$ is the step length. At the end of the minimization step the displaced frames $q_n^{i,M}$ have been computed.

2. Reparametrization step

Let $\|\cdot\|$ be the norm induced by a chosen metric, the displacements between the frames are defined as $\Delta s_n = \|\hat{q}_n^i - q_{n-1}^i\|$. The parametrization is then computed as

$$s_n = \frac{\sum_p \Delta s_p}{\sum_j \Delta s_j}.$$  \hspace{1cm} (16)

In this way the curve is parametrized as $q_s = q(s_n)$ with $s \in [0,1]$. Using the input set $I = \{(s_n, q_n)\}$ the interpolating function $\hat{q}(s)$ is estimated. Finally, a new set of equidistant frames is generated by

$$q_n^{i+1} = \hat{q} \left( \frac{n}{F - 1} \right).$$ \hspace{1cm} (17)

**Metric and Gauge Invariance**

The key point in our work is finding the saddle points in a system with gauge symmetry. If we consider a generic path in the phase space $q(s)$, the system may evolve in $s$ changing the gauge of the solution without affecting the observable quantities of the system. In other words, the string gets twisted in the gauge degree of freedom crossing zones of the configuration space where there is no movement in the physical fields. This can be better understood thinking of the role of the metric, necessary to calculate the distances $\Delta s_n = \|q_n^i - q_{n-1}^i\|$ needed for the reparametrization step. In a straightforward extension of the prescription of the simplified string method to a Hilbert space, the metric for the Ginzburg-Landau free energy is the distance defined as:

$$\Delta s_n^{gd} = \left( \|a_n - a_{n-1}\|^2 + \|\psi_n - \psi_{n-1}\|^2 \right)^{1/2},$$  \hspace{1cm} (18)

where $\|\cdot\|$ is the standard $L^2$ norm. The problem arising with this choice is the use of the gauge dependent fields $a$ and $\psi$. This means that two configurations of the same physical system expressed in two different gauges are considered as two distinct systems. Hence, the string can move in the gauge degree of freedom, resulting in artifacts. There can be a region of the string where the fields $a$ and $\psi$ are changing, but there is no variation in the observable quantities, such as $b$ and $j$. The approach we use is to define a new gauge-invariant metric. With respect to the gauge transformation in Eq. (6) a possible choice, based on Eq. (18) reads:

$$\Delta s_n^{ph} = \left( \|\psi_n - \psi_{n-1}\|^2 + \left\| \left( \frac{2}{c} \nabla \theta_n - a_n \right) - \left( \frac{2}{c} \nabla \theta_{n-1} - a_{n-1} \right) \right\|^2 \right)^{1/2}.$$  \hspace{1cm} (19)

Eq. (19) entails some limitations. In fact, let us suppose to be interested in studying samples with particular geometry. Inside holes, or other domain exclusion, the order parameter $\psi$ is not defined. Hence, Eq. (19) becomes $\Delta s_n^{ph} = \left( \|a_n - a_{n-1}\|^2 \right)^{1/2}$, which is clearly not gauge invariant. Therefore, we can modify the definition of the metric in Eq. (19), to obtain a gauge invariant quantity which is related to the order parameter $\psi$ and simultaneously defined both in the domain and geometrical exclusions. By using the observables $b$ and $j$ we define:

$$\Delta s_n^{ph} = \left( \|b_n - b_{n-1}\|^2 + \|j_n - j_{n-1}\|^2 \right)^{1/2}.$$ \hspace{1cm} (20)

In the development of our method, we compared the outcomes of choosing different metrics. The sphaleron does not depend on it, as in Fig. 8 displays. In fact, the height of the barrier is the same for $s^{gd}$ (continuous line) and $s^{ph}$ (dashed line), with the definition of Eq. (20) [28]. If we focus on the line obtained using the metric $s^{gd}$, we notice that the first part, highlighted in red, is an artifact that corresponds to pure gauge evolution.

**FIG. 8.** The same Minimum Free Energy path $f(s)$ is plotted with the gauge dependent metric $s^{gd}$ defined in Eq. (19) and gauge independent metric $s^{ph}$ defined in Eq. (20). The red highlighted zone at the beginning of the $f(s^{ph})$ path collapses to a single point in the $f(s^{ph})$. This means that the pseudomotion in that zone is consists of gauge twisting.
Details of the numerical method developed

The energy landscape of the GL model is a system far more complex than the usual molecular dynamics problems addressed by the string method. The problem for 2D systems involves four different fields, is strongly nonlinear, and has a local gauge symmetry. For this reason, some expedients have to be introduced to apply the string method to this problem. One is the gauge-independent metric described above, and the others concern the numerical implementation of the algorithm.

In our computation, the string $q(s)$ is discretized as a vector of $F$ frames $q_n$. The number of frames we employ ranges between 80 and 120, depending on the transition we are considering. Each of these frames, $q_n = (a_x, a_y, \text{Re}{\psi}, \text{Im}{\psi})$ represents a state of the system and is discretized on a mesh grid with a minimum of $400 \times 400$ lattice sites. We adopted a second-order finite difference scheme for the discretization of the functional. Then the gradient force is computed by simple analytical derivation of the function obtained by the discretization process.

For the minimization step, we applied the Nonlinear Conjugate Gradient (NLCG) method with the Polak-Ribibi condition with automatic reset and exact line search. NLCG is necessary as the steepest gradient descent is too slow for this type of problem. Notice that, since the frames are displaced in the reparametrization step, the conjugacy is lost, and the conjugate direction needs to be reset at each iteration. In the final steps of the simulation, NLCG can be switched off. By doing this, the algorithm applies the steepest gradient as descent direction, which is more mathematically rigorous. For what concerns the reparametrization step, we decided to use a linear interpolation step. Linear interpolation is computationally cheaper than the usual cubic interpolation, used within the string method, and more numerically stable. The only negative side of this choice is that the continuity up to the second derivative of $q(s)$ is lost. However, the loss of analytical smoothness is counterbalanced by an increased number of frames, which results in a more dense discretization along $s$, generating a regular and well-behaved MEP.

The initial guess we used the ansatz for a single vortex $\psi(r) = \text{tanh}\left(-r - r_0\right)^2(x - x_0 + iy(y_0))/|r - r_0|$ where $r_0$ is the center of the vortex and it varies frame by frame. It starts from a point outside the superconductor at $s = 0$ and moves toward the center of the specimen for $s = 1$. Concerning the numerical extrema of the Hamiltonian (5), the current density perpendicular to the boundary may slightly deviate from zero due to the limited accuracy of the finite-difference scheme. This discrepancy tends to zero with increasing mesh density. Strictly speaking, for non-extremum cases, i.e., configurations along the MEP except initial, sphaleron (saddle point) and final states, this behavior is not guaranteed. Therefore, we monitored the perpendicular component of the current, and it turned out that this value is negligible. The computer implementation is developed using the General Purpose GPU (GPGPU) paradigm. In particular, the core of the tool is implemented in CUDA C++ language and run on a NVIDIA Quadro P6000 GPU.

Quantitative analysis of the planar edge problem

We simulated a 2D square system with side length $L = 24\lambda$. In such a vast domain, the interactions between the entering vortex and the other edges of the sample are negligible, allowing the study of the surface barrier of a flat edge, which is the standard case studied in the previous literature.

The minimum free energy path of the vortex nucleation process, in this case, presents only one sphaleron whose free energy is $F_{\text{Sphaleron}} = \max_s F(s)$. Once we identify the sphaleron, we compute the nucleation and escape barriers according to:

$$\Delta F_n = F_{\text{Sphaleron}} - F_{\text{Meissner}}$$
$$\Delta F_e = F_{\text{Sphaleron}} - F_{\text{Shubnikov}}$$

where $F_{\text{Meissner}} = F(s = 0)$ is the energy of the Meissner state while $F_{\text{Shubnikov}} = F(s = 1)$ is the energy of the system with a vortex in the bulk. The nucleation barrier can easily be interpreted as the energy cost of inserting a vortex inside the domain while the escape barrier is the activation energy of the opposite transition.

![FIG. 9. Sketch of a Minimum Free Energy Path for vortex nucleation with the definition of nucleation barrier $\Delta F_n$ and the escape barrier $\Delta F_e$.](image-url)
filling the sample until inter-vortex repulsion force prevents further nucleations. When \( H_n \) is applied to the superconductor, solutions with vortices are not stable anymore, and they spontaneously escape from the bulk. Notice that, in principle, \( H_n \) and the superheating field \( H_{sh} \) are different quantities. The former is computed studying the entry process of the first vortex, while the latter is the mathematical stability limit of the Meissner state. These two quantities are strictly the same only for type-II superconductors.

We have simulated this transition in a wide region of the \( \kappa - H \) region, and show the results in Fig. 10. From

![Image](Image)

**FIG. 10.** Nucleation barrier \( \Delta F_n = \Delta F_{n0}/F_0 \) in log units as a function of the external field \( H \) and GL parameter \( \kappa \). The space of parameters in the hatched zone in the upper right is unstable as \( H > H_n \) and therefore a single vortex state is not a stable solution as there is no barrier preventing additional vortices to enter in the bulk. Notice that the contour-plot is cut just below for numerical reasons.

the computed \( \Delta F_n \) is possible to extrapolate the nucleation field \( H_n \). To do that, we interpolate the data points with the ansatz \( \Delta F_{n0}^{(H)}(H)/F_0 = C_1 \exp(-(C_2(H - H_n))) \) where \( C_1 \), \( C_2 \) and \( H_n \) are the coefficients to be estimated for each value of \( \kappa \). The calculated nucleation field is within a 2% error compared the superheating field computed in [6], which is the most advanced analytical study available.

We defined the escape barrier \( \Delta F_e = F_{\text{Sphaleron}} - F_{\text{Shubnikov}} \) as the barrier crossed in the event of the vortex exit from the bulk. The results for the barrier height in the \( \kappa - H \) diagram are shown in Fig. 11.

![Image](Image)

**FIG. 11.** Escape barrier \( \Delta F_e = \Delta F_{e0}/F_0 \) as a function of the external field \( H \) and GL parameter \( \kappa \). The space of parameters in the hatched zone in the upper right is unstable as \( H > H_n \) and therefore a single vortex state is not a stable solution as there is no barrier preventing additional vortices to enter in the bulk. Notice that the contour-plot is cut just below for numerical reasons.

Studying the escape barrier as a function of the external field \( H \), we can notice as the barrier is exactly zero only for null external fields. This is in agreement with experimental results showing that weak external magnetic fields are sufficient to keep a vortex inside a superconductor. This result fixes the escape field \( H_e = 0 \) meaning that an applied field in the opposite direction is needed to expel a vortex from a sample.

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