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TEXTO SISTEMÁTICO-CRÍTICO DE LIVRE-DOCÊNCIA

SOLUÇÃO NUMÉRICA DAS EQUAÇÕES DE GINZBURG-LANDAU
DEPENDENTES DO TEMPO

Aplicações a Materiais Supercondutores Mesoscópicos

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“Para todo problema complexo existe sempre uma solução simples, elegante e completamente errada.”

“Explanations exist; they have existed for all time; there is always a well-known solution to every human problem – neat, plausible, and wrong.”

Henry Louis Mencken

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Este documento é um texto sistemático-crítico de minha produção literária nos últimos dez anos.

Desde o início de meu doutorado em Física em 1988 na [University of Manchester](#) ([Shuster Laboratory](#)), quando me afastei da [UNESP-Faculdade de Engenharia de Ilha Solteira](#), comecei a escrever e publicar trabalhos científicos. Os primeiros artigos foram na área de Física Estatística aplicada a sistemas fora do equilíbrio usando o método de operador de projeção de Hazime Mori [1]. Esta é uma poderosa técnica para o cálculo de funções de correlação a qual exerce um papel central na teoria da função resposta de Ryogo Kubo [2]. Uma forma muito comum de se investigar as propriedades física dos materiais é perturba-lo com algum tipo de força externa tais como campo elétrico, campo magnético, radiação eletromagnética, etc. A teoria de Kubo estabelece uma relação entre a propriedade física e a força externa, bem como entre a função admitância (susceptibilidade) e a função de correlação.

Ao mesmo tempo trabalhei na investigação de supercondutores anisotrópicos, sobretudo os de alta temperatura crítica. Minha contribuição nesta área foi no estudo das constantes elásticas da rede de vórtices. Os artigos deste período basearam-se fundamentalmente na teoria de elasticidade de Ernest Helmut Brandt da rede de vórtices consagrada na série de artigos publicados no Journal of Low Temperature Physics [3, 4, 5, 6]. Esta teoria foi proposta para supercondutores isotrópicos. Quando aplicada para supercondutores anisotrópicos, novas constantes elásticas aparecem além dos coeficientes de compressão, de cisalhamento e de curvatura das linhas de vórtices [7].

Com efeito, minha tese de doutorado foi dividida em duas partes, uma sobre aplicações do método de operador de projeção e a outra sobre a teoria de elasticidade da rede de vórtices. A tese foi orientada pelo Professor [Michel A. Moore](#) ([wiki](#)) da The University of Manchester. A banca avaliadora foi composta pelos Professores [Alan Mckane](#) da University of Manchester e [J. M. F. Gunn](#) da University of Birmingham. O primeiro avaliou a parte da tese que versou sobre Física Estatística e o segundo sobre a parte que versou sobre Supercondutividade.

No início de 1994, quando retornei ao Brasil, permaneci pouco mais de um ano no [IFGW](#) da [UNICAMP](#) com bolsa do [CNPq](#) na modalidade Recém-Doutor. Naquele momento fiz uma escolha, decidi que iria trabalhar somente em Supercondutividade. Durante este período de readaptação não tive nenhuma publicação científica. Mas continuei trabalhando em alguns

problemas de teoria elástica da rede de vórtices em supercondutores anisotrópicos. Em Abril de 1995 fui contratado pela [UNESP-Faculdade de Ciências de Bauru](#), lotado no [Departamento de Física](#), onde me encontro até hoje. No início deste período consegui transformar em artigos científicos boa parte dos estudos que fiz durante minha permanência na UNICAMP.

Até 2006, os estudos que desenvolvi eram predominantemente analíticos. A partir deste ano, mudei meus estudos inteiramente de foco e comecei a estudar métodos numéricos de solução das equações de Ginzburg-Landau dependentes do tempo (TDGL) aplicados a sistemas supercondutores em escala de tamanho mesoscópica. Com a melhora nas técnicas de microfabricação de supercondutores, cresceu sobremaneira o interesse no estudo das propriedades eletrônicas destes materiais. A matéria de vórtice em supercondutores mesoscópicos é fortemente influenciada pelas geometria e pelo seu tamanho. Inicialmente, os Professores [André Luiz Malvezzi](#), [Paulo Noronha Lisboa-Filho](#), e [Wilson Ayres Ortiz](#) foram meus grandes incentivadores e colaboradores nesta empreitada. Mais tarde, outros Professores tornam-se meus profícuos colaboradores; destaco os Professores [José José Barba Ortega](#), [Rafael Zadorosny](#), e [José Albino Aguiar](#), e em menor grau, porém não menos importante os Professores [Ernest Helmut Brandt](#), [Clécio Clemente de Souza Silva](#), [Leonardo Ribeiro Eulálio Cabral](#), [François M. Peeters](#), e [Milorad V. Milošević](#).

No Capítulo 2 apresentaremos uma breve descrição da Teoria Clássica de Campos onde obtemos as equações de Euler-Lagrange para campos escalares e vetoriais. No Capítulo 3 empregaremos estas equações para obter as equações de London e de Ginzburg-Landau. Ainda no Capítulo 3 obtemos os comprimentos fundamentais da Supercondutividade e generalizamos as equações de Ginzburg-Landau para fenômenos fora do equilíbrio. No Capítulo 4 desenvolvemos o algoritmo de solução numérica das equações TDGL. No Capítulo 5 apresentamos os artigos mais significativos dos últimos dez anos. Cada um deles é acompanhado de breve comentário do próprio autor sobre o respectivo trabalho.

Teoria Clássica de Campos

2.1 Introdução

Iniciaremos este Capítulo com uma breve introdução à teoria clássica de campos, onde obtemos as equações de Euler-Lagrange para campos escalares e vetoriais. No Capítulo 3 iremos usar estas equações para obter as equações de London e de Ginzburg-Landau que descrevem o fenômeno da Supercondutividade em nível macroscópico.

2.2 Teoria Clássica de Campos

A teoria clássica de campos é uma teoria que descreve a interação entre um campo atribuído a uma quantidade física com a matéria. Nessa descrição, utiliza-se o conceito de ação, a qual diz que de todos os caminhos possíveis que um sistema dinâmico pode se mover de um ponto a outro no espaço de configurações, em um determinado intervalo de tempo, corresponde a aquele que minimiza a ação.

Nessa seção obtemos alguns resultados da teoria clássica de campos [8] os quais utilizaremos posteriormente na minimização dos funcionais de London e Ginzburg-Landau. O ferramental matemático utilizado aqui é o cálculo variacional, o qual lida com minimização de funcionais.

2.2.1 Equação de Lagrange

Seja $\psi = \psi(\mathbf{r}, t)$ um campo escalar que representa alguma quantidade física em um determinado ponto do espaço e tempo. Definimos a ação como

$$L = \int_{t_1}^{t_2} \int_V \mathcal{L}[\psi, \nabla\psi, \dot{\psi}, t] d^3r dt, \quad (2.2.1)$$

onde $\dot{\psi} = \partial\psi/\partial t$ e $\mathcal{L}$ é a *densidade Lagrangeana*, a qual depende do campo e suas derivadas espaciais e temporal; V é um domínio (volume) do espaço limitado por uma superfície Ω . Trataremos ψ , $\nabla\psi$ e $\dot{\psi}$ como variáveis independentes e, a partir disso, supomos que exista um campo ψ que minimize a ação L .

Seja $\delta\psi$, $\delta(\nabla\psi)$ e $\delta\dot{\psi}$ mudanças infinitesimais do campo escalar e suas derivadas. Consequentemente, isto produz uma mudança infinitesimal δL da ação

$$\delta L = \int_{t_1}^{t_2} \int_V \left\{ \mathcal{L}[\psi + \delta\psi, \nabla\psi + \delta(\nabla\psi), \dot{\psi} + \delta\dot{\psi}, t] - \mathcal{L}[\psi, \nabla\psi, \dot{\psi}, t] \right\} d^3r dt. \quad (2.2.2)$$

A ação mínima é determinada através da condição $\delta L/\delta\psi = 0$. Expandindo o funcional em uma série de Taylor, até primeira ordem, temos que

$$\begin{aligned} \mathcal{L}[\psi + \delta\psi, \nabla\psi + \delta(\nabla\psi), \dot{\psi} + \delta\dot{\psi}, t] &= \mathcal{L}[\psi, \nabla\psi, \dot{\psi}, t] + \frac{\partial\mathcal{L}}{\partial\psi}\delta\psi \\ &+ \frac{\partial\mathcal{L}}{\partial(\nabla\psi)} \cdot \delta(\nabla\psi) + \frac{\partial\mathcal{L}}{\partial\dot{\psi}}\delta\dot{\psi}. \end{aligned} \quad (2.2.3)$$

A quantidade $\partial\mathcal{L}/\partial(\nabla\psi)$ deve ser entendida como um vetor cujas componentes são dadas por $\partial\mathcal{L}/\partial\psi_i, i = x, y, z$. Substituindo a expansão em (2.2.2), vem que

$$\delta L = \int_{t_1}^{t_2} \int_V \left\{ \frac{\partial\mathcal{L}}{\partial\psi}\delta\psi + \frac{\partial\mathcal{L}}{\partial(\nabla\psi)} \cdot \delta(\nabla\psi) + \frac{\partial\mathcal{L}}{\partial\dot{\psi}}\delta\dot{\psi} \right\} d^3r dt. \quad (2.2.4)$$

O segundo e o terceiro termos podem ser simplificados usando integração por partes e assumindo que nos pontos extremos as flutuações em torno do mínimo são nulas em qualquer ponto r_Ω da superfície $\Omega, \forall t$, e nos instantes inicial e final $\forall \mathbf{r} \in V$. Temos que

$$\delta\psi(\mathbf{r}_\Omega, t) = \delta\psi(\mathbf{r}, t_1) = \delta\psi(\mathbf{r}, t_2) = 0. \quad (2.2.5)$$

Desde que existam, a ordem da diferencial funcional e da derivada parcial podem ser invertidas, $\delta\dot{\psi} = \partial\delta\psi/\partial t$. Logo, temos que

$$\begin{aligned} \int_{t_1}^{t_2} \frac{\partial\mathcal{L}}{\partial\dot{\psi}}\delta\dot{\psi} dt &= \int_{t_1}^{t_2} \frac{\partial\mathcal{L}}{\partial\dot{\psi}} \frac{\partial\delta\psi}{\partial t} dt \\ &= \left. \frac{\partial\mathcal{L}}{\partial\dot{\psi}}\delta\psi \right|_{t_1}^{t_2} - \int_{t_1}^{t_2} \frac{\partial}{\partial t} \left(\frac{\partial\mathcal{L}}{\partial\dot{\psi}} \right) \delta\psi dt. \end{aligned} \quad (2.2.6)$$

Usando as condições (2.2.5), obtemos

$$\int_{t_1}^{t_2} \frac{\partial\mathcal{L}}{\partial\dot{\psi}}\delta\dot{\psi} dt = - \int_{t_1}^{t_2} \frac{\partial}{\partial t} \left(\frac{\partial\mathcal{L}}{\partial\dot{\psi}} \right) \delta\psi dt. \quad (2.2.7)$$

Analogamente, podemos mostrar que

$$\int_{x_1}^{x_2} \frac{\partial\mathcal{L}}{\partial\psi_x}\delta\psi_x dx = - \int_{x_1}^{x_2} \frac{\partial}{\partial x} \left(\frac{\partial\mathcal{L}}{\partial\psi_x} \right) \delta\psi dx. \quad (2.2.8)$$

Substituindo os resultados (2.2.7) e (2.2.8) em (2.2.4), obtemos

$$\delta L = \int_{t_1}^{t_2} \int_V \left\{ \frac{\partial \mathcal{L}}{\partial \psi} - \nabla \cdot \left[\frac{\partial \mathcal{L}}{\partial (\nabla \psi)} \right] - \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial \dot{\psi}} \right) \right\} \delta \psi d^3r dt . \quad (2.2.9)$$

Considerando $\delta \psi$ arbitrário em qualquer ponto do espaço e instante de tempo, a condição de extremo é equivalente a

$$\frac{\partial \mathcal{L}}{\partial \psi} - \nabla \cdot \left[\frac{\partial \mathcal{L}}{\partial (\nabla \psi)} \right] - \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial \dot{\psi}} \right) = 0 , \quad (2.2.10)$$

a qual é conhecida como equação de Euler-Lagrange.

A equação de Euler-Lagrange pode ser estendida para um funcional que depende de um campo vetorial $\mathbf{A}$ e seu rotacional $\nabla \times \mathbf{A}$. Temos que

$$\frac{\partial \mathcal{L}}{\partial \mathbf{A}} + \nabla \times \left[\frac{\partial \mathcal{L}}{\partial (\nabla \times \mathbf{A})} \right] - \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{A}}} \right) = 0 . \quad (2.2.11)$$

Teoria Fenomenológicas de Supercondutividade

3.1 Introdução

A Supercondutividade foi descoberta por Kamerlingh Onnes em 1911 [9]. Ele descobriu que a resistência elétrica do mercúrio sólido cai para um valor incomensuravelmente pequeno quando o material é resfriado abaixo de uma determinada temperatura, chamada de *temperatura crítica* T_c . O mercúrio de fato vai de um estado normal para um estado *supercondutor* para temperaturas abaixo de $T_c = 4.2^\circ \text{ K}$ (ver figura 3.1).

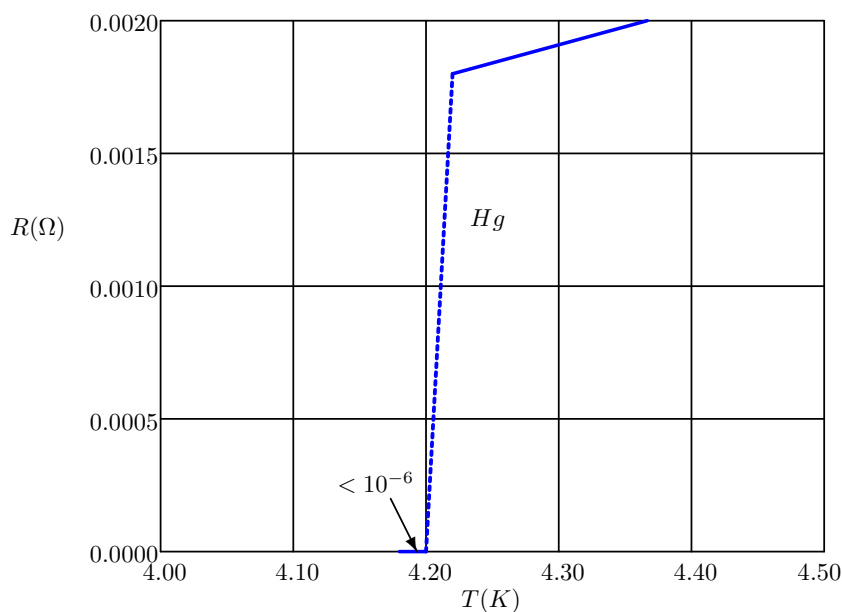


Figura 3.1: Gráfico histórico de Onnes: resistência do mercúrio sólido em função da temperatura (Elaborada por Mauro César Videira Pascolati).

Muitos outros elementos, compostos e amorfos, desde têm sido descobertos serem supercondutores com temperaturas críticas mais alta. Até 1986, o limite superior conhecido era de $T_c = 23^\circ \text{ K}$ para o Nb_3Ge . Neste ano, Bednorz e Müller construíram um complexo material cerâmico que era supercondutor a 30° K [10]. Esta fascinante descoberta rapidamente levou à descoberta de materiais com temperaturas críticas tão alta quanto 98° . Esta descoberta despertou um grande interesse pela Supercondutividade que até então estava sendo considerada uma área de estudo praticamente esquecida.

Duas décadas depois da descoberta de Kamerlingh Onnes, Meissner e Ochsenfeld, em 1933, observaram que quando um composto supercondutor é resfriado abaixo de sua temperatura crítica na presença de um campo magnético aplicado, ele expulsa o fluxo de seu interior [11]. Por outro lado, se o campo magnético é aplicado posteriormente ao material ser resfriado abaixo de T_c , o campo magnético também é excluído do seu interior. Este efeito é conhecido como *efeito Meissner*. Em outras palavras, os materiais supercondutores são diamagnéticos perfeitos. A figura 3.2 ilustra esta propriedade e a diferença de supercondutores com condutores perfeitos.

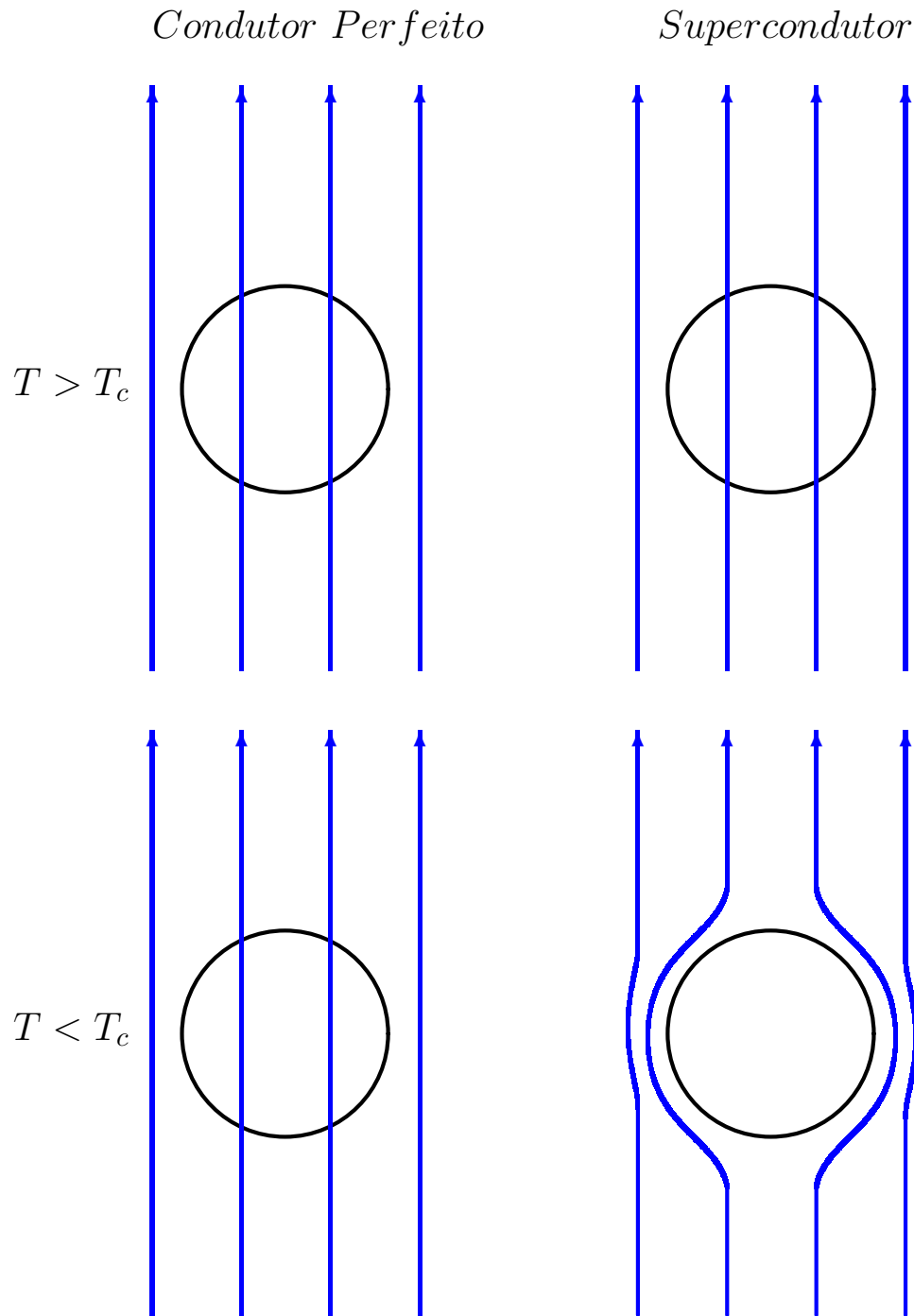


Figura 3.2: Condutor perfeito e supercondutor (Elaborada por Mauro César Videira Pascolati).

Os supercondutores são divididos em dois tipos. Os do primeiro tipo, *supercondutores do tipo I*, expulsam o fluxo magnético até que campo aplicado alcança um determinado valor,

chamado de *campo crítico termodinâmico* $H_c(T)$, e depende da temperatura. Uma vez que o campo magnético aplicado excede este campo crítico, o supercondutor retorna ao seu estado normal (ver painel (a) da figura 3.3).

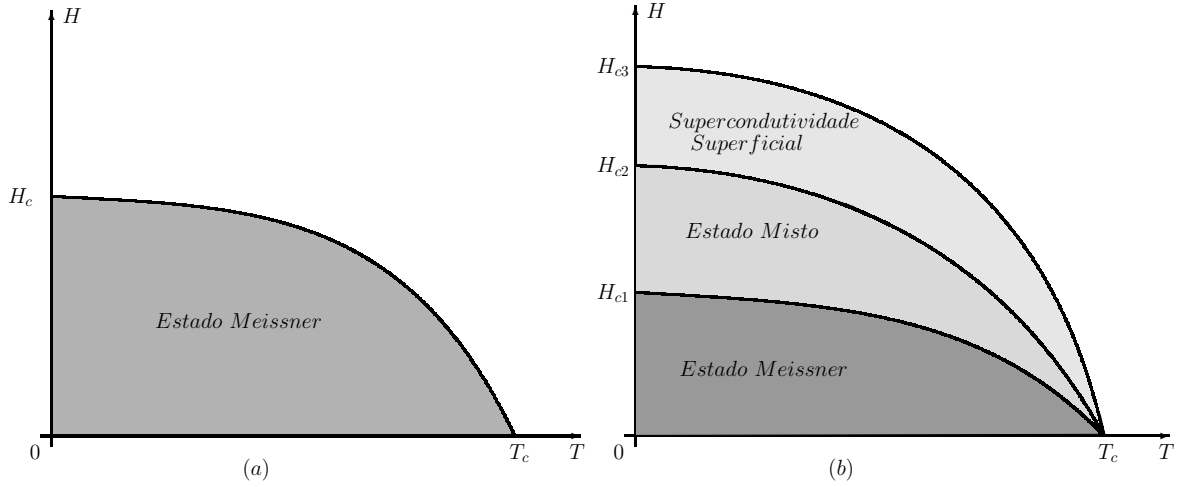


Figura 3.3: Diagramas de fase H-T para supercondutores do tipo-I (a) e do tipo-II (b) (Elaborada por Mauro César Videira Pascolati).

Os supercondutores do tipo II comportam-se de maneira ligeiramente diferente. Para os materiais do tipo II, existe um segundo campo crítico, $H_{c2}(T)$ com valores que o primeiro campo crítico, $H_{c1}(T)$. Abaixo de $H_{c1}(T)$ o supercondutor encontra-se no estado de Meissner. Quando o campo aplicado excede o *campo crítico inferior* $H_{c1}(T)$ o supercondutor não expulsa o fluxo magnético por completo. Entretanto, o material continua supercondutor em determinadas regiões até que o campo magnético aplicado excede o *campo crítico superior* $H_{c2}(T)$. Quando a intensidade do campo aplicado encontra-se entre $H_{c1}(T)$ e $H_{c2}(T)$, ocorre penetração parcial de fluxo, exibe uma *estrutura de domínio* de regiões normais e supercondutoras, conhecido *estado misto* (ver painel (b) da figura 3.3). Acima de $H_{c2}(T)$, somente próximo à superfície o material permanece supercondutor. Para valores de campo aplicado superior a $H_{c3}(T)$, chamado de *campo crítico de superfície*, a supercondutividade é totalmente destruída.

Em 1957, um discípulo de Landau, Alexei Alexeevich Abrikosov, propôs uma teoria que descrevia os supercondutores do tipo I e II [?, 13]. Ele demonstrou que no estado misto o campo magnético aplicado penetra parcialmente na amostra na forma de filamentos de fluxo de um determinado raio $\xi(T)$ (ver Seção 3.4). No interior deste filamento a supercondutividade é inteiramente suprimida. Fora do caroço, o material permanece supercondutor em uma região de raio $\lambda(T)$ (ver Seção 3.4), contendo *supercondutores*. A esta estrutura filamentar damos o nome de *vórtice*. Abrikosov demonstrou que cada vórtice carrega um fluxo dado por $\Phi_0 = hc/2e = 2 \times 10^{-7} \text{ G cm}^2$. Ele ainda demonstrou que as linhas de fluxo agrupam-se em um arranjo regular na forma de uma rede triangular. A figura 3.4 ilustra esta geometria. Esta teoria foi posteriormente comprovada por experimento de decoração magnética conduzido por Essmann e Trauble [14].

A quantidade $\kappa = \lambda(T)/\xi(T)$ é conhecido como *parâmetro de Ginzburg-Landau*. Abrikosov mostrou que, para $\kappa \geq 1/\sqrt{2}$, o supercondutor é do tipo II e, caso contrário é do tipo I; κ é uma

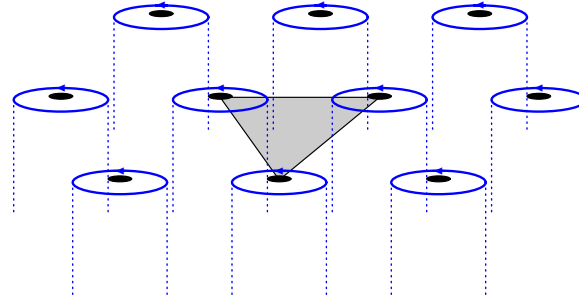


Figura 3.4: Rede de vórtices de Abrikosov (Elaborada por Mauro César Videira Pascolati).

característica de cada material. Esta classificação é válida para supercondutores de dimensão infinita. Recentemente tem sido observado que supercondutores mesoscópicos com $\kappa < 1/\sqrt{2}$ exibem estado misto [15, 16]. Assim, o valor de κ que distingue os supercondutores do tipo I e II está sendo revisto [17].

Nas próximas Seções descreveremos as principais teoria fenomenológica que descrevem a supercondutividade, a saber, teorias de London e de Ginzburg-Landau.

3.2 Teoria de London

Para baixas temperaturas, próximas do zero absoluto, um sistema se comporta como a mistura de dois fluidos: um fluido com viscosidade nula, superfluido, e um fluido com viscosidade finita. Considerando que a energia livre do superfluido consiste em três partes, podemos escrever

$$F = F_0 + F_T + F_B \quad (3.2.1)$$

onde F_0 é a energia associada ao fluido no estado normal, F_T a energia cinética do superfluido e F_B a energia associada ao campo magnético local. Explicitamente, temos que

$$F_B = \frac{1}{8\pi} \int_V h^2 d^3r, \quad (3.2.2)$$

e

$$F_T = \frac{1}{2}mv^2 = \frac{1}{2} \int_V \rho v^2 d^3r, \quad (3.2.3)$$

onde ρ é a densidade associada ao superfluido. Escrevendo $\rho = nm$, sabendo que $\mathbf{J} = ne\mathbf{v}$ e de acordo com a lei de Ampère $\nabla \times \mathbf{h} = (4\pi/c)\mathbf{J}$, a expressão (3.2.3) torna-se

$$F_B = \frac{1}{8\pi} \int_V \frac{mc^2}{4\pi ne^2} (\nabla \times \mathbf{h})^2 d^3r, \quad (3.2.4)$$

onde n é a densidade de elétrons. Colecionando todas as contribuições, obtemos

$$F = F_0 + \int_V \frac{1}{8\pi} \left\{ h^2 + \frac{mc^2}{4\pi ne^2} (\nabla \times \mathbf{h})^2 \right\} d^3r = 0. \quad (3.2.5)$$

Definindo $\lambda^2 = mc^2/4\pi ne^2$, finalmente obtemos o funcional de London

$$\mathcal{F}_L = \frac{1}{8\pi} [h^2 + \lambda^2 (\nabla \times \mathbf{h})^2]. \quad (3.2.6)$$

Assim, introduzindo as derivadas funcionais

$$\frac{\partial \mathcal{F}_L}{\partial \mathbf{h}} = \frac{1}{4\pi} \mathbf{h}, \quad \frac{\partial \mathcal{F}_L}{\partial (\nabla \times \mathbf{h})} = -\frac{\lambda^2}{4\pi} \nabla \times \mathbf{h}, \quad \frac{\partial \mathcal{F}_L}{\partial \dot{\mathbf{h}}} = 0, \quad (3.2.7)$$

na equação de Euler-Lagrange (2.2.11), encontramos

$$\lambda^2 \nabla \times (\nabla \times \mathbf{h}) + \mathbf{h} = 0, \quad (3.2.8)$$

que é conhecida como equação de London [18, 19].

3.3 Teoria de Ginzburg-Landau

A teoria proposta por Vitaly Lazarevich Ginzburg e Lev Davidovich Landau é uma teoria semi-clássica capaz de descrever o fenômeno da supercondutividade do ponto de vista macroscópico [20, 21]. Ela resolve alguns problemas que a teoria de London apresenta na escala de comprimento muito menor que λ . Ginzburg e Landau observaram que a transição para o estado supercondutor poderia ser descrita através da teoria de Landau para transições de segunda ordem baseada em um *parâmetro de ordem*. Esse parâmetro possui comportamento semelhante à magnetização estudada na teoria de Landau. O parâmetro de ordem, denotado por ψ , será tal que

$$\psi = \begin{cases} 0, & T > T_c, \\ \neq 0, & T < T_c, \end{cases} \quad (3.3.1)$$

onde T_c é a temperatura crítica, abaixo da qual o material passa do estado normal para o estado supercondutor; ψ representa uma função de onda complexa e o quadrado de seu módulo indica a densidade de pares de Cooper. Considere um supercondutor uniforme na ausência de um campo magnético e suponha que ψ independa da posição. De acordo com a teoria de transição de fase de segunda ordem, para T próximo de T_c , a densidade de energia livre é dada por

$$\mathcal{F} = \mathcal{F}_0 + \alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4, \quad (3.3.2)$$

onde $\mathcal{F}_0$ é energia (por unidade de volume) do estado normal, enquanto α é uma função que depende da temperatura, e que β independe da temperatura. Ambas as constantes fenomenológicas satisfazem as seguintes condições

$$\begin{aligned} \beta &> 0, \\ \alpha(T) &= \begin{cases} \alpha_0(T - T_c), & \text{para } T < T_c \\ 0, & \text{para } T \geq T_c \end{cases} \end{aligned} \quad (3.3.3)$$

onde α_0 é uma constante positiva.

Para um supercondutor na ausência de campo magnético e corrente de transporte, a condição de mínima energia é dada por

$$\frac{\partial \mathcal{F}}{\partial \psi} = 0, \quad (3.3.4)$$

de onde se obtém

$$\psi(\alpha + \beta|\psi|^2) = 0, \quad (3.3.5)$$

onde a barra indica o complexo conjugado da função complexa.

Descartando a solução trivial $\psi = 0$, obtemos

$$|\psi|^2 = n_s = -\frac{\alpha}{\beta}. \quad (3.3.6)$$

Note que, fosse α positiva, teríamos a solução trivial e portanto não haveria o estado supercondutor. Os painéis da figura 3.5 ilustram esta consideração sobre as constantes fenomenológica α e β . A fase supercondutora em que o parâmetro de ordem é constante em todo o espaço é dado pela equação (3.3.6) é conhecida como estado de Meissner.

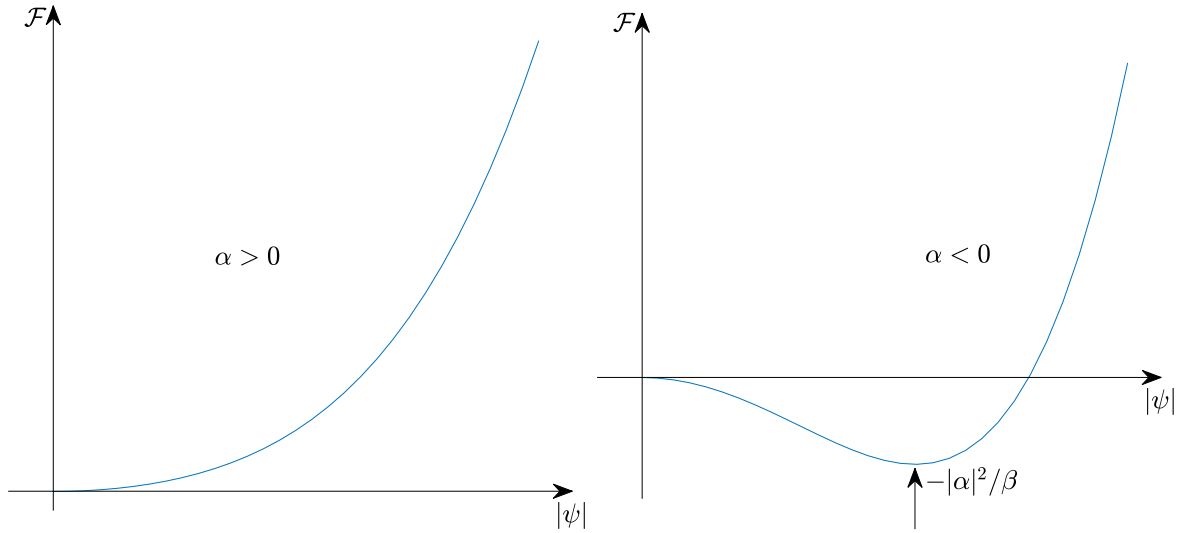


Figura 3.5: Energia livre do estado de Meissner em função do parâmetro de ordem.

Agora, para um supercondutor na presença de um campo magnético devemos somar duas contribuições: a energia do campo externo, $\mathcal{F}_B$, e a energia de um gradiente de ψ por influência do campo externo, $\mathcal{F}_G$, o qual induz uma supercorrente. Para a segunda contribuição podemos escrever

$$\mathcal{F}_G = \frac{1}{2m^*} \left| \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} \mathbf{A} \right) \psi \right|^2, \quad (3.3.7)$$

onde m^* e e^* são a massa e a carga efetivas do par de Cooper, respectivamente, e $\mathbf{A}$ o potencial vetor.

A energia associada ao campo magnético externo é dada por

$$\mathcal{F}_B = \frac{1}{8\pi} h^2 . \quad (3.3.8)$$

Assim, a energia livre total fica escrita como:

$$F = F_0 + \int_V (\mathcal{F}_C + \mathcal{F}_G + \mathcal{F}_B) d^3r , \quad (3.3.9)$$

$$F = F_0 + \int_V \left\{ \alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \frac{1}{2m^*} \left| \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} \mathbf{A} \right) \psi \right|^2 + \frac{1}{8\pi} h^2 \right\} d^3r . \quad (3.3.10)$$

Portanto, o funcional de Ginzburg-Landau é definido por

$$\mathcal{F}_{GL} = \alpha |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \frac{1}{2m^*} \left| \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} \mathbf{A} \right) \psi \right|^2 + \frac{1}{8\pi} (\nabla \times \mathbf{A})^2 , \quad (3.3.11)$$

onde $\mathbf{h} = \nabla \times \mathbf{A}$.

As derivadas funcionais são dadas por

$$\begin{aligned} \frac{\partial \mathcal{F}_{GL}}{\partial \bar{\psi}} &= \alpha \psi + \beta \psi |\psi|^2 + \frac{1}{2m^*} \left(-\frac{e^*}{c} \right) \mathbf{A} \cdot \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} \mathbf{A} \right) \psi , \\ \frac{\partial \mathcal{F}_{GL}}{\partial \dot{\bar{\psi}}} &= 0 , \\ \frac{\partial \mathcal{F}_{GL}}{\partial (\nabla \bar{\psi})} &= -\frac{1}{2m^*} \frac{\hbar}{i} \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} \mathbf{A} \right) \psi . \end{aligned} \quad (3.3.12)$$

Substituindo as equações (3.3.12) na equação de Euler-Lagrange (2.2.10), encontramos

$$\alpha |\psi| + \beta |\psi|^2 \psi + \frac{1}{2m^*} \left(-\frac{e^*}{c} \mathbf{A} \right) \cdot \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} \mathbf{A} \right) \psi + \frac{1}{2m^*} \left(\frac{\hbar}{i} \nabla \cdot \right) \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} \mathbf{A} \right) \psi = 0 . \quad (3.3.13)$$

Rearranjando os termos, obtemos a primeira equação de Ginzburg-Landau

$$\frac{1}{2m^*} \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} \mathbf{A} \right)^2 \psi + \alpha \psi + \beta |\psi|^2 \psi = 0 . \quad (3.3.14)$$

Agora, iremos encontrar uma equação para o potencial vetor que minimize o funcional de Ginzburg-Landau (3.3.11). As derivadas funcionais são dadas por

$$\begin{aligned} \frac{\partial \mathcal{F}_{GL}}{\partial \mathbf{A}} &= \frac{1}{2m^*} \left[\left(-\frac{e^*}{c} \right) \psi \left(-\frac{\hbar}{i} \nabla - \frac{e^*}{c} \mathbf{A} \right) \bar{\psi} + \left(-\frac{e^*}{c} \right) \bar{\psi} \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} \mathbf{A} \right) \psi \right] \\ &= -\text{Re} \left[\frac{e^*}{m^* c} \bar{\psi} \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} \mathbf{A} \right) \psi \right] , \\ \frac{\partial \mathcal{F}_{GL}}{\partial (\nabla \times \mathbf{A})} &= \frac{1}{4\pi} \nabla \times \mathbf{A} , \\ \frac{\partial \mathcal{F}_{GL}}{\partial \dot{\mathbf{A}}} &= 0 , \end{aligned} \quad (3.3.15)$$

onde Re indica a parte real de uma função complexa. Substituindo estes resultados na equação de Eule-Lagrange para campos vetoriais (2.2.11), encontramos

$$\nabla \times \mathbf{h} = \frac{4\pi}{c} \mathbf{J}_s, \quad (3.3.16)$$

onde a densidade de corrente supercondutora é dada por

$$\mathbf{J}_s = \frac{e^*}{m^*} \text{Re} \left[\bar{\psi} \left(\frac{\hbar}{i} \nabla - \frac{e^*}{c} \mathbf{A} \right) \psi \right]. \quad (3.3.17)$$

Assim, a segunda equação de Ginzburg-Landau (3.3.16) nada mais é do que a lei de Àmpere.

3.4 Comprimentos Fundamentais

Nesta Seção manipularemos as equações de Ginzburg-Landau em dois limites distintos. Obteremos duas escalas de comprimentos fundamentais desta teoria, o *comprimento de coerência* ξ e o *comprimento de penetração* de London λ , os quais descrevem as distâncias em que o parâmetro de ordem e o campo magnético local variam, respectivamente.

3.4.1 Comprimento de Penetração de London

Partindo da formulação semi-clássica de Ginzburg-Landau, e supondo que o parâmetro de ordem é constante em todo o espaço, a densidade de corrente supercondutora (3.3.17) pode ser escrita como

$$\mathbf{J}_s = -\frac{(e^*)^2}{m^* c} n_s \mathbf{A}, \quad (3.4.1)$$

onde $n_s = |\psi|^2$ é a densidade de pares de elétrons supercondutores. Substituindo este resultado na lei de Àmpere (3.3.16) encontramos

$$\nabla \times \mathbf{h} + \frac{4\pi(e^*)^2 n_s}{m^* c^2} \mathbf{A} = 0. \quad (3.4.2)$$

Aplicando o rotacional de ambos os lados obtemos a equação de London

$$\lambda^2 \nabla \times (\nabla \times \mathbf{h}) + \mathbf{h} = 0, \quad (3.4.3)$$

onde comprimento de penetração de London agora é dado por

$$\lambda = \sqrt{\frac{m^* c^2}{4\pi(e^*)^2 n_s}}. \quad (3.4.4)$$

Note que a equação de London é um caso especial da teoria de Ginzburg-Landau, exceto pelo fato de que agora o comprimento de penetração de London incorpora a carga e massa efetivas.

Agora, usando a seguinte identidade vetorial $\nabla \times \nabla \times \mathbf{h} = \nabla(\nabla \cdot \mathbf{h}) - \nabla^2 \mathbf{h}$ e da lei de Gauss do magnetismo $\nabla \cdot \mathbf{h} = 0$, então obtemos

$$\nabla^2 \mathbf{h} = -\frac{1}{\lambda^2} \mathbf{h}. \quad (3.4.5)$$

Para entendermos o significado desse parâmetro, suponha o caso um supercondutor semi-infinito preenchendo o espaço $x > 0$. A região $x < 0$ é o vácuo onde aplicamos um campo magnético uniforme $\mathbf{H}$ paralelo ao plano yz . Assim, $\mathbf{h} = (0, 0, h_z(x))$ no interior do supercondutor e, fora dele, $\mathbf{h} = H\mathbf{k}$. Sendo assim, podemos reduzir a equação (3.4.5) ao caso unidimensional

$$\frac{d^2 h_z}{dx^2} - \frac{1}{\lambda^2} h_z = 0, \quad (3.4.6)$$

cujas solução é simplesmente dada por

$$h_z(x) = H e^{-x/\lambda}. \quad (3.4.7)$$

O que significa que o campo magnético externo, cuja intensidade é H , decai exponencialmente à medida que penetra na amostra supercondutora. Portanto, o campo magnético local é atenuado no interior do material supercondutor e o comprimento característico dessa atenuação é representado pelo parâmetro λ (ver figura 3.6).

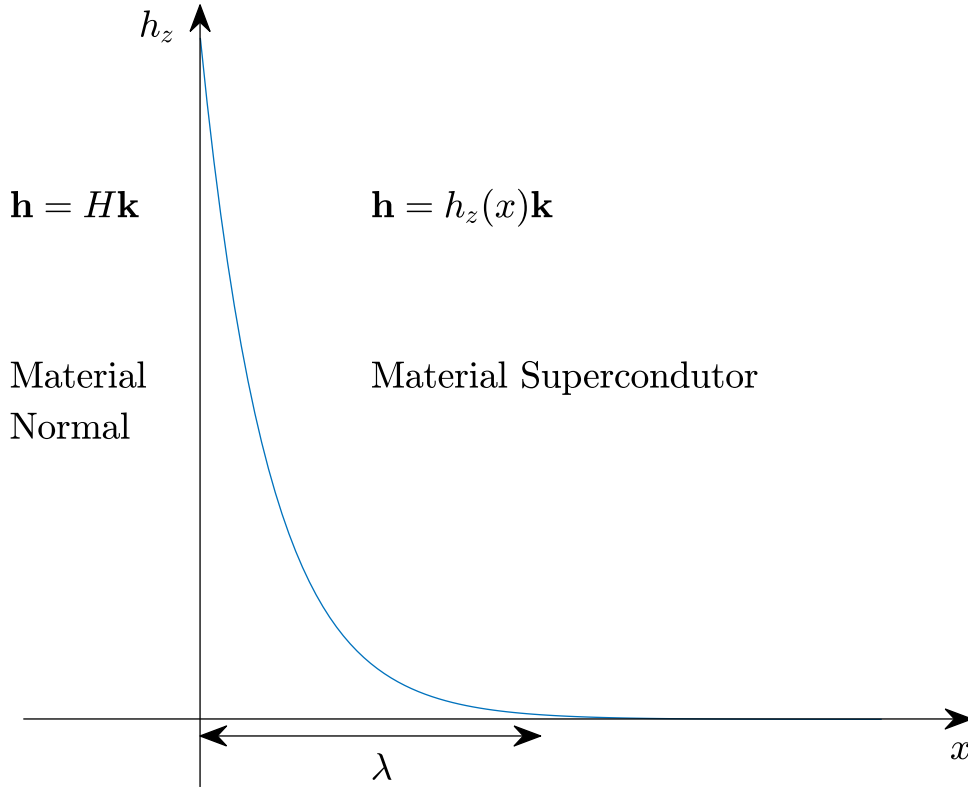


Figura 3.6: Campo magnético local no interior da amostra supercondutora. O comprimento de penetração λ representa o decaimento no interior do supercondutor.

3.4.2 Comprimento de Coerência

Quando minimizamos o funcional de Ginzburg-Landau com relação a ψ , obtivemos uma equação que descreve a densidade dos elétrons supercondutores no interior do material supercondutor (ver equação (3.3.14)). Uma quantidade intrinsecamente associada a esta equação é

o assim chamado comprimento de coerência que descreve o domínio de variação do parâmetro de ordem. Embora a equação diferencial (3.3.14) é não-linear, em alguns casos especiais possui solução exata conforme veremos adiante. Considere um material supercondutor semi-infinito preenchendo todo espaço $x > 0$ na ausência de um campo magnético externo, $\mathbf{A} = 0$. Neste caso, é suficiente considerar $\psi = \psi(x)$ uma função real,

$$-\frac{\hbar^2}{2m^*} \frac{d^2\psi}{dx^2} + \alpha\psi + \beta\psi^3 = 0 . \quad (3.4.8)$$

No estado supercondutor, a constante α é negativa. Então, escrevemos $\alpha = -|\alpha|$. Substituindo esta relação na equação anterior e dividindo todos os termos por $|\alpha|$, encontramos

$$-\frac{\hbar^2}{2m^*|\alpha|} \frac{d^2\psi}{dx^2} - \psi + \frac{\beta}{|\alpha|}\psi^3 = 0 . \quad (3.4.9)$$

Definir

$$\xi = \sqrt{\frac{\hbar^2}{2m^*|\alpha|}} , \quad (3.4.10)$$

conhecido como comprimento de coerência.

Também é conveniente escrevermos o parâmetro de ordem na forma adimensional por meio da seguinte transformação

$$\psi = \sqrt{\frac{|\alpha|}{\beta}} \tilde{\psi} . \quad (3.4.11)$$

Assim, a equação (3.4.9) toma a forma

$$-\xi^2 \frac{d^2\tilde{\psi}}{dx^2} - \tilde{\psi} + \tilde{\psi}^3 = 0 . \quad (3.4.12)$$

Definir $\tilde{\psi}' = d\tilde{\psi}/dx$, tal que

$$-\xi^2 \tilde{\psi}'' - \tilde{\psi} + \tilde{\psi}^3 = 0 . \quad (3.4.13)$$

Agora, multiplicando esta equação por $\tilde{\psi}'$, obtemos

$$-\xi^2 \tilde{\psi}'' \tilde{\psi}' - \tilde{\psi}' \tilde{\psi} + \tilde{\psi}' \tilde{\psi}^3 = 0 , \quad (3.4.14)$$

a qual pode ser reescrita alternativamente como

$$\frac{d}{dx} \left[-\xi^2 \frac{\tilde{\psi}'^2}{2} - \frac{\tilde{\psi}^2}{2} + \frac{\tilde{\psi}^4}{4} \right] = 0 . \quad (3.4.15)$$

De forma que o termo entre colchetes deve ser uma constante

$$C = -\xi^2 \frac{\tilde{\psi}'^2}{2} - \frac{\tilde{\psi}^2}{2} + \frac{\tilde{\psi}^4}{4} . \quad (3.4.16)$$

A constante C pode ser determinada usando as condições de contorno

$$\begin{cases} \text{Para } x \rightarrow \infty \Rightarrow \tilde{\psi}^2 \rightarrow 1 \text{ e } \tilde{\psi}' \rightarrow 0, \\ \text{Para } x \rightarrow 0 \Rightarrow \tilde{\psi}^2 \rightarrow 0, \end{cases} \quad (3.4.17)$$

de onde obtemos $C = -1/4$, de tal modo que

$$-\xi^2 \frac{\tilde{\psi}'^2}{2} - \frac{\tilde{\psi}^2}{2} + \frac{\tilde{\psi}^4}{4} = -\frac{1}{4}, \quad (3.4.18)$$

$$2\xi^2 \tilde{\psi}'^2 = -2\tilde{\psi}^2 + \tilde{\psi}^4 + 1, \quad (3.4.19)$$

$$\xi^2 (\tilde{\psi}')^2 = \frac{1}{2} (1 - \tilde{\psi}^2)^2. \quad (3.4.20)$$

Essa equação diferencial possui solução exata. Temos que

$$\tilde{\psi} = \tanh\left(\frac{x}{\sqrt{2}\xi}\right), \quad (3.4.21)$$

a qual satisfaz as condições de contorno (3.4.17). A figura (3.7) ilustra a variação do parâmetro de ordem próximo à superfície do material supercondutor.

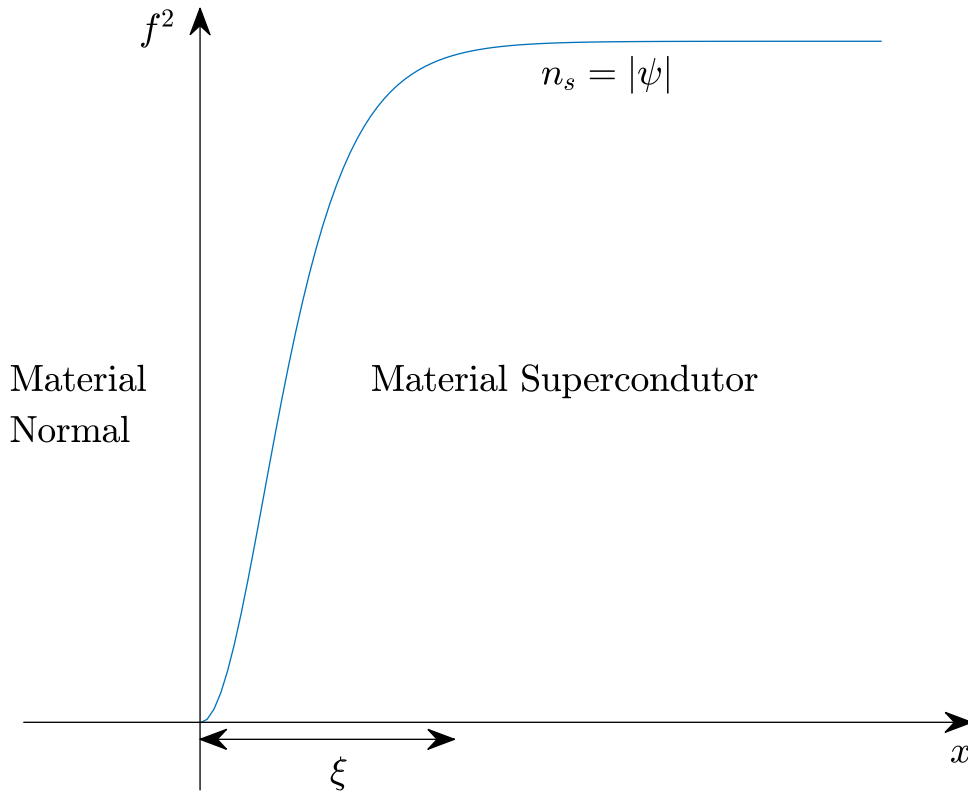


Figura 3.7: Densidade supercondutora $|\psi|^2$, em unidades adimensionais, dentro do material; a região onde ψ é constante, $|\psi|^2$ iguala-se a n_s .

3.5 Equação de Ginzburg-Landau Dependente do Tempo

A equação de Ginzburg-Landau discutida até aqui é uma equação independente do tempo que descreve o equilíbrio termodinâmico do supercondutor. Isso significa que temos conside-

rado casos em que o supercondutor está apenas na presença de um campo magnético estático. Entretanto, nas últimas décadas uma atenção considerável tem sido dado para problemas dependentes do tempo fora do equilíbrio. Dessa maneira, podemos questionar sobre a existência da generalização da teoria de Ginzburg-Landau capaz de descrever variações do parâmetro de ordem com o tempo.

As investigações teóricas para a generalização da equação de Ginzburg-Landau na qual incluem termos dependentes do tempo foram propostas por Stephen e Suhl [22], e suas conclusões confirmadas através de um ponto de vista qualitativo por Anderson [23]. Posteriormente, análises mais detalhas foram realizadas por Stephen [24], Lucas [25], Schmid [26]¹. Estas equações foram largamente exploradas por Abrahams e Tsuneto [27], Caroli e Maki [28, 29].

Com base nestes estudos, as equações de Ginzburg-Landau dependentes do tempo (TDGL) são dadas por

$$\frac{\hbar^2}{2m^*D} \left(\frac{\partial}{\partial t} + \frac{ie^*}{\hbar} \varphi \right) \psi = -\frac{1}{2m^*} \mathbf{\Pi}^2 \psi + \alpha \psi + \beta |\psi|^2 \psi, \quad (3.5.1)$$

$$\frac{4\pi}{c} \sigma \left(\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} + \nabla \varphi \right) = \frac{4\pi}{c} \mathbf{J}_s - \nabla \times \mathbf{h}, \quad (3.5.2)$$

sendo a densidade de supercorrente dada por

$$\mathbf{J}_s = \frac{e^*}{m^*} \text{Re} (\bar{\psi} \mathbf{\Pi} \psi), \quad (3.5.3)$$

onde $\alpha = \alpha(T) = \alpha_0(T - T_c)$ para $T \leq T_c$ e $\alpha = 0$ para $T > T_c$, sendo T_c a temperatura crítica e $\alpha_0 > 0$; β é uma constante positiva e não depende da temperatura; D é o coeficiente de difusão; σ é a condutividade elétrica; $\mathbf{\Pi} = (-i\hbar \nabla - \frac{e^*}{c} \mathbf{A})$ é a derivada covariante; $e^* = 2e$, $m^* = 2m$ onde e e m são a carga e a massa do elétron, respectivamente.

Posteriormente, a equação TDGL (3.3.14) foi generalizadas para supercondutores com *gap* (equação GTDGL). Esta se diferencia da equação TDGL convencional no seguinte aspecto. Quando aplicamos uma corrente de transporte a um supercondutor, acima de uma determinada corrente crítica, inicia-se um regime não-estacionário onde se forma pares de vórtice e anti-vórtice (v-av) que se aniquilam. Na região onde se formam o par v-av, o parâmetro de ordem é consideravelmente depreciado ao longo da linha que separa seus núcleos centrais. A GTDGL incorpora um termo que leva em conta o tempo que o parâmetro de ordem leva para se recompor quando são formados pares v-av. Este termo é dado por $\gamma = 2\tau_E \sqrt{n_s}/\hbar$, onde τ_E é o tempo de colisão inelástico [30, 31]. Temos que

$$\frac{\hbar^2}{2m^*D} \frac{u}{\sqrt{1 + \gamma^2 |\psi|^2 / n_s}} \left(\frac{\partial}{\partial t} + \frac{ie^*}{\hbar} \varphi \right) \psi = -\frac{1}{2m^*} \mathbf{\Pi}^2 \psi + \alpha \psi + \beta |\psi|^2 \psi, \quad (3.5.4)$$

onde $u = 5.79$ é obtido de primeiros princípios (mecânico-quanticamente). Note quando $\gamma = 0$ obtemos as equações TDGL para supercondutores *gapless*, exceto pelo fato de que neste referido caso $u = 1$.

¹Schmid fez a inclusão do potencial escalar elétrico que descreve um supercondutor na presença de uma corrente de transporte.

Mesmo nos caso onde temos a ausência de corrente de transporte, as equações TDGL podem ser utilizadas com equações de relaxação para se determinar as configurações de equilíbrio da rede de vórtices para supercondutores na presença de campo magnético externo aplicado.

No próximo Capítulo iremos escrever um algoritmo que resolve as equações TDGL. A extensão deste procedimento para as equações GTDGL é imediata.

Solução Numérica das Equações de Ginzburg-Landau Dependentes do Tempo

4.1 Equações de Ginzburg-Landau Dependentes do Tempo

Conforme isto no Capítulo anterior, as equações de Ginzburg-Landau dependentes do tempo (TDGL) são dadas por

$$\frac{\hbar^2}{2m^*D} \left(\frac{\partial}{\partial t} + \frac{ie^*}{\hbar} \varphi \right) \psi = -\frac{1}{2m^*} \mathbf{\Pi}^2 \psi - \alpha \psi - \beta |\psi|^2 \psi , \quad (4.1.1)$$

$$\frac{4\pi}{c} \sigma \left(\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} + \nabla \varphi \right) = \frac{4\pi}{c} \mathbf{J}_s - \nabla \times \mathbf{h} , \quad (4.1.2)$$

sendo a densidade de supercorrente dada por

$$\mathbf{J}_s = \frac{e^*}{m^*} \text{Re} (\bar{\psi} \mathbf{\Pi} \psi) , \quad (4.1.3)$$

onde $\alpha = \alpha(T) = \alpha_0(T - T_c)$ para $T \leq T_c$ e $\alpha = 0$ para $T > T_c$, sendo T_c a temperatura crítica e $\alpha_0 > 0$; β é uma constante positiva e não depende da temperatura; D é o coeficiente de difusão; σ é a condutividade elétrica; $\mathbf{\Pi} = (-i\hbar \nabla - \frac{e^*}{c} \mathbf{A})$ é a derivada covariante; $e^* = 2e$, $m^* = 2m$ onde e e m são a carga e a massa do elétron, respectivamente; o potencial vetor e o campo magnético local estão relacionados por $\mathbf{h} = \nabla \times \mathbf{A}$; φ é o potencial escalar.

Suponhamos que o supercondutor encontra-se na ausência de campo magnético aplicado e de corrente de transporte aplicada. Nestes casos

$$\alpha \psi + \beta |\psi|^2 \psi = 0 , \quad (4.1.4)$$

cujas soluções são dadas por $\psi = 0$ e $|\psi|^2 = -\alpha/\beta$. Descartando a solução trivial, ficamos com a segunda solução. Assim, vemos que α necessariamente deve ser uma constante negativa para que $|\psi|^2$ seja positivo. Assim, podemos escrever $|\psi|^2 = |\alpha|/\beta$. Este estado é conhecido como estado de Meissner.

4.2 Unidades Reduzidas

As equações (4.1.1) e (4.1.2) podem ser convenientemente reescritas usando o seguinte sistema de unidades

$$\begin{aligned}
 \psi &= \psi_0 \tilde{\psi}, \\
 T &= T_c \tilde{T}, \\
 \nabla &= \frac{1}{\xi} \tilde{\nabla}, \\
 t &= \frac{\xi^2}{D} \tilde{t}, \\
 \mathbf{A} &= H_{c2} \xi \tilde{\mathbf{A}}, \\
 \varphi &= \frac{H_{c2} D}{c} \tilde{\varphi}, \\
 \mathbf{h} &= H_{c2} \tilde{\mathbf{h}},
 \end{aligned} \tag{4.2.1}$$

onde $\psi_0^2 = |\alpha|/\beta$, $\xi^2 = \hbar^2/2m^*|\alpha|$ e $H_{c2} = \Phi_0/2\pi\xi^2$ é o campo crítico superior (o valor de campo magnético suficiente para destruir a rede de vórtices de Abrikosov), e $\Phi_0 = hc/2e$ é o fluxo quântico.

Multiplicando ambos os lados da equação (4.1.1) por ψ_0 e considerando cada um dos termos separadamente, podemos mostrar que:

1. *Termo do condensado:*

$$-\psi_0(\alpha\psi + \beta\psi|\psi|^2) = \psi_0^2|\alpha|\tilde{\psi}(1 - |\tilde{\psi}|^2); \tag{4.2.2}$$

2. *Campo crítico:*

$$\frac{e^*\xi}{\hbar c} = \frac{1}{H_{c2}\xi}; \tag{4.2.3}$$

3. *Termo cinético:*

$$\frac{\psi_0}{2m^*} \left(-i\hbar\nabla - \frac{e^*}{c}\mathbf{A} \right)^2 \psi = \psi_0^2|\alpha| \left(-i\tilde{\nabla} - \tilde{\mathbf{A}} \right)^2 \tilde{\psi}; \tag{4.2.4}$$

4. *Derivada temporal:*

$$\psi_0 \frac{\hbar^2}{2m^*D} \frac{\partial\psi}{\partial t} = \psi_0^2|\alpha| \frac{\partial\tilde{\psi}}{\partial\tilde{t}}; \tag{4.2.5}$$

5. *Potencial:*

$$\psi_0 \frac{\hbar^2}{2m^*D} \left(i\frac{e^*}{\hbar}\varphi \right) \psi = \psi_0^2|\alpha| i\tilde{\varphi}\tilde{\psi}. \tag{4.2.6}$$

Consequentemente, a equação (4.1.1) pode ser escrita na forma

$$\left(\frac{\partial}{\partial t} + i\varphi\right)\psi = -\mathbf{\Pi}^2\psi + \psi(1 - |\psi|^2), \quad (4.2.7)$$

onde abandonamos os til's, e a derivada covariante agora é dada por $\mathbf{\Pi} = (-i\nabla - \mathbf{A})$.

O comprimento de penetração de London é definido por

$$\lambda^2 = \frac{m^*c^2}{4\pi(e^*)^2\psi_0^2}, \quad (4.2.8)$$

e o parâmetro de Ginzburg-Landau por $\kappa = \lambda/\xi$.

Definindo a constante

$$\beta = \frac{4\pi\sigma D\kappa^2}{c^2}, \quad (4.2.9)$$

de forma análoga podemos proceder com as equações (4.1.2) e (4.1.3) e mostrar que

1. *Termo do campo:*

$$\nabla \times \mathbf{h} = \frac{H_{c2}\xi}{\lambda^2}\kappa^2\tilde{\nabla} \times \tilde{\mathbf{h}}; \quad (4.2.10)$$

2. *Termo da corrente:*

$$\begin{aligned} \frac{4\pi}{c}\mathbf{J}_s &= \frac{H_{c2}\xi}{\lambda^2}\mathbb{R}\text{e}\left[\left(\tilde{\psi} - i\tilde{\nabla} - \tilde{\mathbf{A}}\right)\tilde{\psi}\right] \\ &= \frac{H_{c2}\xi}{\lambda^2}\tilde{\mathbf{J}}_s; \end{aligned} \quad (4.2.11)$$

3. *Termo do potencial:*

$$\frac{4\pi}{c}\sigma\nabla\varphi = \frac{H_{c2}\xi}{\lambda^2}\beta\tilde{\nabla}\tilde{\varphi}; \quad (4.2.12)$$

4. *Termo do potencial vetor:*

$$\frac{4\pi}{c}\sigma\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t} = \frac{H_{c2}\xi}{\lambda^2}\beta\frac{\partial\tilde{\mathbf{A}}}{\partial\tilde{t}}. \quad (4.2.13)$$

Assim, as equações (4.1.2) e (4.1.3), em unidades reduzidas são escritas como

$$\beta\left(\frac{\partial\mathbf{A}}{\partial t} + \nabla\varphi\right) = \mathbf{J}_s - \kappa^2\nabla \times \mathbf{h}, \quad (4.2.14)$$

$$\mathbf{J}_s = \mathbb{R}\text{e}\left[\tilde{\psi}(-i\nabla - \mathbf{A})\psi\right], \quad (4.2.15)$$

onde novamente abandonamos os til's nas equações.

4.3 Campos Auxiliares

Com a finalidade de resolver numericamente as equações (4.2.7), (4.2.14) e (4.2.15) é conveniente introduzirmos o vetor *campo auxiliar* $\mathbf{U} = (\mathcal{U}_x, \mathcal{U}_y)$, cujas componentes são definidas por

$$\mathcal{U}_x = \exp \left(-i \int_{x_0}^x A_x dx \right), \quad (4.3.1)$$

$$\mathcal{U}_y = \exp \left(-i \int_{y_0}^y A_y dy \right), \quad (4.3.2)$$

onde (x_0, y_0) é um ponto de referência arbitrário.

Usando a identidade

$$\frac{\partial \mathcal{U}_x}{\partial x} = -i A_x \mathcal{U}_x, \quad (4.3.3)$$

e usando a propriedade de que os campos auxiliares são funções unimodulares, isto é, $\mathcal{U} \bar{\mathcal{U}} = 1$, encontramos

1.

$$-i \bar{\mathcal{U}}_x \frac{\partial (\mathcal{U}_x f)}{\partial x} = \left(-i \frac{\partial}{\partial x} - A_x \right) f. \quad (4.3.4)$$

A identidade (4.3.4) vale para qualquer função complexa f . Empregando a primeiramente com $f = \psi$ e em segundo com $f = -i \bar{\mathcal{U}}_x \frac{\partial (\mathcal{U}_x \psi)}{\partial x}$, podemos mostrar que

2.

$$\begin{aligned} \left(-i \frac{\partial}{\partial x} - A_x \right)^2 \psi &= \left(-i \frac{\partial}{\partial x} - A_x \right) \left(-i \frac{\partial}{\partial x} - A_x \right) \psi \\ &= -\bar{\mathcal{U}}_x \frac{\partial^2 (\mathcal{U}_x \psi)}{\partial x^2}. \end{aligned} \quad (4.3.5)$$

Analogamente, obtemos

$$\left(-i \frac{\partial}{\partial y} - A_y \right)^2 \psi = -\bar{\mathcal{U}}_y \frac{\partial^2 (\mathcal{U}_y \psi)}{\partial y^2}. \quad (4.3.6)$$

Assim, a equação (4.2.7) pode ser escrita como

$$\left(\frac{\partial}{\partial t} + i\varphi \right) \psi = \bar{\mathcal{U}}_x \frac{\partial^2 (\mathcal{U}_x \psi)}{\partial x^2} + \bar{\mathcal{U}}_y \frac{\partial^2 (\mathcal{U}_y \psi)}{\partial y^2} + \psi(1 - |\psi|^2). \quad (4.3.7)$$

As componentes da densidade de corrente (4.2.15) também podem ser expressas em termos dos campos auxiliares. Usando a identidade (4.3.4), temos que

$$J_{sx} = \text{Re} \left[\bar{\psi} \left(-i \bar{\mathcal{U}}_x \frac{\partial (\mathcal{U}_x \psi)}{\partial x} \right) \right]. \quad (4.3.8)$$

Uma vez que $\Re(-iz) = \Im(z)$, obtemos

$$J_{sx} = \Im \left[\bar{\mathcal{U}}_x \bar{\psi} \frac{\partial(\mathcal{U}_x \psi)}{\partial x} \right]. \quad (4.3.9)$$

De maneira análoga, encontramos

$$J_{sy} = \Im \left[\bar{\mathcal{U}}_y \bar{\psi} \frac{\partial(\mathcal{U}_y \psi)}{\partial y} \right]. \quad (4.3.10)$$

4.4 Resumo

Nesta Seção resumimos as equações que serão discretizadas e as respectivas condições de contorno. A geometria que estudaremos é a de um supercondutor retangular na presença de um campo magnético externo aplicado H conforme ilustrado na figura 4.1. Assumiremos que não há corrente de transporte aplicada. Assim, podemos usar o calibre de Coulomb $\varphi = 0$.

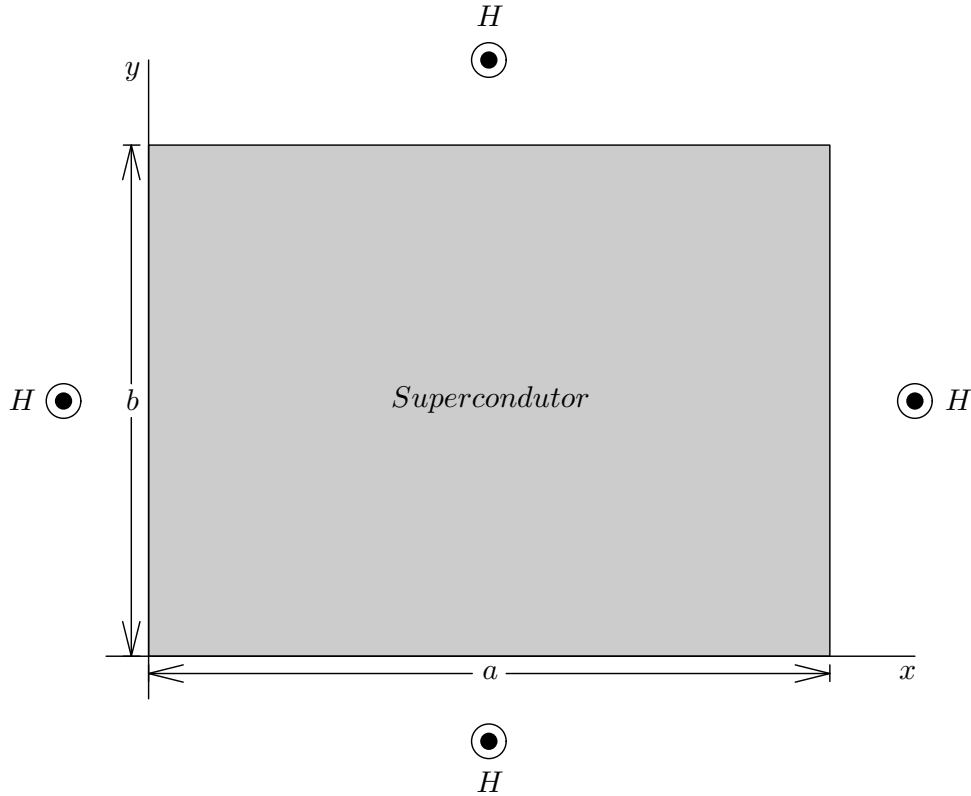


Figura 4.1: Geometria do problema.

1. *Primeira equação TDGL:*

$$\frac{\partial \psi}{\partial t} = \bar{\mathcal{U}}_x \frac{\partial^2(\mathcal{U}_x \psi)}{\partial x^2} + \bar{\mathcal{U}}_y \frac{\partial^2(\mathcal{U}_y \psi)}{\partial y^2} + \psi(1 - |\psi|^2). \quad (4.4.1)$$

2. *Equações das componentes da densidade de corrente:*

$$J_{sx} = \Im \left[\bar{\mathcal{U}}_x \bar{\psi} \frac{\partial(\mathcal{U}_x \psi)}{\partial x} \right], \quad (4.4.2)$$

$$J_{sy} = \Im \left[\bar{\mathcal{U}}_y \bar{\psi} \frac{\partial(\mathcal{U}_y \psi)}{\partial y} \right]. \quad (4.4.3)$$

3. Segunda equação TDGL:

$$\beta \frac{\partial \mathbf{A}}{\partial t} = \mathbf{J}_s - \kappa^2 \nabla \times \mathbf{h} . \quad (4.4.4)$$

$$(4.4.5)$$

4. Condições de contorno para ψ :

$$\frac{\partial(\mathcal{U}_x \psi)}{\partial x} = 0 \quad \text{para os lados oeste e leste do retângulo ,} \quad (4.4.6)$$

$$\frac{\partial(\mathcal{U}_y \psi)}{\partial y} = 0 \quad \text{para os lados sul e norte do retângulo .} \quad (4.4.7)$$

Estas condições garantem que a componente perpendicular da densidade de corrente é nula em todos os lados do retângulo.

5. Condições de contorno para $\mathbf{h}$:

$$h_z = H , \quad \text{nos lados do retângulo .} \quad (4.4.8)$$

4.5 Discretização das Equações TDGL

4.5.1 Malha de Discretização

Nas duas últimas décadas, várias técnicas de discretização das equações TDGL foram desenvolvidas (ver por exemplo referências [32, 33, 34]). Todas elas baseiam-se no *método de variáveis de ligação* [35, 36]. No que segue descrevemos esta técnica e então no próximo Capítulo apresentaremos aplicações que fizemos para supercondutores mesoscópicos.

Para discretizar as equações de Ginzburg-Landau substituímos as variáveis (x, y) por suas discretas equivalentes (x_i, y_j) . Considerando (a, b) os lados de um retângulo, dividimos estes em intervalos de tamanhos $(\Delta x, \Delta y)$, respectivamente. Assim, os pontos de vértice da malha de discretização são dados por $x_i = (i - 1)\Delta x$, e $y_j = (j - 1)\Delta y$, para todo $\{i = 1, \dots, N_x + 1, j = 1, \dots, N_y + 1\}$, onde $N_x = a/\Delta x$, e $N_y = b/\Delta y$ são os números de células unitárias nas direções x e y , respectivamente. A figura 4.2 ilustra a malha de discretização. O domínio supercondutor Ω_{sc} é limitado pelas linhas tracejadas $\partial\Omega_{sc}$ da figura. Temos que

$$\Omega_{sc} = \left\{ \mathbf{r} = (x, y) : x_1 + \frac{\Delta x}{2} < x < x_{N_x} + \frac{\Delta x}{2}, y_1 + \frac{\Delta y}{2} < y < y_{N_y} + \frac{\Delta y}{2} \right\} . \quad (4.5.1)$$

Os pontos fora da linha tracejada são pontos falsos.

4.5.2 Definições

Antes de discretizarmos as equações TDGL, precisamos de introduzir algumas definições. A principal delas é a de variável de ligação. Consideremos o produto do campo auxiliar $\mathcal{U}_x$ entre dois pontos consecutivos da malha (x_i, y_j) e (x_{i+1}, y_j) . Temos que

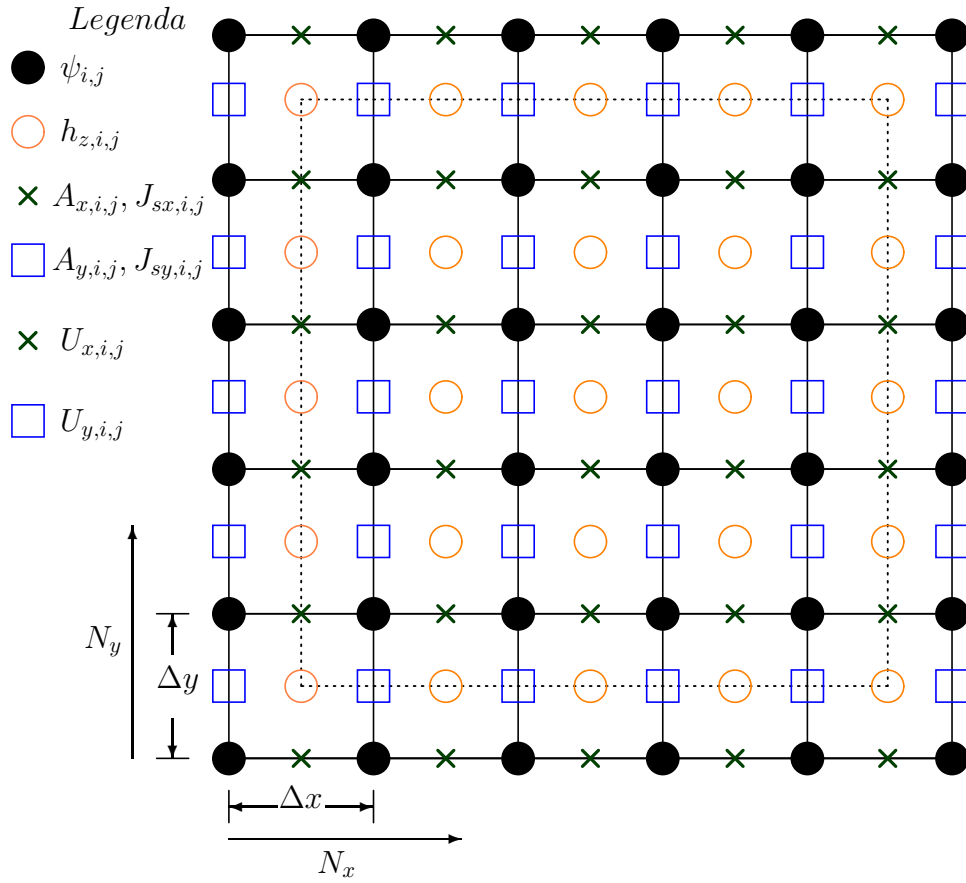


Figura 4.2: Malha de discretização.

$$\begin{aligned}
 U_{x,i,j} &\equiv \mathcal{U}_x(x_{i+1}, y_j) \bar{\mathcal{U}}_x(x_i, y_j) \\
 &= \exp \left(-i \int_{x_0}^{x_{i+1}} A_x(x, y_j) dx \right) \exp \left(i \int_{x_0}^{x_i} A_x(x, y_j) dx \right) \\
 &= \exp \left(-i \int_{x_0}^{x_i} A_x(x, y_j) dx - i \int_{x_i}^{x_{i+1}} A_x(x, y_j) dx + i \int_{x_0}^{x_i} A_x(x, y_j) dx \right) \\
 &= \exp \left(-i \int_{x_i}^{x_{i+1}} A_x(x, y_j) dx \right) \\
 &= \exp(-i \Delta x A_{x,i,j}) ,
 \end{aligned} \tag{4.5.2}$$

onde $A_{x,i,j} \equiv A_x(x_i + \frac{\Delta x}{2}, y_j)$ e usamos a regra do ponto médio para integração. Analogamente, temos que

$$\begin{aligned}
 U_{y,i,j} &\equiv \mathcal{U}_y(x_i, y_{j+1}) \bar{\mathcal{U}}_y(x_i, y_j) \\
 &= \exp(-i \Delta y A_{y,i,j}) ,
 \end{aligned} \tag{4.5.3}$$

onde $A_{y,i,j} \equiv A_y(x_i, y_j + \frac{\Delta y}{2})$. Fica claro então a denominação variável de ligação, pois as variáveis $U_{x,i,j}$ e $U_{y,i,j}$ ligam pontos adjacentes de malha através do potencial vetor no ponto médio.

Outras definições são as seguintes

- $\psi_{i,j} \equiv \psi(x_i, y_j)$,
- $J_{sx,i,j} \equiv J_{sx}(x_i + \frac{\Delta x}{2}, y_j)$,
- $J_{sy,i,j} \equiv J_{sy}(x_i, y_j + \frac{\Delta y}{2})$,
- $h_{z,i,j} \equiv h_z(x_i + \frac{\Delta x}{2}, y_j + \frac{\Delta y}{2})$.

Em resumo, o parâmetro de ordem é calculado nos pontos de vértice da célula unitária; as componentes do potencial vetor e da densidade de corrente são calculados nos pontos médios da célula unitária; o campo magnético local é calculado no centro da célula unitária.

Será mais conveniente escrever as variáveis de ligação na forma

$$U_{x,i,j} = \exp(-i\phi_{x,i,j}) , \quad (4.5.4)$$

$$U_{y,i,j} = \exp(-i\phi_{y,i,j}) , \quad (4.5.5)$$

onde

$$\phi_{x,i,j} = \Delta x A_{x,i,j} , \quad (4.5.6)$$

$$\phi_{y,i,j} = \Delta y A_{y,i,j} . \quad (4.5.7)$$

4.5.3 Aproximações para as Derivadas

Usando expansão em série de Taylor, obtemos

$$f(x + \frac{\Delta x}{2}) = f(x) + \frac{\Delta x}{2} f'(x) + \frac{\Delta x^2}{8} f''(x) + \dots , \quad (4.5.8)$$

$$f(x - \frac{\Delta x}{2}) = f(x) - \frac{\Delta x}{2} f'(x) + \frac{\Delta x^2}{8} f''(x) + \dots , \quad (4.5.9)$$

e

$$f(x + \Delta x) = f(x) + \Delta x f'(x) + \frac{\Delta x^2}{2} f''(x) + \dots , \quad (4.5.10)$$

$$f(x - \Delta x) = f(x) - \Delta x f'(x) + \frac{\Delta x^2}{2} f''(x) + \dots , \quad (4.5.11)$$

1. Das equações (4.5.8) e (4.5.9) encontramos

$$f'(x) = \frac{f(x + \frac{\Delta x}{2}) - f(x - \frac{\Delta x}{2})}{\Delta x} . \quad (4.5.12)$$

2. Das equações (4.5.10) e (4.5.11) temos que

$$f''(x) = \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x^2} . \quad (4.5.13)$$

Estas fórmulas de aproximação das primeira e segunda derivadas serão muito úteis para a discretização das equações TDGL.

4.5.4 Discretização da Primeira Equação TDGL

Usando a aproximação para a derivada segunda (4.5.13), podemos escrever

$$\bar{\mathcal{U}}_x \frac{\partial^2(\mathcal{U}_x \psi)}{\partial x^2} \Big|_{x_i, y_j} = \bar{\mathcal{U}}_x(x_i, y_i) \frac{1}{\Delta x^2} [\mathcal{U}_x(x_{i+1}, y_j) \psi(x_{i+1}, y_j) - 2\mathcal{U}_x(x_i, y_j) \psi(x_i, y_j) + \mathcal{U}_x(x_{i-1}, y_j) \psi(x_{i-1}, y_j)] . \quad (4.5.14)$$

Agora, usando as definições para o parâmetro de ordem, e (4.5.2) para a variável de ligação, obtemos

$$\bar{\mathcal{U}}_x \frac{\partial^2(\mathcal{U}_x \psi)}{\partial x^2} \Big|_{x_i, y_j} = \frac{U_{x,i,j} \psi_{i+1,j} - 2\psi_{i,j} + \bar{U}_{x,i-1,j} \psi_{i-1,j}}{\Delta x^2} . \quad (4.5.15)$$

Procedendo de forma análoga, temos que

$$\bar{\mathcal{U}}_y \frac{\partial^2(\mathcal{U}_y \psi)}{\partial y^2} \Big|_{x_i, y_j} = \frac{U_{y,i,j} \psi_{i,j+1} - 2\psi_{i,j} + \bar{U}_{y,i,j-1} \psi_{i,j-1}}{\Delta y^2} . \quad (4.5.16)$$

Consequentemente, a forma discreta da equação (4.4.1) é dada por

$$\begin{aligned} \frac{\partial \psi_{i,j}}{\partial t} = & \frac{U_{x,i,j} \psi_{i+1,j} - 2\psi_{i,j} + \bar{U}_{x,i-1,j} \psi_{i-1,j}}{\Delta x^2} + \frac{U_{y,i,j} \psi_{i,j+1} - 2\psi_{i,j} + \bar{U}_{y,i,j-1} \psi_{i,j-1}}{\Delta y^2} \\ & + \psi_{i,j} (1 - |\psi_{i,j}|^2) . \end{aligned} \quad (4.5.17)$$

A evolução temporal do parâmetro de ordem é determinada usando-se o método de Euler explícito. Integrando a equação (4.5.17) com relação a t , encontramos

$$\begin{aligned} \psi(t + \Delta t) = & \psi_{i,j}(t) + r_x [U_{x,i,j}(t) \psi_{i+1,j}(t) - 2\psi_{i,j}(t) + \bar{U}_{x,i-1,j}(t) \psi_{i-1,j}(t)] \\ & + r_y [U_{y,i,j}(t) \psi_{i,j+1}(t) - 2\psi_{i,j}(t) + \bar{U}_{y,i,j-1}(t) \psi_{i,j-1}(t)] \\ & + \Delta t \psi_{i,j}(t) (1 - |\psi_{i,j}(t)|^2) , \end{aligned} \quad (4.5.18)$$

para todo $\{i = 2, \dots, N_x, j = 2, \dots, N_y\}$; aqui $r_x = \Delta t / \Delta x^2$ e $r_y = \Delta t / \Delta y^2$.

4.5.5 Discretização da Densidade de Corrente

A componente x da densidade de corrente (4.4.2) envolve o produto dos termos $\bar{\mathcal{U}}_x \bar{\psi}$ e $\frac{\partial(\mathcal{U}_x \psi)}{\partial x}$. Usando a aproximação para a primeira derivada (4.5.12), temos que

$$\begin{aligned} \frac{\partial(\mathcal{U}_x \psi)}{\partial x} \Big|_{(x_i + \frac{\Delta x}{2}, y_j)} = & [\mathcal{U}_x(x_i + \Delta x, y_j) \psi(x_i + \Delta x, y_j) \\ & - \mathcal{U}_x(x_i, y_j) \psi(x_i, y_j)] / \Delta x . \end{aligned} \quad (4.5.19)$$

Aproximamos o outro termo pelo seu valor médio entre os pontos adjacentes na malha. Encontramos

$$\bar{\mathcal{U}}_x \bar{\psi} \Big|_{(x_i + \frac{\Delta x}{2}, y_j)} = \frac{\bar{\mathcal{U}}_x(x_i + \Delta x, y_j) \bar{\psi}(x_i + \Delta x, y_j) + \bar{\mathcal{U}}_x(x_i, y_j) \bar{\psi}(x_i, y_j)}{2} . \quad (4.5.20)$$

Introduzindo a identidade $\mathcal{U}_x(x_i, y_j) \bar{\mathcal{U}}_x(x_i, y_j) = 1$ entre o produto dos termos $\bar{\mathcal{U}}_x \bar{\psi}$ e $\frac{\partial(\mathcal{U}_x \psi)}{\partial x}$, e usando a definição de variável de ligação (4.5.2), obtemos

$$\bar{\mathcal{U}}_x \bar{\psi} \frac{\partial(\mathcal{U}_x \psi)}{\partial x} \Big|_{(x_i + \frac{\Delta x}{2}, y_j)} = \frac{1}{2\Delta x} [\bar{U}_{x,i,j} \bar{\psi}_{i+1,j} + \bar{\psi}_{i,j}] [U_{x,i,j} \psi_{i+1,j} - \psi_{i,j}] . \quad (4.5.21)$$

Substituindo este resultado em (4.4.2), finalmente encontramos

$$J_{sx,i,j} = \frac{1}{\Delta x} Q_{x,i,j} , \quad (4.5.22)$$

onde

$$Q_{x,i,j} = \text{Im} [\bar{\psi}_{i,j} U_{x,i,j} \psi_{i+1,j}] . \quad (4.5.23)$$

Analogamente, podemos determinar a aproximação para a componente J_{sy} . Temos que

$$J_{sy,i,j} = \frac{1}{\Delta y} Q_{y,i,j} , \quad (4.5.24)$$

onde

$$Q_{y,i,j} = \text{Im} [\bar{\psi}_{i,j} U_{y,i,j} \psi_{i,j+1}] . \quad (4.5.25)$$

4.5.6 Discretização da Segunda Equação TDGL

Iremos agora discretizar a segunda equação TDGL (4.4.4). Lembrando que $\mathbf{h} = h_z \mathbf{k}$, vem que

$$\beta \frac{\partial A_x}{\partial t} = J_{sx} - \kappa^2 \frac{\partial h_z}{\partial y} , \quad (4.5.26)$$

$$\beta \frac{\partial A_y}{\partial t} = J_{sy} + \kappa^2 \frac{\partial h_z}{\partial x} . \quad (4.5.27)$$

Agora, usando a aproximação (4.5.12) para a primeira derivada, encontramos

$$\begin{aligned} \frac{\partial h_z}{\partial y} \Big|_{(x_i + \frac{\Delta x}{2}, y_j)} &= \frac{h_z(x_i + \frac{\Delta x}{2}, y_j + \frac{\Delta y}{2}) - h_z(x_i + \frac{\Delta x}{2}, y_j - \frac{\Delta y}{2})}{\Delta y} \\ &= \frac{h_{z,i,j} - h_{z,i,j-1}}{\Delta y} , \end{aligned} \quad (4.5.28)$$

$$\begin{aligned} \frac{\partial h_z}{\partial x} \Big|_{(x_i, y_j + \frac{\Delta y}{2})} &= \frac{h_z(x_i + \frac{\Delta x}{2}, y_j + \frac{\Delta y}{2}) - h_z(x_i - \frac{\Delta x}{2}, y_j + \frac{\Delta y}{2})}{\Delta x} \\ &= \frac{h_{z,i,j} - h_{z,i-1,j}}{\Delta x} . \end{aligned} \quad (4.5.29)$$

Portanto, as equações (4.5.26) e (4.5.27) podem ser aproximadas por

$$\beta \frac{\partial A_{x,i,j}}{\partial t} = J_{sx,i,j} - \frac{\kappa^2}{\Delta y} (h_{z,i,j} - h_{z,i,j-1}) , \quad (4.5.30)$$

$$\beta \frac{\partial A_{y,i,j}}{\partial t} = J_{sy,i,j} + \frac{\kappa^2}{\Delta x} (h_{z,i,j} - h_{z,i-1,j}) . \quad (4.5.31)$$

Finalmente, integrando as duas últimas equações com relação a t , obtemos a evolução temporal do potencial vetor. Temos que

1. *Equação para $\phi_{x,i,j}$:*

$$\phi_{x,i,j}(t + \Delta t) = \phi_{x,i,j}(t) + s_x Q_{x,i,j}(t) - t_{xy} [h_{z,i,j}(t) - h_{z,i,j-1}(t)] , \quad (4.5.32)$$

para todo $\{i = 1, 2, \dots, N_x, j = 2, 3, \dots, N_y\}$, onde $s_x = \Delta t / \beta$, $t_{xy} = \kappa^2 \Delta t \Delta x / \beta \Delta y$.

2. *Equação para $\phi_{y,i,j}$:*

$$\phi_{y,i,j}(t + \Delta t) = \phi_{y,i,j}(t) + s_y Q_{y,i,j}(t) + t_{yx} [h_{z,i,j}(t) - h_{z,i-1,j}(t)] , \quad (4.5.33)$$

para todo $\{i = 2, 3, \dots, N_x, j = 1, 2, \dots, N_y\}$, onde $s_y = \Delta t / \beta$, $t_{yx} = \kappa^2 \Delta t \Delta y / \beta \Delta x$.

4.5.7 Campo Local

Como assumimos invariância ao longo da direção z , temos que calcular apenas $h_z = \partial A_y / \partial x - \partial A_x / \partial y$. Assim, usando a aproximação para a primeira derivada (4.5.12) podemos, sem muita dificuldade discretizar esta equação. Temos que

1. *Equação para o campo local:*

$$h_{z,i,j} = \frac{\phi_{y,i+1,j} - \phi_{y,i,j} - \phi_{x,i,j+1} + \phi_{x,i,j}}{\Delta x \Delta y} , \quad (4.5.34)$$

para todo $\{i = 2, 3, \dots, N_x - 1, j = 2, 3, \dots, N_y - 1\}$.

4.5.8 Discretização das Condições de Contorno

Supondo continuidade do campo na interface $\partial\Omega_{sc}$ podemos escrever

$$h_{z,1,j} = H , \quad (4.5.35)$$

$$h_{z,N_x,j} = H , \quad (4.5.36)$$

$$h_{z,i,1} = H , \quad (4.5.37)$$

$$h_{z,i,N_y} = H , \quad (4.5.38)$$

para todo $\{i = 1, 2, \dots, N_x, j = 2, 3, \dots, N_y - 1\}$.

Usando novamente a aproximação para a primeira derivada (4.5.12), e a definição de variáveis de ligação (4.5.2) e (4.5.3), as expressões (4.4.6) e (4.4.7) podem ser discretizadas. Então obtemos

1. Para o lado oeste:

$$\psi_{1,j} = U_{x,1,j} \psi_{2,j} , \quad (4.5.39)$$

para todo $\{j = 2, 3, \dots, N_y\}$;

2. Para o lado leste:

$$\psi_{N_x+1,j} = \bar{U}_{x,N_x,j} \psi_{N_x,j} , \quad (4.5.40)$$

para todo $\{j = 2, 3, \dots, N_y\}$;

3. Para o lado sul:

$$\psi_{i,1} = U_{y,i,1} \psi_{i,2} , \quad (4.5.41)$$

para todo $\{i = 2, 3, \dots, N_x\}$;

4. Para o lado norte:

$$\psi_{i,N_y+1} = \bar{U}_{y,i,N_y} \psi_{i,N_y} , \quad (4.5.42)$$

para todo $\{i = 2, 3, \dots, N_x\}$.

Assim conhecendo-se os valores do parâmetro de ordem e as variáveis de ligação no interior da malha, determinamos os valores de $\psi_{i,j}$ nas bordas da malha.

4.6 Algoritmo

A implementação do algoritmo funciona da seguinte forma. Suponhamos que conhecemos todas as quantidades em todos os pontos de malha em um determinado instante de tempo t . Então podemos determinar-las em $t + \Delta t$. Em outras palavras, se sabemos $\{\psi_{i,j}, \phi_{x,i,j}, \phi_{y,i,j}, h_{z,i,j}\}$ em t , das equações (4.5.18), (4.5.32) e (4.5.33), podemos calcular todas as quantidades nos pontos interiores da malha. Em seguida aplicamos as condições de contorno (4.5.35-4.5.42). Antes de ir para o próximo instante de tempo, atualizamos todas as quantidades relevantes como as variáveis de ligação, densidade de corrente e o campo local em todos os pontos de malha. Então vamos para o nível de tempo acima. Repetindo este procedimento podemos determinar todas as quantidades físicas relevantes em todos os níveis de tempo até que o sistema atinga o estado estacionário. Infelizmente, este método não converge para qualquer passo de tempo Δt . Usamos a seguinte regra prática

$$\Delta t \leq \min \left\{ \frac{\delta^2}{4}, \frac{\delta^2 \beta}{4\kappa^2} \right\} , \quad (4.6.1)$$

$$\delta^2 = \frac{2}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}} . \quad (4.6.2)$$

5.1 Temperature-dependent vortex motion in a square mesoscopic superconducting cylinder: Ginzburg-Landau calculations ([aqui](#))

Este foi o primeiro artigo sobre supercondutividade mesoscópica que publiquei em colaboração com os Professores [André Luiz Malvezzi](#), [Paulo Noronha Lisboa-Filho](#), e [Wilson Ayres Ortiz](#). O André colaborou sobremaneira com a primeira versão do código computacional que implementa o algoritmo de solução numérica das equações TDGL e sua cultura física vasta. O Paulo Noronha participou da forma efetiva na escrita do artigo e em pesquisa bibliográfica, bem como com sua experiência de laboratório em supercondutividade. O Wilson colaborou como observador e sua rica erudição em supercondutividade.

O trabalho trata dos efeitos da temperatura nas configurações de vórtice em supercondutores de dimensões mesoscópicas. As propriedades da rede de vórtices são fortemente influenciadas pela geometria da amostra e a temperatura. Para dimensões muito reduzidas, da ordem de 10ξ ou menor, os efeitos de confinamento induzem o aparecimento de vórtices gigantes (vórtices com vorticidade maior que 1). Isto não ocorre em supercondutores macroscópicos, pois a interação entre os vórtices é repulsiva. Neste trabalho fizemos um mapeamento amplo de todas as possíveis configurações da rede de vórtices como função da temperatura, bem como de todas as transições de estados para várias temperaturas. Também determinamos o diagrama $H - T$, o qual difere sobremaneira do equivalente macroscópico.

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Temperature-dependent vortex motion in a square mesoscopic superconducting cylinder: Ginzburg-Landau calculations

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In this work we investigate the dynamics of vortices in a square mesoscopic superconductor. As time evolves we show how the vortices are nucleated into the sample to form a multivortex, single vortex, and giant vortex states. We illustrate how the vortices move around at the transition fields before they accommodate into an equilibrium configuration. We also calculate the magnetization and the free energy as functions of the applied magnetic field for several values of temperature. In addition, we evaluate the upper critical field.

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I. INTRODUCTION

The study of superconducting samples in mesoscopic scale presented a remarkable improvement during the last years. Certainly, such interest is based on the fact that when the size of the samples is close to the order of the coherence length ξ and/or the size of the penetration depth λ , there are some significant modifications on the physical properties of the superconducting state. Among such differences, the occurrence and dynamics of vortices have been extensively reported in the literature.^{1,2} Besides size effects, the geometrical configuration of the samples also plays a significant role.¹ Taking into account vortex-vortex interaction and boundary effects, two different types of vortex configurations can be achieved in mesoscopic samples. One of them is the multivortex state (MVS) characterized by the existence of several single quantized vortices. The other possibility is the so-called giant vortex state (GVS) where more than one quantum of flux can be measured.

In terms of the theoretical prediction of GVS and the collapse of MVS into GVS, several studies reported not just the occurrence of GVS, but also a multiple form of a combination of these states.^{1,3} However, the direct experimental observation of GVS and MVS-GVS (coexistence of both states) is still controversial.⁴⁻⁶

One of the most used approaches to study mesoscopic superconductors is the time dependent Ginzburg-Landau equations (TDGL). This theory has been successfully applied for thin square mesoscopic superconductors. For instance, Mel'nikov *et al.*⁷ have used the TDGL equations to study the vortex configurations close to the upper critical field in such systems. Otherwise, Hernandez *et al.*⁸ focused on the effects of thermal fluctuations in the magnetization and free energy as function of the external applied magnetic field.

In the present contribution, we study the time evolution of the superconducting state of a long cylinder of square cross section by slowly increasing the applied external field. Despite our results show some subtle differences compared with recent work on thin mesoscopic squares¹ concerning the formation of GVS, MVS, and MVS-GVS, most of them

strengthen the conclusions of the existence of such vortex configurations. We must stress that the emphasis of our work held on the description of the vortex dynamics for different temperatures in a condition of infinitesimal growing applied external field.

The paper is outlined as follows. In Sec. II we present the theoretical approach which will be used. Our description of the superconducting state is based on the time dependent Ginzburg-Landau equations. We also present the main steps of the ψ - U method used to solve the TDGL equations numerically. In Sec. III, the upper critical field, the magnetization, and energy curves are shown and discussed. In addition, we shall discuss the output of the TDGL equations concerning the GVS, MVS, and MVS-GVS.

II. THE THEORETICAL MODEL AND THE NUMERICAL SETUP

We investigate the dynamics of the vortices for a long and thin superconducting cylinder of square cross section. For the sake of brevity, from now on we will refer to this geometry as a square superconductor. Thus, we are allowed to take the order parameter and the local magnetic field invariant along the z direction. The vortex configurations at the equilibrium can be obtained from the Ginzburg-Landau (GL) equations of superconductivity. Schmid⁹ generalized the GL equations which account for the time evolution of the vortices until the most stable configuration is accomplished. The time evolution was incorporated to the GL equations in such a manner that their gauge invariance is preserved. The TDGL equations for the complex order parameter ψ , the vector potential $\mathbf{A}$, and the scalar electrical potential Φ are given by

$$\frac{\hbar^2}{4mD} \left(\frac{\partial}{\partial t} + \frac{ie}{\hbar} \Phi \right) \psi = - \frac{1}{4m} \left(-i\hbar \nabla - \frac{2e}{c} \mathbf{A} \right)^2 \psi + a\psi - b|\psi|^2\psi, \quad (1)$$

$$\nabla \cdot \left(\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} + \nabla \Phi \right) = \mathbf{J}_s - \frac{c}{4\pi} \nabla \times \mathbf{A},$$

where the supercurrent density is

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$$\mathbf{J}_s = \frac{e}{m} \Re \left[\bar{\psi} \left(-i\hbar \nabla - \frac{2e}{c} \mathbf{A} \right) \psi \right], \quad (2)$$

where $\Re$ indicates the real part and the overbar the complex conjugation. Here, D is the diffusion coefficient, ν is the electrical conductivity, and a and b are two positive phenomenological constants; we use the temperature dependence $a = a(T) = a_0(T_c - T)$, for all temperatures $T \leq T_c$, where T_c is the critical temperature. The quantity $|\psi|^2$ represents the local density of Cooper pairs and the local magnetic field is given by $\mathbf{h} = \nabla \times \mathbf{A}$. We consider the zero-electrical potential gauge at all times, $\Phi = 0$.

We solve the TDGL subject to the following boundary conditions: $(-i\nabla - \mathbf{A})|_n = 0$ normal to the sample surfaces, and $h_z = H$ parallel to the sample surfaces, where H is the external field uniformly applied along the z direction.

It is convenient to write the above equations in dimensionless units. We use the following units for the order parameter, length, time, and magnetic field, respectively:

$$\begin{aligned} \psi_c^2 &= \frac{a}{b} = \frac{a_0 T_c}{b} (1 - T/T_c), \\ \xi^2(0) &= \frac{\hbar^2}{4ma_0 T_c}, \\ \tau &= \frac{\xi^2(0)}{D}, \\ H_{c2}(0) &= \frac{\Phi_0}{2\pi\xi^2(0)}, \end{aligned} \quad (3)$$

and T in units of T_c .

Then, the nondimensional TDGL equations can be rewritten as

$$\frac{\partial \psi}{\partial t} = -(-i\nabla - \mathbf{A})^2 \psi + (1 - T)\psi(1 - |\psi|^2),$$

$$\beta \frac{\partial \mathbf{A}}{\partial t} = \mathbf{J}_s - \kappa^2 \nabla \times \mathbf{A},$$

$$\mathbf{J}_s = (1 - T) \Re [\bar{\psi} (-i\nabla - \mathbf{A}) \psi], \quad (4)$$

where $\kappa = \lambda(T)/\xi(T) = \lambda(0)/\xi(0)$ is the GL parameter and $\beta = 4\pi\nu D/c^2 \xi^2(0)$; here

$$\begin{aligned} \lambda(T) &= \left(\frac{mc^2 b}{8\pi e^2 a(T)} \right)^{1/2}, \\ \xi(T) &= \left(\frac{\hbar^2}{4ma(T)} \right)^{1/2}, \end{aligned} \quad (5)$$

are the London penetration length and the coherence length, respectively.

In order to discretize the TDGL equations we use the ψ - U method.¹⁰ This method has the important characteristic of preserving the gauge invariance of the TDGL equations.

This is accomplished by introducing the auxiliary fields

$$\begin{aligned} U_x(x, y, t) &= \exp \left(-i \int_{x_0}^x A_x(s, y, t) ds \right), \\ U_y(x, y, t) &= \exp \left(-i \int_{y_0}^y A_y(x, s, t) ds \right), \end{aligned} \quad (6)$$

where (x_0, y_0) is an arbitrary point.

Thus, the first of the TDGL equations and the supercurrent density can be written in the following form:

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= U_x \frac{\partial^2 (U_x \psi)}{\partial x^2} + U_y \frac{\partial^2 (U_y \psi)}{\partial y^2} + (1 - T)\psi(1 - |\psi|^2), \\ J_{s\alpha} &= \frac{(1 - T)}{2i} \left[U_\alpha \bar{\psi} \frac{\partial (U_\alpha \psi)}{\partial \alpha} - U_\alpha \psi \frac{\partial (U_\alpha \bar{\psi})}{\partial \alpha} \right] \\ &= (1 - T) \Im \left[U_\alpha \bar{\psi} \frac{\partial (U_\alpha \psi)}{\partial \alpha} \right], \end{aligned} \quad (7)$$

where $\alpha = (x, y)$, and $\Im$ indicates the imaginary part.

The full discretization of the TDGL equations can be found in more detail in Refs. 10 and 11. Here, we only show the results. The discretizations are carried out in a rectangular mesh consisting of $N_x \times N_y$ cell points. We denote by Δt the incremental time, by (a_x, a_y) the lattice spacing between adjacent cell points, and by (x_i, y_j) an arbitrary vertex point in the mesh. Let us define

$$t_n = n\Delta t, \quad n = 0, 1, 2, 3, \dots,$$

$$x_i = (i - 1)a_x, \quad i = 1, 2, 3, \dots, N_x + 1,$$

$$y_j = (j - 1)a_y, \quad j = 1, 2, 3, \dots, N_y + 1,$$

$$\psi_{i,j}^n = \psi(x_i, y_j, t_n),$$

$$U_{x,i,j}^n = U_x(x_{i+1}, y_j, t_n) \bar{U}_x(x_i, y_j, t_n) = \exp \left(-i \int_{x_i}^{x_{i+1}} A_x(s, y, t) ds \right),$$

$$U_{y,i,j}^n = U_y(x_i, y_{j+1}, t_n) \bar{U}_y(x_i, y_j, t_n) = \exp \left(-i \int_{y_j}^{y_{j+1}} A_y(x, s, t) ds \right),$$

$$h_{z,i,j}^n = h_z \left(x_i + \frac{a_x}{2}, y_j + \frac{a_y}{2}, t_n \right). \quad (8)$$

According to these definitions, it can be easily seen that ψ is a vertex variable, h_z is a cell variable, and U is a link variable.

Then, the discretized version of the TDGL equations are given by

$$\begin{aligned}
\psi_{i,j}^{n+1} &= \psi_{i,j}^n + \Delta t \frac{U_{x,i,j}^n \psi_{i+1,j}^n - 2\psi_{i,j}^n + \bar{U}_{x,i-1,j}^n \psi_{i-1,j}^n}{a_x^2} \\
&+ \Delta t \frac{U_{y,i,j}^n \psi_{i,j+1}^n - 2\psi_{i,j}^n + \bar{U}_{y,i,j-1}^n \psi_{i,j-1}^n}{a_y^2} \\
&+ \Delta t (1-T) \psi_{i,j}^n (1 - |\psi_{i,j}^n|^2), \\
U_{x,i,j}^{n+1} &= U_{x,i,j}^n + \Delta t \frac{(1-T)}{i\beta} U_{x,i,j}^n \gamma [\bar{\psi}_{i,j}^n U_{x,i,j}^n \psi_{i+1,j}^n] \\
&- \Delta t \frac{\kappa^2}{\beta a_y^2} U_{x,i,j}^n (\bar{L}_{i,j-1}^n L_{i,j}^n - 1), \\
U_{y,i,j}^{n+1} &= U_{y,i,j}^n + \Delta t \frac{(1-T)}{i\beta} U_{y,i,j}^n \gamma [\bar{\psi}_{i,j}^n U_{y,i,j}^n \psi_{i,j+1}^n] \\
&- \Delta t \frac{\kappa^2}{\beta a_x^2} U_{y,i,j}^n (\bar{L}_{i,j}^n L_{i-1,j}^n - 1),
\end{aligned} \quad (9)$$

where

$$L_{i,j}^n = U_{x,i,j}^n \bar{U}_{x,i,j+1}^n U_{y,i+1,j}^n \bar{U}_{y,i,j}^n = \exp(-ia_x a_y h_{z,i,j}^n). \quad (10)$$

The discretized boundary conditions are

$$\begin{aligned}
\psi_{1,j}^n &= U_{x,1,j}^n \psi_{2,j}^n, \quad \psi_{N_x+1,j}^n = \bar{U}_{x,N_x,j}^n \psi_{N_x,j}^n, \\
\psi_{i,1}^n &= U_{y,i,1}^n \psi_{i,2}^n, \quad \psi_{i,N_y+1}^n = \bar{U}_{y,i,N_y}^n \psi_{i,N_y}^n.
\end{aligned} \quad (11)$$

The auxiliary fields U and L are updated at any (i,j) surface cell point by using the boundary condition $L_{i,j}^n = \exp(-ia_x a_y H)$, whatever the instant n .

Starting from some initial conditions for ψ and the auxiliary fields U , and upon using the TDGL Eqs. (9) and the boundary conditions (11), the new order parameter and the local magnetic field are determined. This process is repeated until a stationary state is achieved. Our procedure consists of starting from a certain value of H and then we ramp up the applied external field in small intervals of $\Delta H = 10^{-3}$. The stationary state found for a fixed value of H is then used as the initial condition for $H + \Delta H$. For the first value of H , the system is initialized at the Meissner state where $\psi_{i,j}^0 = 1$, $U_{x,i,j}^0 = 1$, $U_{y,i,j}^0 = 1$. We must emphasize that no *a priori* vortex configuration is assumed to determine $(\psi, \mathbf{A}, \mathbf{h})$. In other words, the applied magnetic field is increased slowly from zero up to the upper critical field where the superconductivity is completely destroyed. At each fixed applied field we follow the time evolution of the local magnetic field and the superconducting order parameter until we obtain a steady state solution. Then, this stationary solution is used as the initial condition for the next applied field. Thus, as the applied magnetic field increases and the time changes, we preserve the magnetic history of the system. That is, we study the time evolution of the system at each fixed applied magnetic field by assuming that there is already some penetrated magnetic flux inside the sample.

The Gibbs free energy and the magnetization are very sensitive to changes in the vortex configurations. So, any

physical relevant phenomenon should manifest into these quantities. The TDGL equations describe the gradient flow for the Gibbs free energy. Thus, in principle, the output of the TDGL should correspond to the global minimum of the energy of the system. The energy, in units of $G_0 = a_0^2 T_c^2 / b$, is given by

$$\begin{aligned}
G &= \frac{1}{V} \int \left[(1-T) |(-i\nabla - \mathbf{A})\psi|^2 + (1-T)^2 |\psi|^2 \left(\frac{1}{2} |\psi|^2 - 1 \right) \right. \\
&\quad \left. + \kappa^2 ((\nabla \times \mathbf{A})_z - H)^2 \right] dV.
\end{aligned} \quad (12)$$

The discrete version of this equations is

$$\begin{aligned}
G_n &= \frac{1}{N_x N_y} \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \left\{ \frac{(1-T)}{2} \left[\frac{|U_{x,i,j}^n \psi_{i+1,j}^n - \psi_{i,j}^n|^2}{a_x^2} \right. \right. \\
&\quad + \frac{|U_{x,i,j+1}^n \psi_{i+1,j+1}^n - \psi_{i,j+1}^n|^2}{a_x^2} + \frac{|U_{y,i,j}^n \psi_{i,j+1}^n - \psi_{i,j}^n|^2}{a_y^2} \\
&\quad + \frac{|U_{y,i+1,j}^n \psi_{i+1,j+1}^n - \psi_{i+1,j}^n|^2}{a_y^2} \left. \right] + \frac{(1-T)^2}{4} \left[|\psi_{i,j}^n|^2 \left(\frac{1}{2} |\psi_{i,j}^n|^2 \right. \right. \\
&\quad \left. \left. - 1 \right) + |\psi_{i+1,j}^n|^2 \left(\frac{1}{2} |\psi_{i+1,j}^n|^2 - 1 \right) + |\psi_{i,j+1}^n|^2 \left(\frac{1}{2} |\psi_{i,j+1}^n|^2 \right. \right. \\
&\quad \left. \left. - 1 \right) + |\psi_{i+1,j+1}^n|^2 \left(\frac{1}{2} |\psi_{i+1,j+1}^n|^2 - 1 \right) \right] + (h_{z,i,j}^n - H)^2 \left. \right\}. \quad (13)
\end{aligned}$$

The magnetization $4\pi M = B - H$, where B is the induction (the spatial average of the local magnetic field), is

$$-4\pi M_n = \frac{1}{N_x N_y} \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} h_{z,i,j}^n - H. \quad (14)$$

We calculate the energy and the magnetization at each instant n , although we are most interested in their values at the stationary state. The stationary state is accepted when the absolute value of the order parameter does not change within

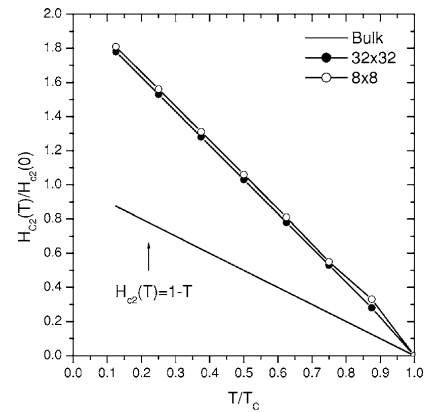


FIG. 1. The upper critical field for two superconducting square: S_1 (open circles); S_2 (filled circles), and bulk (solid straight line).

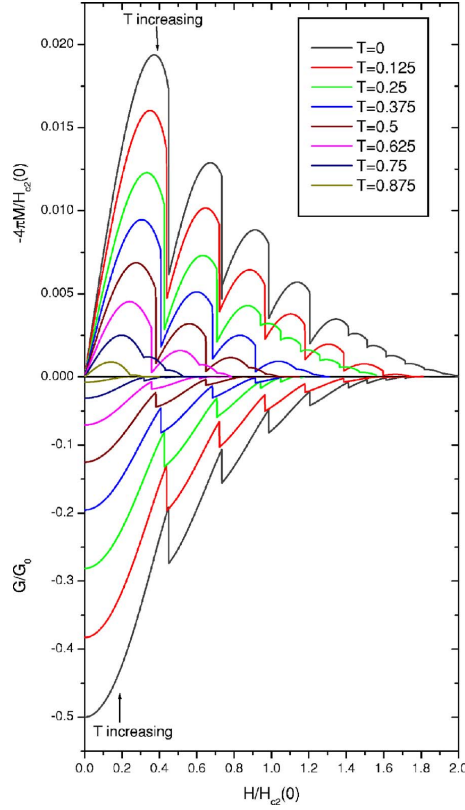
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FIG. 2. (Color online) The magnetization (upper graphics) and the energy (lower graphics) as functions of the applied external field for several values of temperature for the S_1 superconductor.

a certain precision. The highest difference $\|\psi_{i,j}^{n+1} - \psi_{i,j}^n\|$ we allowed was 10^{-5} over a few thousand time steps.

For each fixed value of field and instant n , the output data of Eqs. (9)–(11) were stored in matrices and visualized in order to observe the dynamics of the vortices. The visualization process allows us to see how many vortices are nucleating inside the sample as the applied magnetic field increases. However, a more reliable manner of counting the number of vortices can be found by integrating Eq. (4) along a rectangle containing the superconducting square. This leads us to

$$\oint \frac{1}{|\psi|^2} \Re[\bar{\psi}(-i\nabla - \mathbf{A})\psi] \cdot d\mathbf{r} = (2\pi N - \Phi), \quad (15)$$

where N is the number of vortices (vorticity) and Φ is the total penetrated flux. The discrete counterpart of this equation is

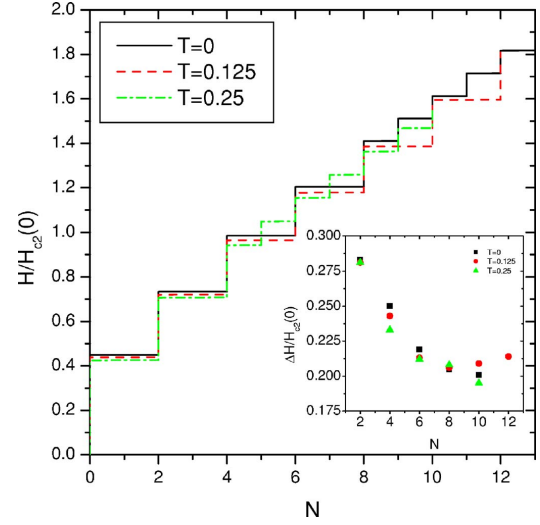


FIG. 3. (Color online) The applied magnetic field as a function of the number of vortices for three different temperatures. Inset: the values of applied magnetic field sufficient to change the vorticity from N to $N+2$, with N even.

$$\begin{aligned} N_n = & \frac{\Phi_n}{2\pi} + \frac{1}{2\pi} \sum_{i=1}^{N_x} \left\{ \frac{1}{|\Psi_{i,1}^n|^2} \Im[\bar{\psi}_{i,1}^n U_{x,i,1}^n \psi_{i+1,1}^n] \right. \\ & - \frac{1}{|\Psi_{i,N_y+1}^n|^2} \Im[\bar{\psi}_{i,N_y+1}^n U_{x,i,N_y+1}^n \psi_{i+1,N_y+1}^n] \Big\} \\ & + \frac{1}{2\pi} \sum_{j=1}^{N_y} \left\{ \frac{1}{|\Psi_{N_x+1,j}^n|^2} \Im[\bar{\psi}_{N_x+1,j}^n U_{y,N_x+1,j}^n \psi_{N_x+1,j+1}^n] \right. \\ & - \frac{1}{|\Psi_{1,j}^n|^2} \Im[\bar{\psi}_{1,j}^n U_{y,1,j}^n \psi_{1,j+1}^n] \Big\}, \end{aligned} \quad (16)$$

where, for instance,

$$|\Psi_{i,1}^n|^2 = \frac{1}{2} (|\psi_{i,1}^n|^2 + |\psi_{i+1,1}^n|^2). \quad (17)$$

Notice that (16) has not been derived in Refs. 10 and 11.

III. RESULTS AND DISCUSSION

In order to carry out the numerical simulations we have chosen two superconducting squares of parameter areas $S_1=8 \times 8$ and $S_2=32 \times 32$. The Ginzburg-Landau parameter used for both samples was $\kappa=5$, and $\beta=1$. Since the core size of the vortices diminishes as the temperature is lowered we have used two different meshes. For $T \geq 0.25$, a mesh with 32×32 cell points was sufficient to describe the detailed configuration of the vortices. Nevertheless, for lower temperatures we had to increase the number of cell points to 64×64 .

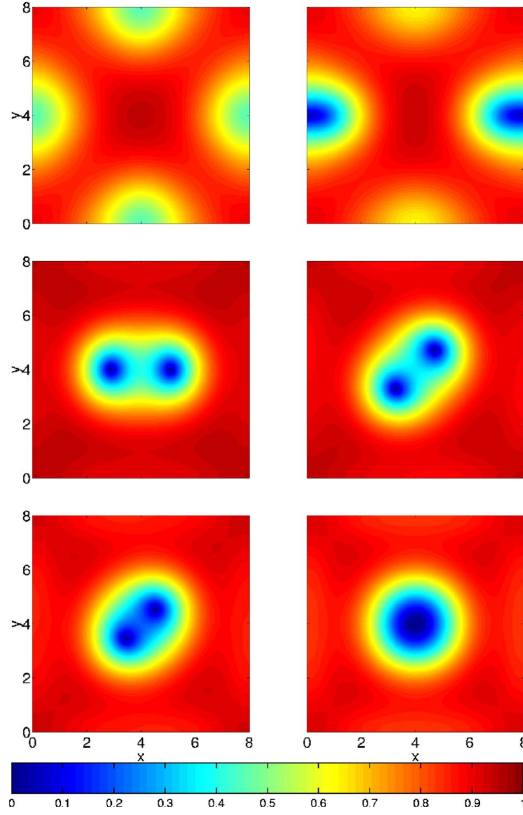


FIG. 4. (Color online) Sequence of pictures for the first phase transition in the S_1 superconductor at $T=0$; the sequence should be followed from the top to the bottom and from the left to the right. The colorbar indicates the magnitude of the order parameter.

A. The upper critical field

First of all, we calculated the upper critical field for the S_1 and S_2 superconductors. This result was useful in guiding us in which field window we had to work with in order to determine the other physical quantities. The criterion we have used for the total destruction of superconductivity is that at any (i,j) vertex point and instant n the magnitude of the order parameter $|\psi_{i,j}^n| < 10^{-4}$. We slowly increased the applied magnetic field and kept track of the converged solution of the TDGL equations. Once the above criterion was fulfilled the corresponding values of the applied magnetic field was the upper critical field. The results are shown in Fig. 1. Notice that within the mesoscopic regime, the $H_{c2}(T)$ curves do not change significantly with the surface area and they are both linear with respect to the temperature. To confirm that finite size effects are small we also have determined the upper critical field for $S_3=128 \times 128$ and $T=0.875$ and found no significant difference from S_2 . Considering the linear dependence seen in Fig. 1, it is safe to affirm that the

same is true for all temperatures. Figure 1 also shows the bulk values of $H_{c2}(T)$, which is roughly half of its typical values for the systems we have studied. This tell us that, even though the mesoscopic behavior has been well characterized, it is still very distant from the thermodynamic limit. Since computational limitations preclude us from arbitrarily increasing system size, we were not able to determine the frontier between the two regimes.

B. The energy and the magnetization

On using Eqs. (13) and (14) we have evaluated the energy and the magnetization respectively, for several values of temperature ranging from $T=0$ to $T=0.875$. From now on we will restrict ourselves to the S_1 superconductor. The results for the magnetization and energy curves as functions of the applied external field are depicted in Fig. 2. As can be seen, the energy exhibits a series of discontinuities. Each of these discontinuities signals a vortex entrance. We attribute these abrupt reductions in the energy to flux expulsion. This point

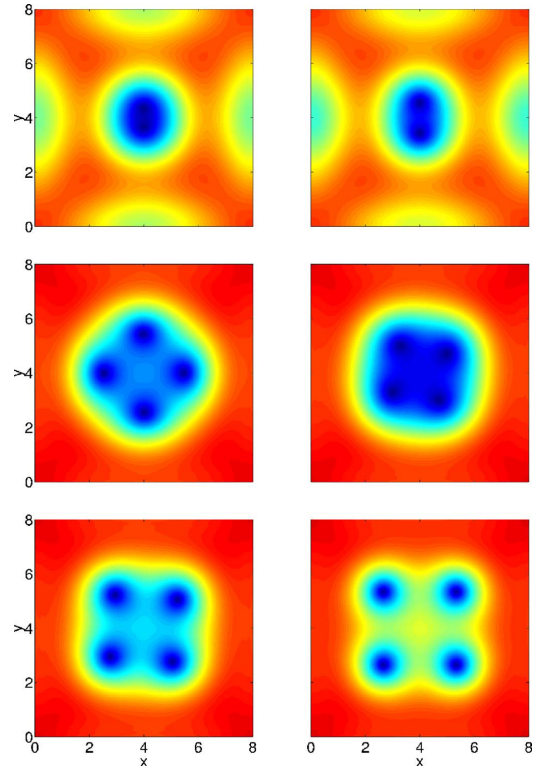


FIG. 5. (Color online) Sequence of pictures for the second phase transition in the S_1 superconductor at $T=0$; the sequence should be followed from the top to the bottom and from the left to the right. The magnitude of the order parameter is given by the colorbar of Fig. 4.

SARDELLA *et al.*PHYSICAL REVIEW B **74**, 014512 (2006)TABLE I. The vortex configurations we have observed for each fixed temperature for the S_1 superconductor; the minus sign indicates that no configuration was observed with the respective vorticity. The nomenclature used is explained in the text.

Vorticity	Temperature							
	0	0.125	0.25	0.375	0.5	0.625	0.75	0.875
1	—	—	—	—	—	—	1S	1S
2	$2S \rightarrow 1G_2$	$2S \rightarrow 1G_2$	$1G_2$	$1G_2$	$1G_2$	$1G_2$	$1G_2$	—
3	—	—	—	—	—	$1G_3$	—	—
4	4S	4S	4S	4S	4S	4S	—	—
5	—	—	5S	—	5S	—	—	—
6	$4S1G_2$	$4S1G_2$	$4S1G_2$	$4S1G_2$	$4S1G_2$	—	—	—
7	—	—	$4S1G_3$	$4S1G_3$	—	—	—	—
8	$4S1G_4$	$4S1G_4$	$4S1G_4$	$4S1G_4$	—	—	—	—
9	$4S1G_5$	—	$4S1G_5$	—	—	—	—	—
10	$4S1G_6$	$4S1G_6$	$4S1G_6$	—	—	—	—	—
11	$4S1G_7$	—	—	—	—	—	—	—
12	$4S1G_8$	$4S1G_8$	—	—	—	—	—	—
13	$4S1G_9$	—	—	—	—	—	—	—
14	$4S1G_{10}$	—	—	—	—	—	—	—
15	$4S1G_{11}$	—	—	—	—	—	—	—

will be better justified later on when we describe how the vortex motion occurs inside the sample.

We observed that for $T \leq 0.625$ the first vortex entrance always corresponds to a phase transition from $N=0$ to $N=2$ vortex state, and, similarly to the energy, the magnetization also decreases abruptly at the transition field. For $T \geq 0.75$ the energy also shows discontinuities as the applied field increases. Nevertheless, at the transitions the magnetization is continuous. In addition, only one vortex enters the sample at the first phase transition. This seems to be consistent with the fact that the dimension of the vortex tends to increase as we approach the critical temperature. So, there is less space available for the vortices to populate the sample. Notice that the field windows in which the magnetization is nonvanishing, vary with the temperature. At the zero temperature the system has the longest mixed state phase which is consistent with the phase diagram of Fig. 1. Furthermore, the magnetization does not scale with the temperature, that is, the behavior of this quantity is distinct for different temperatures.

For a fixed temperature, both the magnetization and the energy curves are composed of several field windows. Each window corresponds to a certain vorticity N . In Fig. 3 we illustrate the $N(H)$ curves calculated from Eq. (16) for lower temperatures; the inset of this figure shows the field window ΔH as a function of the vorticity N ; here ΔH represents the amount of applied magnetic field required to take the system from N to $N+2$ vortex state. As can be seen from these figures, the field window decreases as more vortices nucleate into the sample. However, ΔH has a weak dependence on the temperature.

The sequence of phase transitions does not follow the same pattern for different values of temperatures. In general, we have transitions either from N to $N+2$, or from N to $N+1$ vortex state. This may vary for different temperatures or even within a fixed temperature. To describe an N vortex

state we use the following nomenclature. We denote by $N_s S$, a multiple vortex configuration formed by N_s single vortices. A single giant vortex of vorticity N_g is denoted by $1G_{N_g}$; the constraint $N=N_s+N_g$ must be obeyed. For example, the $4S1G_2$ state is formed by four single vortices and a double quantized giant vortex. All vortex configurations are summarized in Table I. Although our magnetization curves are very similar to others presented in the literature,¹ it is necessary to emphasize that the simulations were performed considering the applied external field always increasing, and starting from the previous stationary state as the initial condition for the next value of H (see Sec. II for a detailed explanation). Some differences can be noticed. It can be immediately seen that the 4S state occurs for all temperatures $T \leq 0.625$. For T not too close to the critical temperature, the $1G_2$ state always exists. However, for lower temperatures ($T \leq 0.125$), once two vortices penetrate the sample, first they form a $2S$ state. Next, there is a smooth transition to a $1G_2$ state. This transition is not manifested in the magnetization since there is no change in the vorticity, but only in the vortex arrangement. Notice that this particular scenario is highlighted in Table I. Also, the 1S and 5S states seem to occur less frequently. It can also be noticed that, different from other works,¹ the $N=2$ state is always observed as $1G_2$. Another important result obtained in our simulations is that the 4S state is observed to temperatures up to $T \leq 0.625$, without the evolution from MVS to GVS.

C. The vortex configurations

For all values of the applied magnetic field and between regular intervals of n , the magnitude of the order parameter and the local magnetic field were stored in matrices which were used to generate the time evolution of the vortex configurations. It must be stated that the sequence of figures

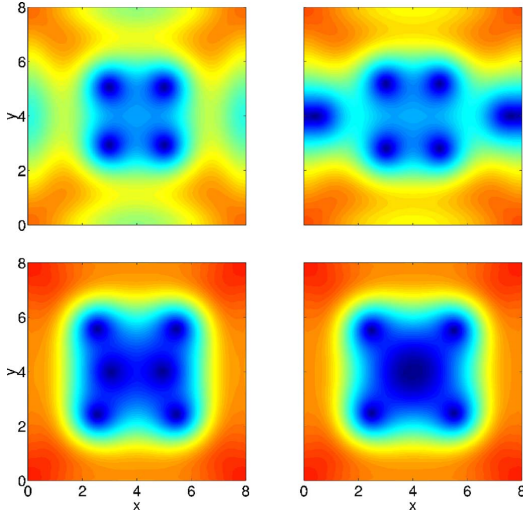


FIG. 6. (Color online) Sequence of pictures for the third phase transition in the S_1 superconductor at $T=0$; the sequence should be followed from the top to the bottom and from the left to the right. The magnitude of the order parameter is given by the colorbar of Fig. 4.

shown hereafter do not necessarily represent a collection of stationary states. To illustrate how the vortices evolve in time, first we chose the $T=0$ case. In Fig. 4, the phase transition from the Meissner to the $N=2$ state is presented. First, there are four vortices trying to nucleate at the surfaces, but only two will succeed to enter the sample, and the other two are driven out. This explains the reduction in the value of the free energy as we have stressed previously. Once the two vortices have completely penetrated the sample, they form a $2S$ state aligned as shown in Fig. 4. Next, they will try to align along the square diagonal. Since this configuration is double degenerated, they stay in a significant range of applied magnetic field aligned perpendicular to the vertical sides of the square, before they go to the square diagonal. As the applied external field increases, the vortices will slowly rotate until they are along the square diagonal. Such a result was also found by Mel'nikov *et al.*⁷ In their work, the vortices also accommodate in the diagonal configuration. However, since we follow the time evolution, we were able to notice that the $2S$ configuration collapses into a $1G_2$ state. This also occurs for $T=0.125$, although in a smaller field window. Otherwise, for the values of $0.25 \leq T \leq 0.625$, the $1G_2$ state is formed straightway, that is, no additional applied field is required to collapse into this state after the phase transition occurs.

In opposition to the situation described above, all the phase transitions we sketch below occurs at a fixed applied magnetic field.

Now we discuss the phase transition $1G_2 \rightarrow 4S$, which occurs for a wide range of temperature (see Fig. 5). Initially, there are four vortices trying to nucleate at the surface. As in the previous case described above, only two vortices can

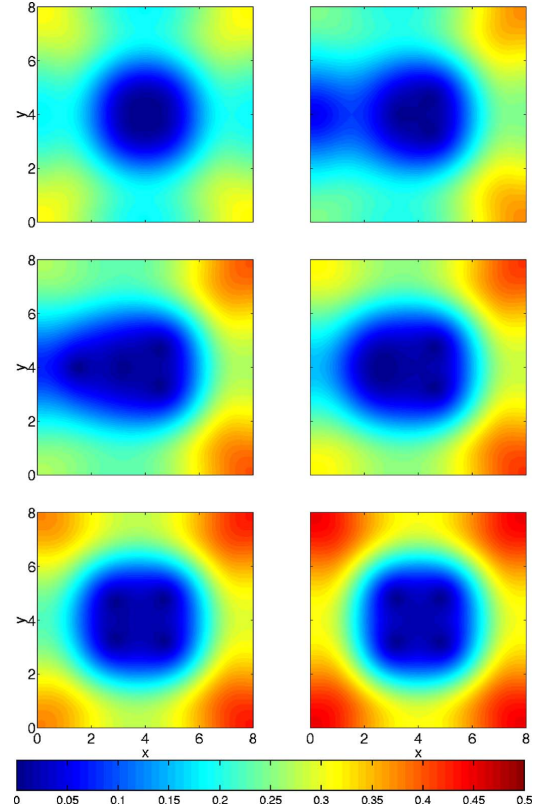


FIG. 7. (Color online) Sequence of pictures for the second phase transition in the S_1 square superconductor at $T=0.625$; the sequence should be followed from the top to the bottom and from the left to the right. The colorbar indicates the magnitude of the order parameter.

enter the sample. While these two vortices are moving toward the center, the giant vortex in the center is breaking off. Just after the two new vortices have completed penetrating the sample, the $4S$ state is created forming a square. Then, they will rotate in order to fit into the sample. We have found that this rotation occurs very rapidly until the $4S$ state stabilizes. Notice that while the $4S$ square is rotating, the vortices keep moving forward and then backward.

Let us show how the phase transition $4S \rightarrow 4S1G_2$ takes place (see Fig. 6). Similar to the previous situations, among four vortices, two move back and the other two enter the sample. The two new vortices will pass through the $4S$ square and collapse at the center of the superconducting square and, consequently, a $1G_2$ state is formed.

As can be seen from Table I, the state $3S$ was not observed. This is in agreement with the work of Mel'nikov *et al.* In fact, they constructed the state $N=3$, either considering a $4S$ state plus an antivortex at the center of the square or a single $3S$ state with a broken symmetry caused by a defect.

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Finally, it is interesting to describe a quite unique phase transition $1G_3 \rightarrow 4S$, which happens only at $T=0.625$ (see Fig. 7). In this case, only one vortex is able to enter the sample. Once it is inside the superconductor, the $1G_3$ state will break off into a triangle-like $3S$ state. The inner vortex of the $3S$ state collides with the penetrated vortex, coming from the left-hand side of the square superconductor. Just after the collision, they move to the vertices of a square ($4S$) which fits into the sample.

In Ref. 12 we have provided animations which describe the vortex motions from the beginning of the Meissner phase until the superconductivity is completely suppressed for all temperatures.

IV. SUMMARY

We have solved numerically the TDGL equations for a square mesoscopic superconductor by using the ψ - U method.

Our implementation of the algorithm provides all possible configurations of the vortices for a wide range of temperatures. Furthermore, our approach makes it possible to observe the time evolution of the vortex configurations, that is, we have been able to see how GV and MV states are formed and how the transitions from GV into MV states (and vice versa) may occur. We also have demonstrated that the temperature has a crucial role in the formation of these states. In spite of some slight differences, our results agree well with previous works.^{1,6} Perhaps these differences may be attributed to the different geometry and the parameters used.

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¹²See <http://www.fc.unesp.br/superconductores>

5.2 Vortex-antivortex annihilation dynamics in a square mesoscopic superconducting cylinder (aqui)

Neste trabalho, novos pesquisadores apareceram como meus colaboradores, os Professores [Clécio Clemente de Souza Silva](#) e [Leonardo Ribeiro Eulálio Cabral](#), ambos da UFPE. Todas as simulações foram por mim conduzidas. Os demais colaboraram com a escrita do artigo, resposta aos relatores do Physical Review, dentre outras tarefas relevantes.

Normalmente a colisão entre vórtices e anti-vórtices (v-av) é produzida em supercondutores por aplicação de campo elétrico (injeção e ejeção de uma corrente de transporte através de dois eletrodos simetricamente posicionados no filme). Do ponto de vista teórico, este estudo foi primeiramente conduzido no trabalho pioneiro de Andronov e outros [37] e investigado em mais detalhes na referência [38]. Até então, as investigações de correntes críticas eram conduzidas em fios supercondutores finos [30, 31]. Os pares v-av alcançam a velocidade de 10^5 m/s, duas ordens de grandeza maior que a velocidade de um vórtice de Abrikosov. Devido a esta alta velocidade eles não mantêm a forma circular. São alongados e muitas vezes comparados com um *phase slip line*, embora ambos os vórtices carregam uma singularidade da fase (*vortex core*). Este par v-av é comumente chamado de *vórtice cinemático*. Posteriormente à previsão de Andronov, eles foram observados experimentalmente em um filme fino de Sn [39]. O nosso trabalho é uma proposta de estudo dos pares v-av magneticamente ativados, criados apenas por meio de aplicação de campo magnético, embora na época não tínhamos conhecimento da referência [37]. O trabalho de Berdiyorov [38] foi publicado quase que simultaneamente ao nosso. O resultado para a velocidade dos pares v-av são exatamente iguais. A proposta é de criar artificialmente um defeito no interior de um filme e aplicar campo magnético. Então, construímos o laço de histerese completo. Quando há fluxo retido no defeito, no ramo negativo da curva $M \times H$, o anti-vórtice que penetra dentro da amostra irá se colidir com o vórtice preso no defeito. Num trabalho mais recente, fizemos um mapeamento completo de quando as colisões ocorrem dentro do feito, na região supercondutora, ou se ainda não há aniquilação do par v-av. Isto depende do tamanho da amostra e da temperatura. Efeitos de dissipação de calor na colisão também foram estudados [40]. Este artigo foi escolhido como capa do fascículo 40, volume 29, de 2017 da revista *Journal of Physics: Condensed Matter*.

PHYSICAL REVIEW B **80**, 012506 (2009)**Vortex-antivortex annihilation dynamics in a square mesoscopic superconducting cylinder**Edson Sardella,¹ Paulo Noronha Lisboa Filho,¹ Clécio C. de Souza Silva,²Leonardo Ribeiro Eulálio Cabral,² and Wilson Aires Ortiz³¹*Departamento de Física, Faculdade de Ciências, UNESP—Universidade Estadual Paulista, Caixa Postal 473, 17033-360 Bauru, SP, Brazil*²*Departamento de Física, Universidade Federal de Pernambuco, 50670-901 Recife, PE, Brazil*³*Departamento de Física, Universidade Federal de São Carlos, 13565-905 São Carlos, SP, Brazil*

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The dynamics of the annihilation of a vortex-antivortex pair is investigated. The pair is activated magnetically during the run of a simulated hysteresis loop on a square mesoscopic superconducting cylinder with an antidot inserted at its center. We study the nucleation of vortices and antivortices by first increasing the magnetic field, applied parallel to the axis of the sample, from zero until the first vortex is created. A further increase in the field pulls the vortex in, until it reaches the antidot. As the polarity of the field is reversed, an antivortex enters the scene, travels toward the center of the sample, and eventually the pair is annihilated. Depending on the sample size, its temperature, and Ginzburg-Landau parameter, the vortex-antivortex encounter takes place at the antidot or at the superconducting sea around it. The position and velocity of the vortex and antivortex singularities were evaluated as a function of time. The current density, magnetization, and order-parameter topology were also calculated.

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PACS number(s): 74.78.Na, 74.20.De, 74.25.-q

Achieving a deep understanding of the nucleation and propagation of vortices in real superconductors is a truly complex task, since these entities interact with almost everything: first, with the surface of the specimen, to surpass it; upon entrance, with other vortices that might have already penetrated, and also with defects, which might attract them and even act as pinning centers. Additional difficulties to emulate the problem arise from the fact that vortices generate heat while propagating, what can be harmful to the robustness of the superconducting properties, if not catastrophic, as is the case of vortex avalanches observed in some superconducting films.^{1–6} It is quite common, however, that the existence of pinning potentials represent a beneficial feature, since vortices can thus be prevented from undergoing dissipative motion. An interesting approach to the problem, which enables one to address most specificities without excessive complexity, is to work in the small universe of mesoscopic samples. In such an ambient, one can accommodate the essential ingredients: relatively important surface-to-volume ratio, only a few vortices on scene, and a number of defects—the so-called antidots—usually arranged in a regular pattern. Furthermore, one can study the interaction of an individual vortex-antivortex (V-AV) pair and, eventually, witness their mutual annihilation.

Recently, there have been many studies about V-AV configurations in mesoscopic superconductors (see for instance Refs. 7–11). The authors of these references have found that vortices and antivortices may coexist in equilibrium in configurations which look like a V-AV molecule. A somewhat common approach is to assume an *a priori* configuration and minimize the free energy in terms of some relevant parameter for which the V-AV molecule is a stable configuration. Here, we will focus in a rather different approach concerning more with the dynamics of a V-AV encounter. The aim of the present work is to elucidate the details involved in the process of creation of pairs, following their time evolution and ultimate disappearance. We opted to do this making no use of

a priori assumptions regarding symmetries, but simply varying the applied magnetic field, allowing for the spontaneous nucleation of a vortex and, cycling the field, of an antivortex, which form a pair of interacting entities, whose subsequent time evolution is monitored.

In this Brief Report we present the dynamics of the annihilation of a V-AV pair activated magnetically during a short hysteresis loop. The geometry we consider is a square mesoscopic superconducting cylinder with an antidot placed at its center. Simulations are made in the presence of an applied magnetic field parallel to the axis of the cylinder. We study the nucleation of vortices and antivortices by first increasing the magnetic field from zero until the first vortex is created. The field was then decreased toward negative values. During this process the vortex travels heading the center of the sample, is trapped by the antidot and is then annihilated by an antivortex as the polarity of the applied field is reversed. To monitor the whole process, we evaluate the position and velocity of the vortex and antivortex singularities as a function of time. We also calculate the order-parameter topology, the current density, and the magnetization. In order to follow the dynamics of the physical quantities we use the gauge-invariant time-dependent Ginzburg-Landau (TDGL) equations. These equations describe the time evolution of the complex order parameter ψ and the vector potential $\mathbf{A}$, which is related to the local magnetic field through the expression $\mathbf{h} = \nabla \times \mathbf{A}$. In dimensionless units these equations are given by

$$\begin{aligned} \left(\frac{\partial}{\partial t} + i\phi \right) \psi &= -(-i\nabla - \mathbf{A})^2 \psi + (1 - T)\psi(1 - |\psi|^2), \\ \beta \left(\frac{\partial \mathbf{A}}{\partial t} + \nabla \phi \right) &= \mathbf{J}_s - \kappa^2 \nabla \times \mathbf{h}, \end{aligned} \quad (1)$$

where the supercurrent density is

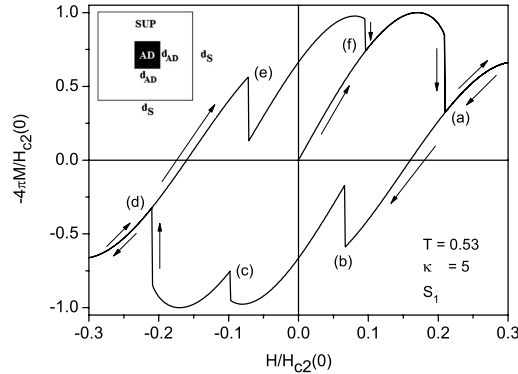


FIG. 1. The magnetization curve normalized to its maximum value as a function of the external applied magnetic field. The meaning of the points marked in the figure are explained in the text. The arrows indicate the direction of the hysteresis loop. The inset illustrates the geometry of the problem.

$$\mathbf{J}_s = (1 - T)\Re[\psi^*(-i\nabla - \mathbf{A})\psi]. \quad (2)$$

Here, the distances are measured in units of the coherence length at zero temperature $\xi(0)$; the magnetic field is in units of the upper critical field at zero temperature $H_{c2}(0)$; the temperature is in units of the critical temperature T_c ; the time is in units of the characteristic time $t_0 = \pi\hbar/8K_B T_c$; κ is the Ginzburg-Landau parameter; β is the relaxation time of the vector potential and is related to the conductivity; and ϕ is the scalar potential. Notice that Eqs. (1) and (2) are gauge invariant since they do not change under the transformation $\bar{\psi} = \psi e^{i\chi}$, $\bar{\mathbf{A}} = \mathbf{A} + \nabla\chi$, and $\bar{\phi} = \phi - \partial\chi/\partial t$. We choose the zero-scalar potential gauge, that is, $\bar{\phi} = 0$ at all times. We have solved the TDGL equations upon using the link-variables method.^{13–15} Since we consider invariance of the system along the z direction, our approach could only be applied to a square mesoscopic superconducting cylinder. However, it might also be used for a very thin superconducting film of thickness d , provided that the effective penetration length $\Lambda = 2\lambda^2/d$ is larger than the lateral dimensions L of the film.^{16,17} In this scenario, the z component of the magnetic field outside the film is nearly the same as the applied magnetic field, so the demagnetization factor can be neglected. The dimensions of the samples used in the present work are within this limit.¹⁸ The geometry we have considered is depicted at the top left corner of Fig. 1: the lateral sizes are d_S for the sample and d_{AD} for the antidot.

For the study presented in this paper, the relaxation time is kept fixed at $\beta = 1$. The GL parameter was also maintained at $\kappa = 5$. For $T = 0.53$, Fig. 1 shows a short hysteresis loop which was made for a mesoscopic superconducting square (hereafter referred to as sample S_1) of dimensions $d_S = 12$, with a small antidot at the center, with size $d_{AD} = 2$. Points marked with letters, (a), ..., (f), indicate the values of H where a vortex (antivortex) either enters or exits the sample. The magnetic field is increased from zero until a value somewhat above that at which the first two vortices penetrate in

(a). It is then reversed until the opposite value is achieved and then reversed once more. At point (d), two antivortices penetrate the superconductor. Points (b) and (e) correspond to the exit of a vortex and an antivortex, respectively, immediately after which one flux quantum still remains in the antidot. The point we will be mainly focusing on is (c) [or, equivalently, (f)]. This point corresponds to the entrance of an antivortex, which will encounter a vortex trapped in the antidot. The V-AV pair will annihilate either inside or outside the antidot.

We have made a systematic study of the V-AV annihilation process, varying the experimentally accessible relevant parameters: T , d_S , and d_{AD} . The other parameters were kept fixed as specified above.

We turn now into a brief discussion of our results. First, we found that for d_S and d_{AD} fixed, the V-AV annihilation occurs at a limited temperature interval. Above the upper limit of such interval, the vortex trapped at the antidot leaves the sample before the entrance of the antivortex, and no collision can possibly occur. For the sample S_1 this upper threshold is somewhat above $T = 0.53$. As a matter of fact, since the penetration length increases as the temperature approaches T_c , the supercurrent density associated with the pinned vortex spreads to distances large enough to reach the external border of the sample. This enhances an attractive interaction between the surface and the trapped vortex, facilitating its escape.

At a given temperature, there is a minimum width of the superconducting frame to allow for a V-AV collision outside the antidot. For example, for $T = 0.23$ and $d_{AD} = 2$ the minimum size of the frame¹⁹ is 6 (these dimensions define sample S_2 : $d_S = 8$ and $d_{AD} = 2$). Our reasoning is as follows: the antivortex nucleated at the external border is kept pinned by the surface barrier at the external border while, in turn, the vortex remains pinned at the antidot. Both entities attract each other and the interaction is larger for smaller superconducting frames. It is then easier to pull the vortex out of the antidot for shorter distances. On the other hand, if the superconductor width is increased, the antivortex starts its excursion toward the center before the V-AV attraction becomes appreciable. Being thus less anchored by the surface, the antivortex travels all the way to the antidot and the annihilation process completes there. In support to this argument, Fig. 2 depicts the values of the x component of the supercurrent density at the surfaces $y = 12$ and $y = 8$ for both samples S_1 and S_2 , respectively. These values of J_{sx} were calculated in the absence of applied field, $H = 0$, and thus represent the supercurrent due *only* to the vortex inside the antidot. The V-AV attraction (Lorentz force) will be proportional to J_{sx} . Notice that, for both samples, the absolute value of J_{sx} is maximum at the center of the square edge. One can clearly see that, in the middle of the sample edge, $x = d_S/2$, the intensity of the Lorentz force is larger for the sample S_2 than for S_1 .

Figure 3 shows the dynamics of the V-AV collision for the sample S_1 at $T = 0.53$. Immediately after entering the sample, only the antivortex is in the superconducting sea. As it moves forward to the antidot, at some instant the trapped vortex will come out and both will collide and annihilate.

Another interesting characteristic we have found was that

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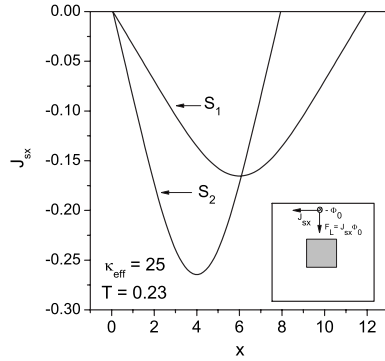
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FIG. 2. The supercurrent density along the top surface of the superconductor. The parameters used are specified in the figure. The inset shows the Lorentz force on the antivortex due to the vortex in the antidot.

as the antivortex penetrates, its interaction with the vortex is so strong that both appear entirely deformed. Usually, vortices look like a composition of core surrounded by whirling supercurrents. However, when the vortex and the antivortex approach one another while still partially pinned at the corresponding surfaces, they become elongated, as if squashed, and form a narrow channel between the external surface and the antidot. This can be seen in Fig. 4, which represents the topology of the order parameter ψ and the supercurrent distribution at the very moment when the collision takes place for the sample S_1 at $T=0.53$. Very recently, Gurevich and

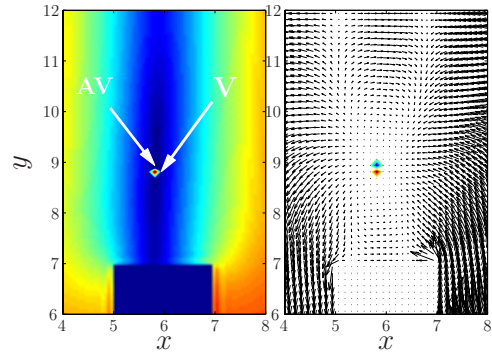


FIG. 4. (Color online) The absolute value of the order parameter (left) and the supercurrent distribution (right) for the sample S_1 ; very dark color means order parameter is very depreciated. The size of the arrows (right) are not real; they were enlarged for better viewing.

Ciovati²⁰ have studied a V-AV collision in a semi-infinite sample in the context of rf fields. However, they were not able to observe the dramatic deformation of the V-AV cores since their analysis is based on rigid circular-shaped vortex cores.

We also have estimated the instantaneous velocity of the vortex on its way from nucleation at the surface through its capture by the antidot [point (a) of Fig. 1]. In addition, the velocities of both the antivortex entering the sample and that of the vortex exiting the antidot, on their route to annihilation

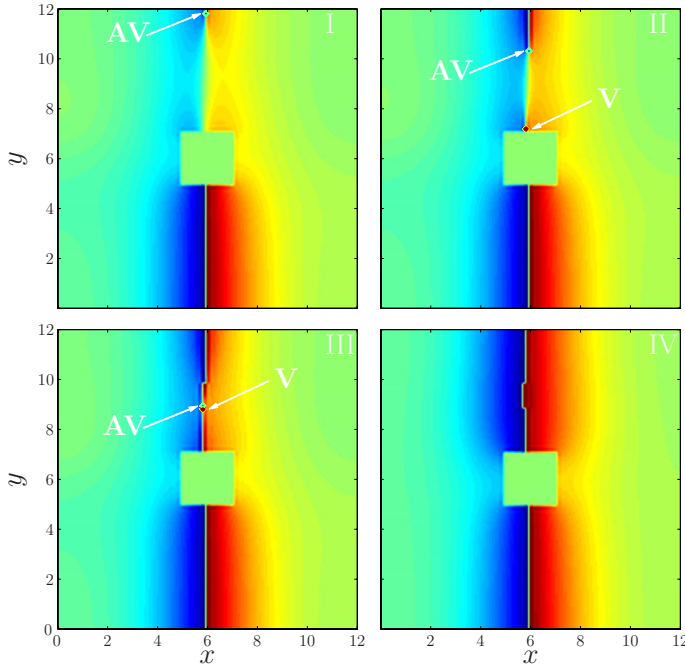


FIG. 3. (Color online) The pictures show the topological shape of the phase of the order parameter; the phase goes from $-\pi$ (blue/dark gray) to π (red/mid gray). The last picture (IV) corresponds to the stationary state of point (c) of the hysteresis loop of Fig. 1.

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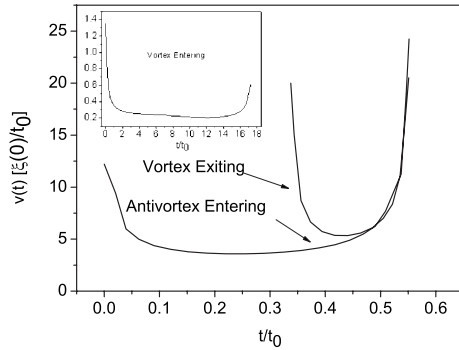
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FIG. 5. The modulus of the velocity of the vortex and the antivortex for the sample S_1 at $T=0.53$ as a function of time [point (c) of Fig. 1]; the inset corresponds to point (a).

[point (c) of Fig. 1], were also determined. The results are shown in Fig. 5. It is clearly seen that the velocities achieved during the collision process are much larger than those of a vortex penetrating the sample (at least one order of magnitude, as shown in the inset).

As we have observed previously, during the V-AV collision the order parameter is very small along a straight line but is zero only at two distinct points. The oscillations of the order parameter connected by these two singularities are usually called *kinematic vortices* and it was proposed in Ref. 21 and experimentally observed by Sivakov *et al.*²² In this last reference it was estimated that a kinematic vortex can achieve a velocity $v_{kv} \approx 10^5$ m/s which is two orders of

magnitude higher than the velocity of an Abrikosov vortex $v_{Av} \approx 10^3$ m/s. On the other hand, the velocity of a kinematic vortex is two orders of magnitude smaller than that of a Josephson vortex $v_{Jv} \approx 10^7$ m/s. For the sample S_1 , the window during which the antivortex remains visible is $\Delta t = 0.5517t_0$ and the distance it travels is $\Delta y = 2.875\xi(0)$; inserting $T_c = 3.72$ K and $\xi(0) = 230$ nm (the relevant parameters for Sn, which were used by Sivakov *et al.*²²), the average velocity is $v_{AV} = 1.5 \times 10^5$ m/s. On the other hand, for the vortex exiting the antidot we obtain $\Delta t = 0.2135t_0$ and $\Delta y = 1.625\xi(0)$; which gives $v_{Vs} = 2.2 \times 10^5$ m/s. Thus, the velocities involved in the annihilation process are very similar to those of kinematic vortices. It is worth noticing that the large velocities anticipated for the V-AV pair along the collision process, are similar to those developed during the early stage of a vortex avalanche, as observed by the authors of Ref. 6, who reported velocities as large as 1.8×10^5 m/s for avalanches in YBCO films. Very recently, Berdiyrov *et al.*²³ have investigated the activation of a kinematic vortex by using a transport current along a superconducting stripe, obtaining experimental results very close to our estimates.

For the vortex first entering the antidot we found an average velocity slightly larger than that for a regular Abrikosov vortex: $\Delta t = 17.2792t_0$, and $\Delta y = 4.125\xi(0)$, which yields $v_{Ve} = 6.8 \times 10^3$ m/s. This somewhat larger value—although in the same order of magnitude—might be attributed to the additional attraction exerted by the antidot.

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5.3 Vortices in a mesoscopic superconducting disk of variable thickness [\(aqui\)](#)

Este trabalho resultou de uma colaboração com o Professor [Ernest Helmut Brandt](#), fruto de uma visita dele a Bauru e São Carlos ao final de 2008. Infelizmente esta colaboração não prosperou, não por falta de vontade das partes mas sim pela infelicidade do Helmut ter adoecido no início de 2011 e falecido em setembro do mesmo ano. Tivesse ele sobrevivido, não tenho dúvidas de que ele seria um dos coautores de um artigo que publicamos em 2013 [\[42\]](#). O referido trabalho, que foi tema da tese de mestrado de meu aluno, Fábio Rogeri, era uma extensão de um estudo feito pelo Helmut com geometria SQUID [\[43, 44\]](#).

No trabalho em tela investigamos as configurações de vórtices em discos supercondutores mesoscópicos levando em conta a rugosidade da superfície. Mostramos que a variabilidade da superfície pode ser um dificultador para a observação de vórtices gigantes [\[45\]](#).

Vortices in a mesoscopic superconducting disk of variable thickness

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Abstract

In this paper we study the formation of vortices in a mesoscopic superconducting disk of thickness equal to or of the same order as the coherence length $\xi(T)$. The roughness of the lower and upper surfaces of the disk is taken into account. We also compute the total induced current and the magnetization for the disk in the presence of an external applied magnetic field.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In the last two decades mesoscopic superconducting structures have been widely studied from both experimental and theoretical points of view. The critical superconducting current density can be largely enhanced for samples of small size comparable to the coherence length and the London penetration length. The vortex configurations on mesoscopic samples can be strongly influenced by their geometry. In addition, a giant vortex state can occur in very confined geometries [1]. This is most unusual since the interaction between vortices is repulsive.

In superconducting films, defects such as magnetic dots, twin boundaries, and variable thickness, are always present and they can act as pinning centers. In this paper we will study the effects of surface roughness in the formation of vortices and how it influences the induced superconducting current for a disk geometry. To this end, we use the time dependent Ginzburg–Landau (TDGL) equations.

This paper is organized as follows. In section 2 we adapt the theoretical formalism of the TDGL equations for a disk of variable thickness. In section 3, a numerical algorithm is proposed in order to solve the TDGL equations for a disk of variable thickness. In section 4 we present the main results of this work and discuss them.

2. The theoretical formalism

Many phenomena in superconductivity can be described by the TDGL equations. These are a set of two equations

which couples the order parameter ψ and the vector potential $\mathbf{A}$, which are the two fundamental quantities describing the superconducting state. The superconducting electronic density of Cooper pairs is given by $|\psi|^2$ and the local magnetic field profile is obtained through $\mathbf{h} = \nabla \times \mathbf{A}$. The nondimensional version of these equations is given by

$$\begin{aligned} \left(\frac{\partial}{\partial t} + i\phi \right) \psi &= -(-i\nabla - \mathbf{A})^2 \psi + \psi(1 - |\psi|^2), \\ \beta \left(\frac{\partial \mathbf{A}}{\partial t} + \nabla \phi \right) &= \mathbf{J}_s - \kappa^2 \nabla \times \mathbf{h}, \end{aligned} \quad (1)$$

where the supercurrent density is

$$\mathbf{J}_s = \text{Re}[\bar{\psi}(-i\nabla - \mathbf{A})\psi]. \quad (2)$$

The boundary conditions are

$$\begin{aligned} \hat{\mathbf{n}} \cdot (-i\nabla - \mathbf{A})\psi &= 0, & \text{on } \partial\Omega, \\ \nabla \times \mathbf{A} &\rightarrow \mathbf{H}_0, & \text{as } |\mathbf{r}| \rightarrow \infty, \end{aligned} \quad (3)$$

where $\mathbf{H}_0$ is the external magnetic field which is applied uniformly; Ω is the domain occupied by the superconducting material and $\hat{\mathbf{n}}$ is a unit vector outward normal to the superconductor–vacuum interface $\partial\Omega$.

Here, the distances are measured in units of the coherence length $\xi(T)$ which depends on the temperature T ; the magnetic field is in units of the upper critical field $H_{c2}(T)$; the time is in units of the characteristic time $t_0 = \pi\hbar/8K_B T_c$ [2]; $\kappa = \lambda(T)/\xi(T)$ is the Ginzburg–Landau parameter; β is the

relaxation time of the vector potential; the Ginzburg–Landau parameter is $\kappa = \xi(T)/\lambda(T)$, where $\lambda(T)$ is the London penetration depth; and the symbol Re denotes the real part of a complex function. Notice that equations (1) and (2) are gauge invariant since they do not change under the transformation $\bar{\psi} = \psi e^{i\chi}$, $\bar{\mathbf{A}} = \mathbf{A} + \nabla\chi$, $\bar{\phi} = \phi - \partial\chi/\partial t$. We choose the zero-scalar potential gauge, that is, $\bar{\phi} = 0$ at all times.

It is well known that superconductors are divided into two types. The first type, type-I superconductors, for which $\kappa < 1/\sqrt{2}$, expel magnetic flux until the applied field reaches a certain value. Once the magnetic field exceeds this critical value, the superconductor returns to its normal state. It was first demonstrated by Abrikosov [3] that there is another class of superconducting materials, type-II superconductors, for which $\kappa > 1/\sqrt{2}$. They allow entry of magnetic flux, though in localized form, when an external magnetic field is applied. That is, we have a coexistence of both normal and superconducting domains. The penetration of magnetic flux occurs in the form of quantized flux lines. Each line consists of a normal core surrounded by circulating superconducting currents, the so-called vortex. Although it was already known a long time ago, it was rigorously demonstrated by some mathematical works [4–6] that for a very thin superconducting film of thickness $\epsilon \leq \xi(T)$ (in real units), the vortex state may be present even in a type-I superconductor. Therefore, even type-I materials will exhibit vortex configurations when they are in the form of a thin film. Within this limit, the solution of the TDGL equations can be strongly simplified, as will be seen later on. The simplifications of [4–6] were extended to the situation in which $\xi(T) \ll \epsilon \ll \lambda(T)$ (in real units) where the London theory can be applied to describe the vortex state [7]. Here, we will work on the former limit of film thickness.

Let a thin superconducting film domain be given by $\Omega_\epsilon = \{(x, y, z) \in \mathbb{R}^3 : (x, y) \in \Omega_0, |z| < \epsilon g(x, y)\}$, where the function $0 < g(x, y) \leq 1$ for all $(x, y) \in \Omega_0$. According to [4–6], to leading order in ϵ the TDGL equations can be reduced to

$$\begin{aligned} \eta \frac{\partial \psi}{\partial t} &= -\frac{1}{g}(-i\nabla - \mathbf{A}_0) \cdot g(-i\nabla - \mathbf{A}_0)\psi \\ &\quad + (1 - T)\psi(1 - |\psi|^2), \quad \text{in } \Omega_0, \\ \hat{\mathbf{n}} \cdot (-i\nabla - \mathbf{A}_0)\psi &= 0, \quad \text{on } \partial\Omega_0, \end{aligned} \quad (4)$$

where, to leading order, the magnetic field is nearly uniform inside the superconductor, that is, $\mathbf{H}_0 = \nabla \times \mathbf{A}_0$. As was proven in [5], equations (4) are good approximations for the superconducting film as long as the condition $\epsilon\xi(T)/\lambda^2(T) \ll 1$ ($\epsilon/\kappa^2 \ll 1$ in our units) is fulfilled. Small corrections to the stray fields have been derived in [5]. Although important, these corrections will not strongly influence the behavior of ψ . So, for the determination of the order parameter, we consider the magnetic field to be uniform everywhere. In fact, Brandt [8] has recently demonstrated that in the limit $\lambda^2(T)/\epsilon a \geq 1$, where a is the half-width of the sample, the magnetization may often be disregarded, that is, the average magnetic field inside the sample is almost equal to the external applied field H_0 . Our choice of parameters will be such that these inequalities are satisfied.

The TDGL equations have been very useful for simulating how vortices can be arranged as an external magnetic field (either abruptly or adiabatically increased) is applied to a superconductor below its critical temperature. Since equations (1) do not have exact solutions, many discretization algorithms have been devised for solving the TDGL equations numerically. One of the most popular approaches is the gauge invariant link variables method (see for instance [9, 10]). In [11], this method was generalized to circular geometries, which will be very useful in our numerical simulations. We will adapt equations (4) to circular geometries, so that we can use them to solve the problem of vortices in a mesoscopic superconducting disk of variable thickness.

To continue, it is now convenient to introduce the auxiliary vector field $\mathbf{U} = (\mathcal{U}_\rho, \mathcal{U}_\theta)$ in polar coordinates, which is defined by

$$\begin{aligned} \mathcal{U}_\rho(\rho, \theta) &= \exp\left(-i \int_{\rho_0}^{\rho} A_{0\rho}(\theta, \xi) d\xi\right), \\ \mathcal{U}_\theta(\rho, \theta) &= \exp\left(-i \int_{\theta_0}^{\theta} A_{0\theta}(\xi, \rho) \rho d\xi\right), \end{aligned} \quad (5)$$

where (ρ_0, θ_0) is an arbitrary reference point. For the sake of brevity we did not write here the time dependence on the fields.

Also, for brevity, let us denote $\mathbf{D} = -i\nabla - \mathbf{A}_0$. Thus, we can notice that

$$\frac{\partial \mathcal{U}_\rho}{\partial \rho} = -iA_{0\rho}\mathcal{U}_\rho, \quad \frac{1}{\rho} \frac{\partial \mathcal{U}_\theta}{\partial \theta} = -iA_{0\theta}\mathcal{U}_\theta, \quad (6)$$

and that

$$D_\rho \psi = -i\bar{\mathcal{U}}_\rho \frac{\partial(\mathcal{U}_\rho \psi)}{\partial \rho}, \quad D_\theta \psi = -i\frac{\bar{\mathcal{U}}_\theta}{\rho} \frac{\partial(\mathcal{U}_\theta \psi)}{\partial \theta}. \quad (7)$$

Upon using these two last equations recursively, we obtain

$$\begin{aligned} D_\rho(g D_\rho \psi) &= -\bar{\mathcal{U}}_\rho \frac{\partial}{\partial \rho} \left[g \frac{\partial(\mathcal{U}_\rho \psi)}{\partial \rho} \right], \\ D_\theta(g D_\theta \psi) &= -\bar{\mathcal{U}}_\theta \frac{\partial}{\partial \theta} \left[g \frac{\partial(\mathcal{U}_\theta \psi)}{\partial \theta} \right]. \end{aligned} \quad (8)$$

As a consequence, we obtain for the kinetic term in the first TDGL equation

$$\begin{aligned} \mathbf{D} \cdot (g \mathbf{D} \psi) &= D_\rho(g D_\rho \psi) + D_\theta(g D_\theta \psi) - \frac{i}{\rho} g D_\rho \psi \\ &= -\frac{\bar{\mathcal{U}}_\rho}{\rho} \frac{\partial}{\partial \rho} \left[\rho g \frac{\partial(\mathcal{U}_\rho \psi)}{\partial \rho} \right] - \frac{\bar{\mathcal{U}}_\theta}{\rho^2} \frac{\partial}{\partial \theta} \left[g \frac{\partial(\mathcal{U}_\theta \psi)}{\partial \theta} \right]. \end{aligned} \quad (9)$$

On using equations (7), the superconducting current density from (2) can also be written as

$$J_{s\rho} = \text{Im} \left[\bar{\mathcal{U}}_\rho \psi \frac{\partial(\mathcal{U}_\rho \psi)}{\partial \rho} \right], \quad J_{s\theta} = \text{Im} \left[\frac{\bar{\mathcal{U}}_\theta \psi}{\rho} \frac{\partial(\mathcal{U}_\theta \psi)}{\partial \theta} \right], \quad (10)$$

where Im indicates the imaginary part.

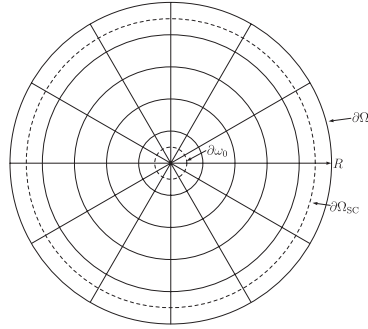


Figure 1. The computational mesh in polar coordinates used for the evaluation of $\psi_{i,j}$. The superconducting domain is delimited by the dashed lines $\partial\Omega_{SC}$, and the superconducting layer is surrounded by the solid line $\partial\Omega$; the surface $\partial\omega_0$ is used to integrate equation (11) in order to find ψ at the center of the disk. More details of this picture are described in the text.

Finally, by using equations (7) and (9) the TDGL equations of (4) can be rewritten as

$$\begin{aligned} \eta \frac{\partial \psi}{\partial t} &= \frac{1}{g} \left\{ \frac{\bar{\mathcal{U}}_\rho}{\rho} \frac{\partial}{\partial \rho} \left[\rho g \frac{\partial (\mathcal{U}_\rho \psi)}{\partial \rho} \right] + \frac{\bar{\mathcal{U}}_\theta}{\rho^2} \frac{\partial}{\partial \theta} \left[g \frac{\partial (\mathcal{U}_\theta \psi)}{\partial \theta} \right] \right\} \\ &+ \psi(1 - |\psi|^2), \quad \text{in } \Omega_0, \\ -i\bar{\mathcal{U}}_\rho \frac{\partial (\mathcal{U}_\rho \psi)}{\partial \rho} &= 0, \quad \text{on } \partial\Omega_0. \end{aligned} \quad (11)$$

In polar coordinates we have $A_\rho = 0$ and $A_\theta = H_0 \rho / 2$, where $\mathbf{H}_0 = H_0 \mathbf{k}$ is perpendicular to the mesoscopic superconducting disk. Consequently, we obtain $\mathcal{U}_\rho = 1$. An additional periodic boundary condition will be used, $\psi(\rho, \theta + 2\pi) = \psi(\rho, \theta)$.

The TDGL equations as in (11) are important for numerical discretization since they are gauge invariant. If gauge invariance is not strictly satisfied in numerics, one may obtain non-physical numerical results.

3. The numerical setup

We will discretize the TDGL equations of (11) inside a circular area of radius R as illustrated in figure 1. The mesh consists of $N_\rho \times N_\theta$ unit cells with size (a_ρ, a_θ) in polar coordinates. Let (ρ_i, θ_j) be a vertex point in the mesh, where $\rho_{i+1} = \rho_i + a_\rho$, $\theta_{j+1} = \theta_j + a_\theta$, for all $\{1 \leq i \leq N_\rho, 1 \leq j \leq N_\theta\}$; $\rho_1 = 0$, $\rho_{N_\rho+1} = R$, $\theta_1 = 0$, and $\theta_{N_\theta+1} = 2\pi$. The superconducting domain is comprehended by $\Omega_{SC} = \{\rho_1 \leq \rho \leq \rho_{N_\rho} + a_\rho/2, 0 \leq \theta \leq 2\pi\}$. The superconducting region is surrounded by a thin superconducting layer, of width $a_\rho/2$, conveniently detached from the superconductor. We will also detach a small circle $\partial\omega_0$ of radius $\rho = a_\rho/2$ for the purpose of determining ψ at the origin of the disk. All regions are inside the domain $\Omega = \{0 \leq \rho \leq R, 0 \leq \theta \leq 2\pi\}$. The boundary conditions will be employed at the outer $\partial\Omega_{SC}$ interface rather than $\partial\Omega$. Actually, the real interface is superconductor–vacuum $\partial\Omega$. However, we introduce a very thin superconducting layer in between the superconductor and

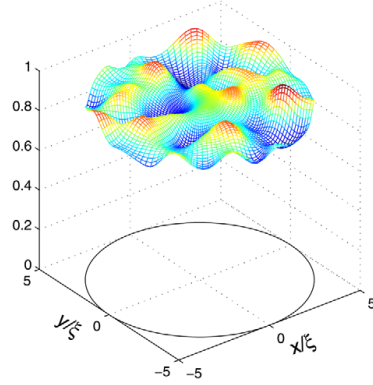


Figure 2. (Color online) the surface generated randomly which was used in the simulations for the 20% roughness.

the vacuum just as an artifact to avoid the divergence of the derivative of the order parameter at the $\partial\Omega$ interface, although both regions consist of the same superconducting material. This is the usual procedure employed in the link variable formalism, not only to avoid divergence of the derivative of the order parameter at the $\partial\Omega$ interface, but also to obtain a discretization of the Ginzburg–Landau equations which preserves the gauge invariance of these equations (see [9] and [12] for more details). The thinner the superconducting layer is, the better our approximation will be.

Let us denote $\psi_{i,j} = \psi(\rho_i, \theta_j)$ and $g_{i,j} = g(\rho_i, \theta_j)$. Also, we denote $\psi_0 = \psi_{1,j}$ for all $1 \leq j \leq N_\theta + 1$ which is the value of the order parameter at the center of the circle. Then, by following the same procedure as in [11], the order parameter can be obtained by the following recurrence relation:

$$\begin{aligned} \psi_{i,j}(t + \Delta t) &= \psi_{i,j}(t) + \mathcal{F}_{i,j}(t) \Delta t, \quad \text{in } \Omega_{SC}, \\ \text{except } j &= N_\theta + 1, \end{aligned} \quad (12)$$

where

$$\begin{aligned} \mathcal{F}_{i,j} &= \frac{\rho_i a_\rho^2}{\rho_i a_\rho^2} (\psi_{i+1,j} - \psi_{i,j}) + \rho_{i-1/2} g_{i-1/2,j} (\psi_{i-1,j} - \psi_{i,j}) \\ &+ \frac{g_{i,j+1/2} (U_{\theta,i,j} \psi_{i,j+1} - \psi_{i,j}) + g_{i,j-1/2} (\bar{U}_{\theta,i,j-1} \psi_{i,j-1} - \psi_{i,j})}{\rho_i^2 a_\theta^2} \\ &+ \psi_{i,j} (1 - |\psi_{i,j}|^2), \end{aligned} \quad (13)$$

and $U_{\theta,i,j} = \exp(-iH_0 \rho_i^2 a_\theta / 2)$. Care must be taken when we use the recurrence relation for $j = 1$. In this case, $\psi_{i,0}$ must be replaced by ψ_{i,N_θ} .

From the second equation of (11), we can obtain at the interface $\partial\Omega$

$$\psi_{N_\rho+1,j}(t + \Delta t) = \psi_{N_\rho,j}(t + \Delta t), \quad \text{except } j = N_\theta + 1. \quad (14)$$

We may obtain the value of ψ_0 by integrating both sides of the first equation of (11) over the area $\pi a_\rho^2 / 4$ limited by the inner interface $\partial\omega_0$ (see figure 1), and using the periodicity of the functions ψ and g . We have

$$\psi_0(t + \Delta t) = \psi_0(t) + \mathcal{F}_0(t) \Delta t, \quad (15)$$

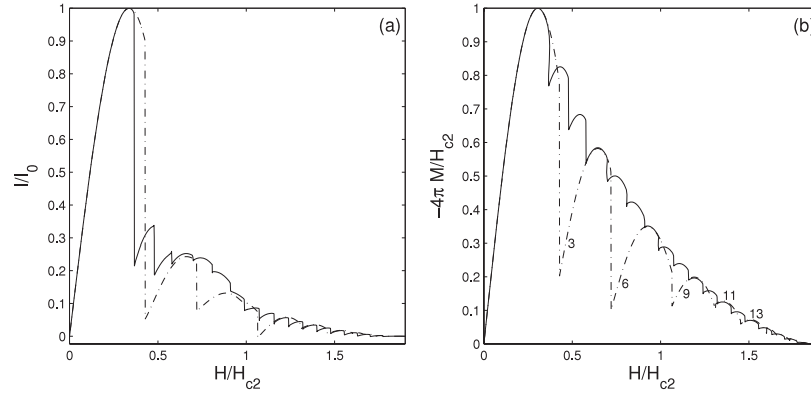


Figure 3. (a) The total induced current: dot-dashed line for case I, and solid line for case II. (b) The same as (a) for the magnetization. The numbers indicate the vorticity of each phase; the indications are only for case I; for case II, we can figure out the number of vortices for each phase, just by counting the number of jumps of the corresponding curve, since its periodicity is $L = 1$.

where

$$\mathcal{F}_0(t) = \frac{2}{\pi a_\rho^2} \sum_{j=1}^{N_\theta} g_{1/2,j}(\psi_{2,j} - \psi_0) + \psi_0(1 - |\psi_0|^2), \quad (16)$$

Finally, we can obtain the order parameter along the branch $j = N_\theta + 1$, that is, $\theta = 2\pi$, by using the periodic boundary condition

$$\psi_{i,N_\theta+1} = \psi_{i,1}, \quad \text{in } \Omega. \quad (17)$$

Before we close this section, let us compute the total induced current along the transverse direction. We have

$$I = \int_{a_\rho/2}^{R-a_\rho/2} \int_{-\epsilon_g}^{\epsilon_g} J_{s\theta} dz d\rho. \quad (18)$$

By using the second of equations (10), it can be easily demonstrated that the discrete version of I , to leading order, is given by

$$I = 2\epsilon \frac{a_\rho}{a_\theta} \sum_{i=2}^{N_\rho} \text{Im} \left[\frac{g_{i,3/2}}{\rho_i} \bar{\psi}_{i,1} U_{\theta,i,1} \psi_{i,2} \right]. \quad (19)$$

Upon doing this, we have taken all components of the current density perpendicular to the line $\theta = a_\theta/2$; the result for I should not depend on this choice.

Another important physical quantity from the experimental point of view is the magnetization (magnetic moment per unit volume), which in nondimensional units is given by

$$4\pi M = \frac{1}{2\kappa^2} \frac{1}{S} \int_0^{2\pi} \int_0^R g(\rho, \theta) \rho J_{s\theta}(\rho, \theta) \rho d\rho d\theta, \quad (20)$$

where S is the area of the surface $z = g(\rho, \theta)$. Upon using the second of equations (10), the numerical version of the magnetization is

$$4\pi M = \frac{1}{2\kappa^2} \frac{1}{S} \frac{1}{a_\theta} \sum_{i=2}^{N_\rho} \sum_{j=1}^{N_\theta} g_{i,j+1/2} \text{Im}[\bar{\psi}_{i,j} U_{\theta,i,j} \psi_{i,j+1}] A_{i,j}, \quad (21)$$

where $A_{i,j} = a_\rho a_\theta \rho_i$ is the area of a unit cell.

4. Results and discussion

We solve the recurrence relations (12) and (15) under the boundary conditions (14) and (17) as follows. We initialize the simulation at the perfect Meissner state $\psi_{i,j} = 1$ and $U_{\theta,i,j} = 1$ in all points of Ω with $H_0 = 0$. We then increase the applied field by ΔH_0 and use the previous solution as the initial state. Once the recurrence relation converges for a fixed value of H_0 , we use its stationary state as the initial state for $H_0 + \Delta H_0$.

In order to study the effect of the roughness of the surface in the dynamics of the formation of vortices in a mesoscopic superconducting disk we have considered two situations:

- Case I. The thickness of the film is taken constant, $g_{i,j} = 1$ for all points in the domain Ω , except in an arbitrary point where $g = 0.99$; this break of symmetry will be justified further.
- Case II. The upper and lower surfaces of the film present some roughness. In this second case, $g_{i,j}$ is chosen randomly with a 20% roughness, that is, $0.8 \leq g_{i,j} \leq 1$. We illustrate this surface in figure 2.

We have considered only these two scenarios in the present investigation. However, the adaptations of the TDGL equations for films of variable thickness developed in [4–6] could also be applied for a variety of surfaces such as a flat disk with blind-hole defects, or even some very smooth surface described by the $g(x, y)$ function, e.g. a concave surface. The present formalism could not be applied to a through-hole defect, since in this case $g(x, y)$ vanishes inside this region.

The reason for taking the function $g \neq 1$ in just one point for case I is as follows. In the TDGL approach, vortices are spontaneously nucleated at the surface and then penetrate inside the sample. After that, they will adopt an equilibrium configuration in order to minimize the energy. Since in a circle we have infinite symmetry axes, the system cannot decide in which direction it could allow the vortices to penetrate inside the sample. As we increase the applied field H_0 , superconductivity is continuously destroyed without

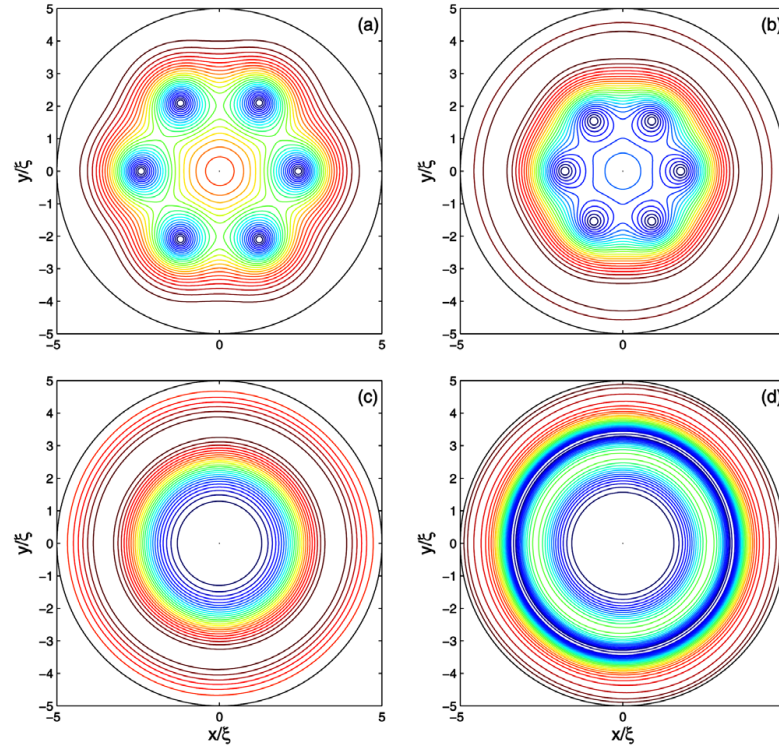


Figure 4. (Color online) the order parameter $|\psi|$ topology for the $L = 6$ state: (a) $H_0/H_{c2} = 0.72$, (b) $H_0/H_{c2} = 0.95$, and (c) $H_0/H_{c2} = 1.064$. (d) The current streamlines for $H_0/H_{c2} = 1.064$.

nucleation of vortices. However, if we make a very small perturbation at the surface we break the symmetry. Otherwise, we would never have a mixed state.

The numerical simulations were carried out for a disk of radius $R = 5\xi$. Figure 3(a) depicts the total induced current in units of length, $\mathcal{J} = I/2\epsilon$ for both cases I and II. Also, we evaluated the magnetization as shown in figure 3(b). It can be clearly noticed that both $\mathcal{J}$ and $-4\pi M$ have a series of discontinuities signaling that one or more vortices have entered the sample. As one can observe, for variable thickness the transitions are more regular than for a flat disk. While for case II all transitions are $L \rightarrow L + 1$, in case I, from $L = 0$ to 9 we have only $L \rightarrow L + 3$ transitions. Then, until $L = 13$, they turn into $L \rightarrow L + 2$ transitions. Subsequently, starting from $L = 14$ to the normal state, we have $L \rightarrow L + 1$ transitions. In other words, with the roughness we can have a better control of the periodicity of the transitions than in a flat disk. In addition, there is a small delay in the penetration of vortices for case I, and the superconductor operates with a higher induced current for most of the applied field intervals.

Let us now move to the study of the vortex configurations. In mesoscopic superconductors we may have the occurrence of a giant vortex state. This state is defined by having a vortex of vorticity equal to or larger than two. Rigorously speaking, all the vortices which constitute a giant vortex would have a

common core center. For $R = 4\xi$, Baelus and Peeters [1] have found that states with vorticity $L \geq 6$ are always giant vortex states. Before this state sets in, the multivortices are positioned on a ring. As the applied field increases, all vortices collapse at the center forming a giant vortex. An additional vortex only increases the vorticity of the giant vortex. Although we have used a larger disk than the one used in [1], we could still observe the same behavior for a flat disk. However, if we take into account the roughness of the surface, some new interesting features of the vortex topology may appear.

In figures 4(a)–(c) we show the topology of the order parameter $|\psi|$ for $L = 6$, case I, at $H_0/H_{c2} = 0.72$, 0.95 , and 1.064 , respectively. It can be clearly observed that, as H_0 increases, all vortices move towards the center and continuously go to a giant vortex state. Several authors have tried to detect this state experimentally, either by using multi-small tunnel junction measurements [13] or scanning SQUID microscopy [14]. Upon using the former technique, the authors have found that, by putting several small tunnel junctions symmetrically distributed on the disk edge, for some vorticities they could not find any significant difference in the voltages at the contacts. This taken as an indication of the occurrence of a giant vortex state. In fact, in figure 4(d) we can see that the current stream lines are entirely uniform once the vortices form a giant vortex state.

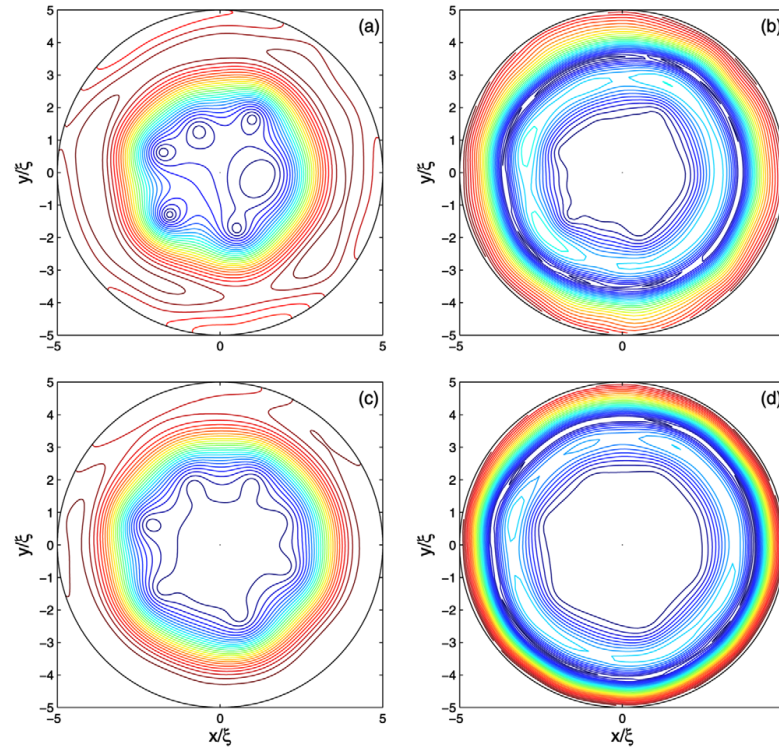


Figure 5. (Color online) the order parameter $|\psi|$ topology ((a) and (c)) and the respective current streamlines ((b) and (d)) for case II. The upper pictures are for $L = 7$ and $H_0/H_{c2} = 1.064$, and the lower ones for $L = 10$ and $H_0/H_{c2} = 1.240$.

We made the same simulation for case II and using the same parameters as previously. It turns out that, if we introduce rugosity, we can hardly observe the giant vortex state, even for very high vorticity. To be certain of this observation, we have used the current streamlines as a guide. In figure 5(a) we illustrate $|\psi|$ for $L = 7$ and $H_0/H_{c2} = 1.064$ and the corresponding current streamlines in figure 5(b).³ Notice that for this value of H_0 , for a flat disk, a giant vortex has already been nucleated as described above, but not for case II as can be seen from this figure. We can observe that the topology of the order parameter still shows the individuality of each vortex. Indeed, it is quite clear that the currents are no longer uniform around the center of the disk. Therefore, we argue that it would be much more difficult to observe a giant vortex state by using the multi-small tunnel junction technique if the surface presents some irregularity. In this scenario the giant vortex state could perhaps be observed only by some imaging technique like scanning SQUID microscopy.

In figures 5(c) and (d), we present the same pictures as the last ones for higher vorticity $L = 10$. Notice that the nonuniformity of the current streamlines still persists. This

³ Notice that, in opposition to bulk superconductors, for mesoscopic superconductors we can still have a vortex lattice for values of the applied field larger than $H_{c2}(T)$. This is so because the barrier for penetration of flux is much larger for small superconductors than for bulk ones (see for instance [1, 15]).

lack of uniformity of the currents tends to disappear as H_0 increases. But then it is difficult to distinguish whether a giant vortex state is nucleating or if the vortex lattice is being destroyed.

In conclusion, we have observed that a small rugosity of the surface of a superconducting film can make it operate in larger induced currents for large fields in the mixed state. Furthermore, we have shown some evidence that the rugosity of a superconducting film would also make the observation of a giant vortex state more difficult.

Acknowledgment

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5.4 Superconducting boundary conditions for mesoscopic circular samples ([aqui](#))

Antes desta publicação, já havia iniciado minha colaboração com os Professores [José José Barba Ortega](#) e [José Albino Aguiar](#). Mas considero que este seja de fato o mais relevante dentre todos que publicamos. Trata-se de uma aplicação da extensão do algoritmo de solução das equações TDGL para geometrias circulares [\[41\]](#), incluindo efeitos de diferentes tipos de superfície. A superfície é modelada usando as condições de contorno de deGennes; interfaces supercondutor/metal normal, supercondutor/vácuo, e supercondutor/supercondutor a mais alta T_c . Neste trabalho, fizemos um detalhado estudo das configurações de vórtices para um setor circular, bem como o diagrama de fase $H - b$, onde b é o comprimento de extrapolação de deGennes. Este diagrama trás informações do estado de Meissner, estado de *mono* e *multivórtices*. Mostramos ainda que para determinados valores de b , um supercondutor do tipo II pode se tornar do tipo I.

Superconducting boundary conditions for mesoscopic circular samples

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Abstract

In the present paper we solve the time dependent Ginzburg–Landau (TDGL) equations by using the link variables technique for two shapes of circular geometry, a circular sector and a disc. The implemented algorithm is applied to a circular geometry surrounded by different kinds of material and immersed in an external magnetic field applied perpendicular to its plane. The properties of these materials are accounted for in the de Gennes boundary conditions with the de Gennes extrapolation length (the so called b parameter). We evaluate the magnetization, the superconducting electron density, the superconducting–normal magnetic field transition, and the applied magnetic field/ b -parameter phase diagram. For the circular sector, our results point out that, under an appropriate choice of the b parameter, the third critical field H_{c3} can be greatly increased. For the disc, we determine the b -limit for the occurrence of the Meissner, single and multi-vortex states in a type-II superconductor. In addition, we show that under an appropriate construction of the boundary, a type-II superconducting disc may behave like a type-I.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Due to advances in nanofabrication techniques the study of confined mesoscopic samples has received a lot of attention in the last few decades. The properties and applications of superconductors are determined by their critical parameters. By nanostructuring a superconductor, one can modify the properties of an existing superconducting structure [1, 2]. Several works have been performed in circular geometries (see [3, 4] and references therein); the authors of these references have shown that, as the angular width of a circular sector (a wedge) is diminished, the nucleation field increases and exhibits an universal behavior regardless of the area of the superconductor.

Another way of either modifying, enhancing or suppressing the properties of superconducting samples can be realized by controlling the sample boundary conditions. Theoretically, one can simulate different types of material by varying the de Gennes extrapolation length b in the boundary conditions for the order parameter. The meaning of this parameter is

as follows: positive b reproduces the interface with normal metals, while negative b reproduces the interface with a superconductor with a higher T_c ; $b = 0$ simulates a high density of defects in the interface and $b \rightarrow \infty$ represents a superconductor/vacuum interface. In a recent work, we studied the flux trapping and paramagnetic effects in superconducting thin films having found that for a superconductor/vacuum interface the order parameter is only slightly suppressed due to the shielding currents. This boundary condition leads to the well known surface barrier which is responsible for the hysteretic behavior of the magnetization and for the paramagnetic effects [5].

It is well known that the phenomenology of superconductivity can be described by the time dependent Ginzburg–Landau (TDGL) equations [6–8]. In the present paper we have made use of the TDGL approach to address the issues above, namely, the magnetization in confined geometries and the behavior of the transition fields for a determined geometry. For this, we have chosen a circular sector (see figure 1 of [4]), where we choose an arbitrary shape for our study.

The discretization of the TDGL equations, by using the link variables technique, has been done only in circular coordinates for the superconductor/vacuum interface ($b \rightarrow \infty$) by Sardella *et al* [4]. So, we will extend this algorithm considering the general boundary conditions for the order parameter, i.e., ($b > 0, b < 0, b = 0$). Our procedure makes it possible to generalize the algorithm to any circular geometry and b value. This simple generalization of the algorithm introduces a variety of novel results which will be described later on. For instance, according to the choice of boundary conditions we will show that the superconductivity can be considerably enhanced, and a new classification of type-I and type-II superconductor may occur.

The paper is outlined as follows. In section 2 we write the dimensionless TDGL equations in a gauge invariant form by using the auxiliary field in polar coordinates with the generalized boundary conditions. In section 3 we present and discuss the results of the numerical simulations for certain parameters of a superconducting circular sector and a disc for a wide range of the de Gennes parameter b (or γ which unifies all types of boundary condition; see section 2.2 for more details).

2. Theoretical formalism

2.1. The TDGL equations

The properties of the superconducting state are usually described by the complex order parameter ψ , for which the absolute square value $|\psi|^2$ represents the superfluid density, and the vector potential $\mathbf{A}$, which is related to the local magnetic field as $\mathbf{h} = \nabla \times \mathbf{A}$. If either a transport current, or an external electric field is present, the scalar potential ϕ must be taken into account. In dimensionless units, the TDGL equations are given by

$$\begin{aligned} \left(\frac{\partial}{\partial t} + i\phi \right) \psi &= -\mathbf{D} \cdot \mathbf{D} \psi + (1 - T) \psi (1 - |\psi|^2), \\ \beta \left(\frac{\partial \mathbf{A}}{\partial t} + \nabla \phi \right) &= (1 - T) \text{Re}[\bar{\psi} \mathbf{D} \psi] - \kappa^2 \nabla \times \mathbf{h}, \end{aligned} \quad (1)$$

where T is the temperature in units of the critical temperature; the lengths are in units of $\xi(0)$, the coherence length at zero temperature, and the fields are in units of $H_{c2}(0)$, the upper critical field at zero temperature; β is the ratio between the relaxation times of the vector potential and the order parameter; κ is the Ginzburg–Landau parameter which is material dependent; the operator $\mathbf{D} = -i\nabla - \mathbf{A}$; Re indicates the real part of a complex variable and the overbar means the complex conjugation; (for more details, see [9, 11–14]). Here, we will neglect the z -dependence on the order parameter. This is reasonable for an infinite homogeneous system along the z -direction. Notice that equations (1) are gauge invariant since they do not change under the transformation $\psi' = \psi e^{i\chi}$, $\mathbf{A}' = \mathbf{A} + \nabla \chi$, $\phi' = \phi - \partial \chi / \partial t$. We choose the zero-scalar potential gauge, that is, $\phi' = 0$ at all times. From now on, we will drop the primes.

The TDGL equations from (1) have been discretized in polar coordinates in [4] by using the link variables technique. Here, we will reproduce some steps of the algorithm developed

in this reference at a minimum level and introduce what is new with respect to the boundary conditions. This procedure will help us to present the results in a more comprehensible manner. At this point, it is convenient to introduce the auxiliary vector field $\mathcal{U} = (\mathcal{U}_\rho, \mathcal{U}_\theta)$ in polar coordinates, which is defined by

$$\begin{aligned} \mathcal{U}_\rho(\rho, \theta) &= \exp\left(-i \int_{\rho_0}^{\rho} A_\rho(\theta, \xi) d\xi\right), \\ \mathcal{U}_\theta(\rho, \theta) &= \exp\left(-i \int_{\theta_0}^{\theta} A_\theta(\xi, \rho) d\xi\right), \end{aligned} \quad (2)$$

where (ρ_0, θ_0) is an arbitrary reference point. On replacing (2) in (1), the TDGL equations can be rewritten as

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= \frac{\bar{\mathcal{U}}_\rho}{\rho} \frac{\partial}{\partial \rho} \left[\rho \frac{\partial (\mathcal{U}_\rho \psi)}{\partial \rho} \right] + \frac{\bar{\mathcal{U}}_\theta}{\rho^2} \frac{\partial^2 (\mathcal{U}_\theta \psi)}{\partial \theta^2} \\ &\quad + (1 - T) \psi (1 - |\psi|^2), \\ \beta \frac{\partial A_\rho}{\partial t} &= (1 - T) \text{Im} \left[\bar{\mathcal{U}}_\rho \bar{\psi} \frac{\partial (\mathcal{U}_\rho \psi)}{\partial \rho} \right] - \kappa^2 \frac{1}{\rho} \frac{\partial h_z}{\partial \theta}, \\ \beta \frac{\partial A_\theta}{\partial t} &= (1 - T) \text{Im} \left[\frac{\bar{\mathcal{U}}_\theta \bar{\psi}}{\rho} \frac{\partial (\mathcal{U}_\theta \psi)}{\partial \theta} \right] - \kappa^2 \frac{\partial h_z}{\partial \rho}. \end{aligned} \quad (3)$$

The grid used for the discretization of the TDGL equations of (3) on a circular sector is illustrated in figure 1 of [4] and the other physical quantities, such as magnetization, free energy, and vortex number, can be found in more detail in [4].

2.2. Circular sector case

Let us now discuss the boundary conditions. Let $\mathbf{n}$ be a unit vector normal to the $\partial\Omega_{\text{SC}}$ interface and directed outward the domain Ω_{SC} . This domain is defined by the internal and external radii, r and R , respectively, and spans an angular width Θ , which can vary from 0 (slit) to 2π (disc) (see figure 1 of [4]). We will assume that the current density normal to $\partial\Omega_{\text{SC}}$ does not vanish at the interfaces, that is $\mathbf{D}\psi \cdot \mathbf{n}|_{\partial\Omega_{\text{SC}}} = b^{-1}\psi|_{\partial\Omega_{\text{SC}}}$. We can show that the discrete implementation of this condition is as follows

$$\begin{aligned} \psi_{1,j} &= \gamma U_{\rho,1,j} \psi_{2,j}, \\ \psi_{N_\rho+1,j} &= \gamma \bar{U}_{\rho,N_\rho,j} \psi_{N_\rho,j}, \end{aligned} \quad (4)$$

and

$$\psi_{i,1} = \gamma U_{\theta,i,1} \psi_{i,2}, \quad \psi_{i,N_\theta+1} = \gamma \bar{U}_{\theta,i,N_\theta} \psi_{i,N_\theta}. \quad (5)$$

We unify the boundary conditions upon introducing the $\gamma = 1 - \delta/b$ parameter, here δ is the mesh size. For convenience, this notation allows us to obtain a better analysis of the results. Thus, $0 < \gamma < 1$ simulates a superconductor/metal interface ($b > 0$); a superconductor/superconductor at higher critical temperature is described with $\gamma > 1$ ($b < 0$); and $\gamma = 1$ simulates a superconductor/vacuum interface ($b \rightarrow \infty$).

2.3. Disc case

A disc, for which $\Theta = 2\pi$, should be treated as a special case. We will assume that the center of the disc contains a small metal of radius r . As before, the boundary condition on the current density across both the internal and external interfaces

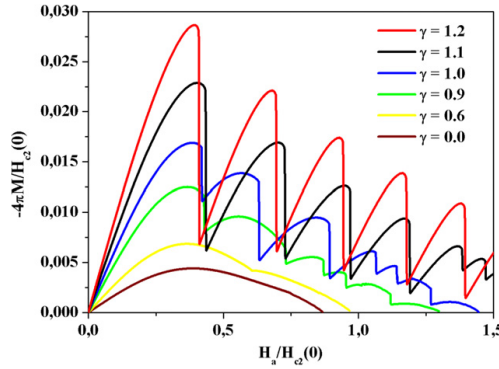


Figure 1. Magnetization curve as a function of the external applied magnetic field H_a for $\gamma = 1.2, 1.1, 1.0, 0.9, 0.6, 0$.

of the disc is $\mathbf{D}\psi \cdot \mathbf{n}|_{\partial\Omega_{SC}} = b^{-1}\psi|_{\partial\Omega_{SC}}$. In this case will consider only $b > 0$ for the disc. We can show that the discrete implementation of this condition is as follows

$$\psi_{1,j} = (1 - a_\rho/b)U_{\rho,1,j}\psi_{2,j}, \quad (6)$$

$$\psi_{N_\rho+1,j} = (1 - a_\rho/b)\bar{U}_{\rho,N_\rho,j}\psi_{N_\rho,j} \quad (7)$$

where a_ρ is the grid size along the radial direction (see [4]). These boundary conditions are supplemented by the additional periodic boundary condition, $\psi(\rho, \theta + 2\pi) = \psi(\rho, \theta)$, whose discrete version is given by $\psi_{i,N_\theta+1} = \psi_{i,1}$.

3. Results and discussion

We started from the Meissner state where $\psi = 1$ and $U_\rho = U_\theta = 1$ everywhere are taken as the initial conditions. Then we let the time evolve until the system achieves a stationary state. This is done by keeping the external applied magnetic field H_a which is taken constant until the system achieves a stationary state. Next, we ramp up the applied field by an amount of ΔH . The stationary solution for H_a is then used as the initial state to determine the solution for $H_a + \Delta H$, and so on. Usually we started from zero field and increased H_a until the superconductivity is entirely destroyed. We use the following criterion to obtain the stationary state: for any vertex point in the mesh, if the highest difference $||\psi(t_m)| - |\psi(t_n)||$ is smaller than a certain precision ϵ , then we go to the next field; usually, this test is made over some thousands of times steps, i.e., $m - n \sim 10^3$. We have worked with a precision of no less than $\epsilon = 10^{-5}$ for the absolute value of the order parameter. The parameters used in our numerical simulations were $\kappa = 5.0$, $T = 0$, and $\beta = 1$.

The internal radius and the area of the circular sector were taken fixed for an angular width $\Theta = 90^\circ$. We used $r = 2\xi(0)$ and $S = 64\xi^2(0)$ for the area, such that the external radius is given by $R = \sqrt{256/\pi + r^2}$ which is equivalent to the area of a square of dimensions $8\xi(0) \times 8\xi(0)$. On the other hand, for the disc, we have considered several external radii varying discretely as follows: $R = 3.0\xi(0), 4.0\xi(0), 5.0\xi(0), 6.0\xi(0), 7.0\xi(0), 8.0\xi(0)$; the internal radius is fixed at $r = 0.1\xi(0)$.

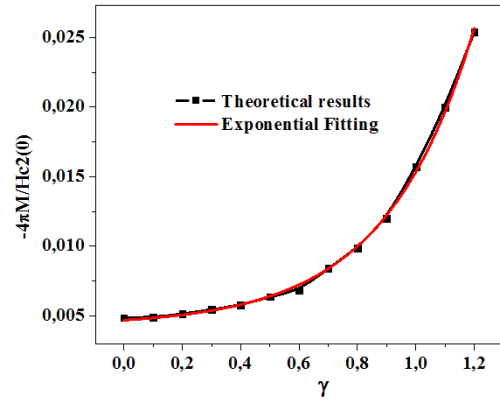


Figure 2. Magnetization as a function of the γ parameter at $H_a = 0.3H_{c2}(0)$: theoretical results and exponential fit.

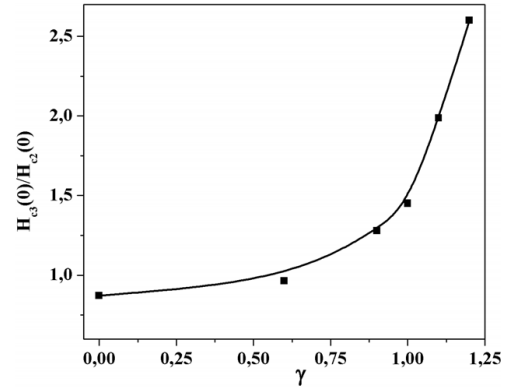


Figure 3. The upper critical field $H_{c3}(0)$ field as a function of the γ parameter.

In both cases, we have taken the length of the largest unit cell to be no larger than $0.25\xi(0) \times 0.25\xi(0)$. Since the order parameter varied most significantly over a distance $\xi(0)$, this choice for the grid space is sufficient to pick the variations of ψ . We ramp up the applied magnetic field adiabatically, typically in steps of $\Delta H = 10^{-3}$.

3.1. Circular sector

In figure 1 we present the magnetization as a function of the external applied magnetic field H_a for a circular sector for several values of the γ parameter. These curves present a typical profile of a magnetization curve of a mesoscopic superconductor. It exhibits a series of discontinuities, in which each jump signals the entrance of one or more vortices into the sample. Notice that the number of jumps and the transition fields vary significantly with γ . We determined the values of the magnetization for an external magnetic field $H_a = 0.3H_{c2}(0)$ as a function of γ (see figure 2). At this magnetic field the superconducting sample is still in the Meissner state,

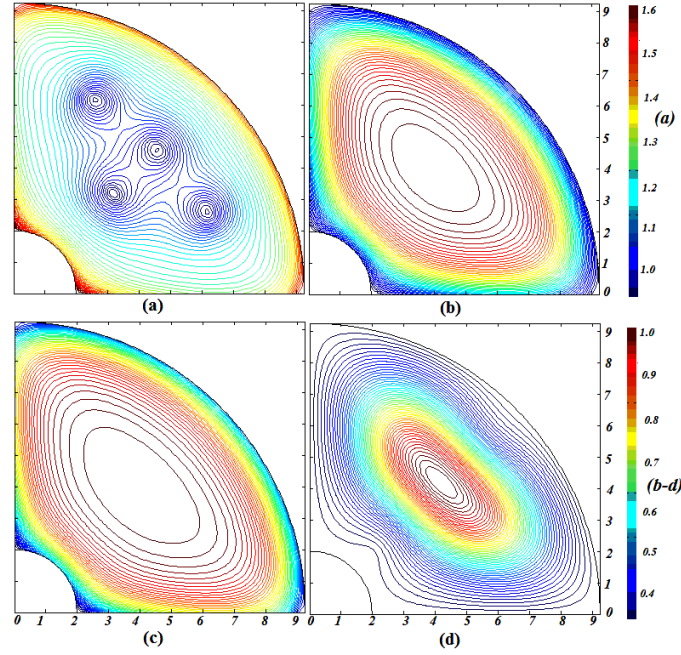


Figure 4. Two-dimensional density contour plot of $|\psi|$ for the boundary conditions with (a) $\gamma = 1.2$ at $H_a = 0.5H_{c2}(0)$, (b) $\gamma = 0$, (c) $\gamma = 0.6$ and (d) $\gamma = 1$ at $H_a = 0.4H_{c2}(0)$. Lengths in the axes are in units of $\xi(0)$.

i.e., there are no vortices. As one can easily notice, the negative magnetization grows strongly with γ . We found an exponential behavior of M as a function of γ . The fitted curve corresponds to $M \approx 0.0042 + 0.0040 \exp(\gamma/0.3)$. The rapid growth with γ means that the less the metallic boundary is the more diamagnetic the material is. This effect can be even more enhanced if the interface is a superconductor of higher T_c ($\gamma > 1$, $b < 0$).

Another interesting feature is shown for the third critical field H_{c3} , the critical field which marks the transition from surface superconductivity to the normal state. In figure 3 we present the $H_{c3}(0) - \gamma$ phase diagram for six samples with $\gamma = 1.2, 1.1, 1.0, 0.9, 0.6, 0$; we found for these cases $H_{c3}(0) = 2.611, 1.987, 1.443, 1.280, 0.965, 0.873$, respectively. The superconductor/normal transition field $H_{c3}(0)$ grows quickly with γ . From an experimental point of view, this is an important result, since the higher the critical field, the higher the critical current density. In fact, we can see a much higher number of jumps in the $M \times H_a$ curve as the γ parameter increases⁴. On the other hand, as γ decreases, the lower critical field increases (see figures 1 and 2). Thus, if we are interested in shielding the first penetration of the magnetic field, a superconductor surrounded by a metallic material should be more useful.

⁴ In [15] it has been observed that the superconductivity can be enhanced if the interface is a superconductor at a higher temperature (b negative) for a disc, but they did not determine an analytical function $H_{c3}(\gamma)$ as in the present work.

Let us now move to the discussion of how the γ parameter influences the topology of the superconducting density of Cooper pairs. In figure 4 we depict $|\psi|$ for the stationary states. We choose different values of the γ parameter to illustrate the role played by the different boundary conditions on the properties of the interfaces. We use (a) $\gamma = 1.2$ at $H_a = 0.5H_{c2}(0)$, and (b) $\gamma = 0$, (c) $\gamma = 0.6$ and (d) $\gamma = 1$ at $H_a = 0.4H_{c2}(0)$. In the superconductor/vacuum interface (see figure 4(d)) we see that $|\psi|$ is slightly suppressed in a region near the surface due to the shielding currents. For the superconductor/metal interface $\gamma = 0.6$ (see figure 4(c)), the order parameter is suppressed in a region near the surface due to contamination with the normal electrons from the metal. For $\gamma = 0$ (see figure 4(b)), the superconductivity is strongly suppressed because we have a surface in the normal state or a superconductor/ferromagnet interface. For $\gamma = 1.2$ (see figure 4(a)) the superconductivity is enhanced in the surface due to the Cooper pairs originating from the superconductor of higher T_c .

In figure 5 we describe the vortex state for three values of vorticity N : for $N = 1$ at $H_a = 0.65H_{c2}(0)$, (a) $\gamma = 0.0$ and (b) $\gamma = 0.6$; for $N = 3$ at $H_a = 0.8H_{c2}(0)$, (c) $\gamma = 0.9$ and (d) $\gamma = 1.0$; and for $N = 4$ at $H_a = H_{c2}(0)$, (e) $\gamma = 1.1$ and (f) $\gamma = 1.2$. For all studied samples we have considered transitions either from N to $N + 1$ or from N to $N + 2$ vortices. In this picture we can also appreciate the enhancement of the surface superconductivity for the samples with $\gamma = 1.1$ and 1.2 .

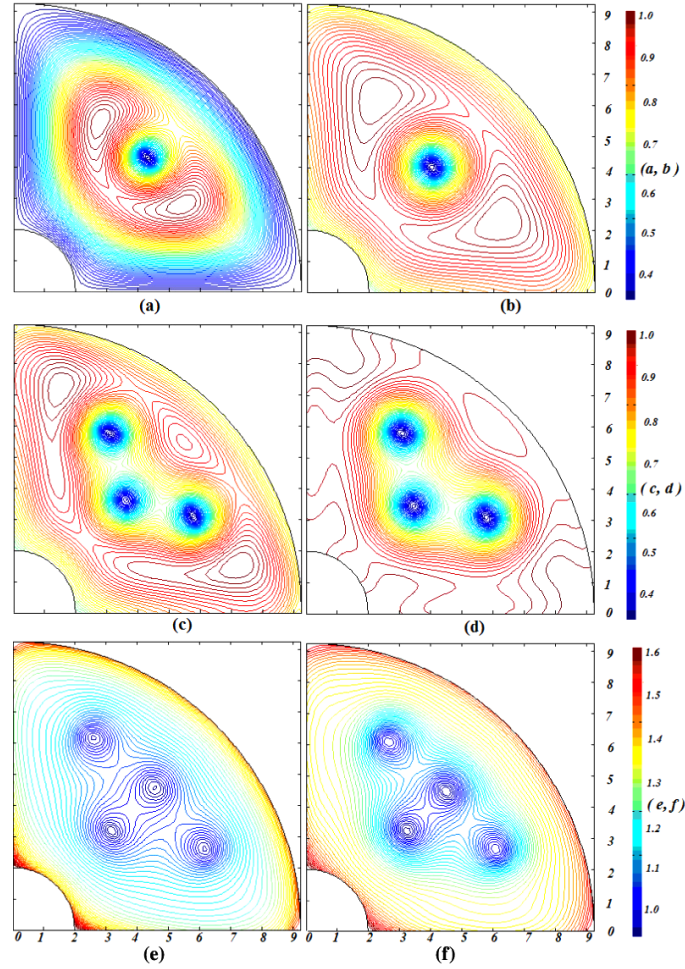


Figure 5. Two-dimensional density contour plot of $|\psi|$ for several type boundaries: the one vortex state at $H_a = 0.65H_{c2}(0)$: (a) $\gamma = 0.0$ and (b) $\gamma = 0.6$; the three vortex state at $H_a = 0.8H_{c2}(0)$: (c) $\gamma = 0.9$ and (d) $\gamma = 1.0$; and the four vortex state at $H_a = H_{c2}(0)$: (e) $\gamma = 1.1$ and (f) $\gamma = 1.2$. Lengths in the scale are in units of $\xi(0)$.

3.2. Disc

We start our discussion from the magnetization curve as a function of the applied magnetic field (see figure 6). This curve shows the usual behavior for a mesoscopic superconductor, exhibiting a series of discontinuities as the vortices are nucleating into the sample. However, this figure shows a rather different feature with respect to the circular sector. From a certain value of b and below, the superconductor behaves as a type-I superconductor [16]. We will explore this characteristic more later on.

In order to find how diamagnetic the disc is, concerning the metallic interfaces, in figure 7 we depict the values of the magnetization, for an external magnetic field of $H_a = 0.75H_{c2}(0)$, as a function of b for a disc of size $R = 3\xi(0)$.

We find that the magnetization grows linearly with b ; the fitted curve corresponds to $M \approx 0.102b + 0.009$. Thus, the circular sector seems to be much more diamagnetic than the disc, since for the former case we have found an exponential behavior for the M - γ phase diagram.

As we anticipated previously, the type of boundary condition may turn the superconductor into a type-I for certain values of b . To see this, in figure 8 we plot the radius of the sample as a function of $\ln(b)$ for an applied magnetic field $H_a = 0.75H_{c2}(0)$. For the six samples with $R = 3\xi(0)$, $R = 4\xi(0)$, $5\xi(0)$, $6\xi(0)$, $7\xi(0)$, $8\xi(0)$, we have found $b = 2.5\xi(0)$, $1.5\xi(0)$, $0.95\xi(0)$, $0.55\xi(0)$, $0.3\xi(0)$, $0.2\xi(0)$ respectively. We can observe a linear behavior of $\ln(b)$ as a function of R . The fitted curve corresponds to $\ln(b) \approx 2.45 - 0.5R$. Thus, a type-II superconductor under the

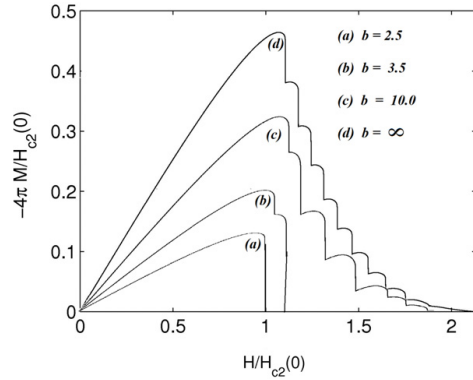


Figure 6. Magnetization curve as a function of the external applied magnetic field for four values of the de Gennes parameter, $b = \infty, 10.0, 3.5, 2.5$ and $R = 3.0\xi(0)$.

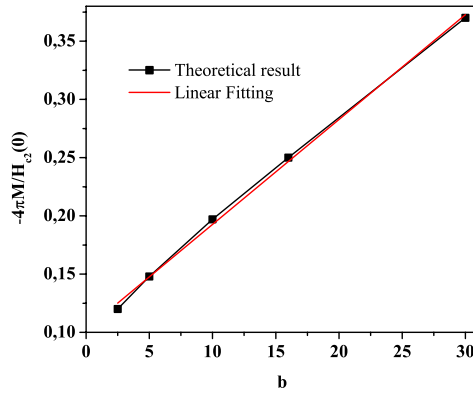


Figure 7. Magnetization curve as a function of the b parameter for $H_a = 0.75H_{c2}(0)$ and $R = 3.0\xi(0)$.

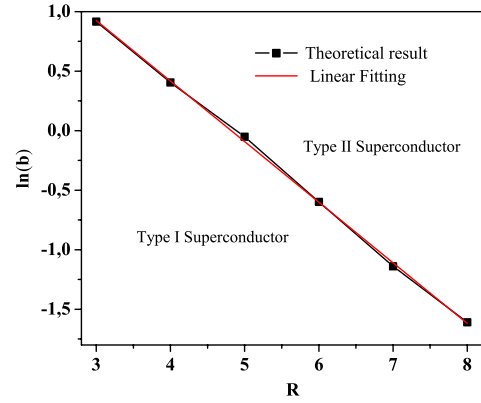


Figure 8. $\ln(b)$ as a function of the radius of the sample, for the absence of a vortex state by using an applied magnetic field $H_a = 0.75H_{c2}(0)$.

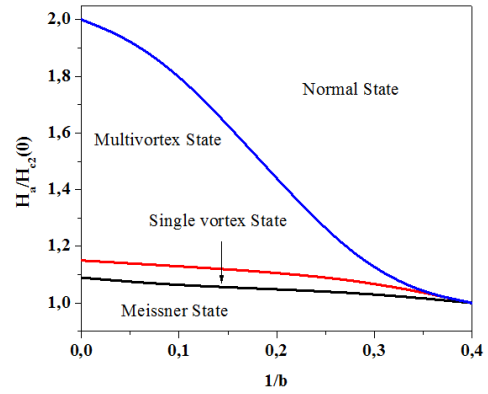


Figure 9. Phase diagram for the applied magnetic field as a function of $1/b$ for a disc of dimension $R = 3\xi(0)$.

appropriate construction of interfaces may become a type-II superconductor. In addition, the curve which delimits the two phases behaves linearly with respect to $\ln(b)$.

We have gone further by determining the critical fields in an H_a-b^{-1} phase diagram for the particular case of $R = 3\xi(0)$ (see figure 9). In this figure we have a variety of phases: the Meissner state, the single vortex state, the multi-vortex state and the normal state. It is remarkable that all critical field lines collapse into a single one for a certain value of b . In the present situation, for $1/b < 0.37$ the sample becomes a type-II superconductor, while for $1/b > 0.37$ behaves like a type-I superconductor for any applied magnetic field.

4. Conclusions

In summary, an algorithm has been devised for solving the time dependent Ginzburg–Landau equations for a circular geometry and general boundary conditions. We have applied

the algorithm to a circular sector and a disc by using the general boundary conditions for the order parameter and have found several configurations for the vortex state in this geometry. Also, the superconducting nucleation field has been evaluated. We have presented some evidence that, if we choose the b parameter accordingly, we can strongly enhance superconductivity. Also, we found an analytical behavior for the magnetization curve as a function of the γ and b parameters; we obtain $M \sim e^\gamma$ for the circular sector and $M \sim b$ for the disc. Finally, we have found an exponential dependence for the Meissner limit $b \sim e^R$ in the disc case.

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5.5 Crossover between macroscopic and mesoscopic regimes of vortex interactions in type-II superconductors (aqui)

Este trabalho foi o primeiro resultado de uma colaboração com o Professor [Rafael Zadorosny](#) da FEIS-UNESP, a qual está se tornando duradoura. Seus alunos de Pós-graduação também têm contribuído significativamente com o aprimoramento do algoritmo de solução numérica das equações TDGL, e com adaptações que geralmente são necessárias para cada tipo de problema abordado, tais como condições de contorno, dissipação de calor, etc.

O trabalho em tela é um minucioso estudo do *crossover* entre supercondutores mesoscópicos e macroscópicos. Mostramos que a fronteira meso-macro depende da temperatura e do valor de κ ; a escala de comprimento que define o *crossover* é dada pela equação $L = L_0(1 - T/T_c)^{-\nu}$, onde ν é um expoente crítico. Esta curva foi extraída de um critério baseado em barreira superfície para a penetração dos primeiros vórtices.

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Crossover between macroscopic and mesoscopic regimes of vortex interactions in type-II superconductors

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In the present work we report the existence of a crossover between the macroscopic and mesoscopic regimes of vortex interactions in type-II superconductors. Our findings rely on a systematic procedure to determine this crossover, which is based on the influence of the surface on the vortex structure of small superconductors. An adjacent result that we have found is that near this regime transformation, the vortex lattice develops a progressive change of symmetry, from square to hexagonal, which is intimately related to the meso-to-macro crossover. Our numerical simulations have been done for a long superconducting cylinder of square cross section for a wide range of length scales and temperatures.

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I. INTRODUCTION

In condensed matter physics, samples are usually considered to be large enough that the influence of finite dimensions on their properties is negligible; therefore, bulk behavior is assumed. This is not the case, however, in many situations of interest. Examples range from quantum size effects in metallic nanoparticles^{1,2} and microfluidics,³ to cluster size effects.⁴ Hallmark physical ingredients in these systems are large surface-to-volume ratio and one or more dimensions of the sample approaching a relevant fundamental scale.

Mesoscopic superconductors also constitute a class of materials where size effects can play a relevant role to determine the vortex arrangement throughout the specimen.^{5–16} In fact, even when only a few quanta of magnetic flux are nucleated into a mesoscopic sample, vortex interactions with other vortices and with the screening currents circulating around the edges give rise to a variety of configurations, such as giant vortices, multivortex states, or even hybrid states of both types. These configurations are strongly influenced by both the geometry and size of the sample. The occurrence of giant vortices in coherence length-sized samples have been predicted by several theoretical calculations,^{17–22} although in some exotic confined geometries, such as a circular sector,²³ they were not observed.

Several authors have tried to detect this state experimentally. Kanda *et al.*^{9–11} used multiple small tunnel junction measurements. They found that, by putting several small tunnel junctions symmetrically distributed on the disk edge, for some vorticities, they could not find any significant difference in the voltages at the contacts. This is taken as an indication of the occurrence of a giant vortex state. Some other authors have attempted to observe giant vortices by direct imaging technique. By using SQUID microscopy, in Refs. 14–16 they could not find giant vortex states in mesoscopic superconducting square and triangle samples. However, on using the Bitter pattern decoration technique in a niobium superconducting disk, Grigorieva *et al.*¹³ observed clusters of multivortex states coexisting with giant vortices. In another work, Cren *et al.*¹²

studied the vortex states in ultrathin single nanocrystals of Pb with random geometries via scanning tunneling microscopy. The images were taken under several values of applied field and at very low temperature. They showed that under certain conditions of magnetic field and sample size, a giant vortex is formed and in the vicinity of the core center the order parameter evolves as $|\psi| \propto r^L$ where L is the vorticity.

In the present work we show strong evidence that there exists a region of crossover between these vortex states in mesoscopic superconductors and the Abrikosov hexagonal vortex lattice in macroscopic superconductors. We have done so by studying the influence of the surface on the vortex configuration as a function of the sample size and temperature. Based on the physics governing the crossover between the mesoscopic and macroscopic behavior, we developed a criterion to determine a length scale that delineates the frontier between those two regimes. One could speculate that this crossover would occur for sample sizes of the order of the penetration depth $\lambda(T)$. As our results will show later on, the length scale that delimits the mesoscopic-macroscopic frontier differs quite significantly from what one might suspect.

The problem treated here was investigated within the scope of the Ginzburg-Landau theory. It is not uncommon to find papers arguing whether the Ginzburg-Landau theory could be applicable or not to the study of superconductivity at a mesoscopic level. This relevant issue has been discussed in detail in Refs. 17, 24, and 25. In the latter, the authors have made a comparative analysis between the phenomenological Ginzburg-Landau theory and the microscopic Bogolyubov-De Gennes theory, for a mesoscopic superconducting square. They conclude that both theories produce very similar results.

The outline of this paper is as follows. First we provide a brief overview of the theoretical model used to obtain the equilibrium configurations of the superconducting state. Then, we describe the numerical method employed to solve the time-dependent Ginzburg-Landau (TDGL) equations for a superconductor in the presence of an external applied magnetic

field. The remainder of the paper is devoted to presentation and discussion of the results that emerge from our numerical simulations.

II. THEORETICAL FORMALISM

The superconducting state is usually described by the complex order parameter ψ . The quantity $|\psi|^2$ represents the electronic density of Cooper pairs. In the regions where $|\psi|^2$ is small, superconductivity is suppressed. At the center of the vortex $|\psi|^2 = 0$, whereas the local magnetic field $\mathbf{h}$ is maximum. The order parameter and the local magnetic field can be determined by the Ginzburg-Landau equations which, in their time-dependent formalism, are expressed by²⁶

$$\begin{aligned} \left(\frac{\partial}{\partial t} + i\Phi \right) \psi &= -(-i\nabla - \mathbf{A})^2 \psi + (1 - T)\psi(1 - |\psi|^2), \\ \beta \left(\frac{\partial \mathbf{A}}{\partial t} + \nabla \Phi \right) &= \mathbf{J}_s - \kappa^2 \nabla \times \mathbf{h}, \end{aligned} \quad (1)$$

where $\mathbf{J}_s = (1 - T)\Re[\psi^*(-i\nabla - \mathbf{A})\psi]$ is the supercurrent density; ψ is the order parameter, $\mathbf{A}$ is the vector potential, related to the local magnetic field as $\mathbf{h} = \nabla \times \mathbf{A}$, and Φ is the scalar potential. Here, the distances are measured in units of the coherence length at zero temperature $\xi(0)$; the magnetic field is in units of the zero temperature upper critical field $H_{c2}(0)$; the temperature T is in units of the critical temperature T_c ; the time is in units of the characteristic time $t_0 = \pi\hbar/8k_B T_c$; κ is the Ginzburg-Landau parameter; β is the relaxation time of $\mathbf{A}$, related to the conductivity. We have adopted a linear dependence with respect to temperature for the phenomenological parameters in the Ginzburg-Landau theory [i.e., $H_{c2}(T) = H_{c2}(0)(1 - T)$]. For small size superconductors this is also valid for temperatures well below T_c , despite the microscopic derivation of the TDGL equations being valid only for T very close to T_c .²⁷ Notice that the TDGL equations and their discretized form^{21,28} are gauge invariant under the transformations $\psi' = \psi e^{i\chi}$, $\mathbf{A}' = \mathbf{A} + \nabla\chi$, $\Phi' = \Phi - \partial\chi/\partial t$. We chose the zero-scalar potential gauge, that is, $\Phi = 0$ at all times and positions.

In order to solve the TDGL equations, we have used the link variables method as delineated in Ref. 28. There are several extensions of this method. For instance, in Ref. 29 it has been adapted for very thin superconductors and in Ref. 23 for circular geometries. The simulations were carried out for samples with square geometry submitted to external magnetic fields applied along the cylinder axis, which is considered infinite. In principle, the TDGL equations can provide all transient states for a fixed external applied magnetic field. However, in this work we are only interested in the stationary states. We solved these equations starting from zero applied field, which was then increased adiabatically in small steps, $\Delta H = 10^{-4}$, until superconductivity was completely destroyed. At each step we let the system attain its equilibrium configuration and use such state as the initial condition for the next applied field.

III. RESULTS AND DISCUSSION

Let us now turn to the presentation of the results that arise from the numerical solution of equations (1). Our simulations have been carried out by using $\beta = 1$ and $\kappa = 5$ for a large number of superconducting square samples of side L , given in units of $\xi(0)$. Since we are interested only in the stationary states, this choice of β is adequate for the purposes. The lateral dimensions of the sample were varied in steps of $\Delta L = 1$ [also expressed in units of $\xi(0)$] and the temperature of simulations ranged from $T = 0$ to $T = 0.9375$ (in units of T_c).

The crucial issue here is to define a robust criterion to determine the characteristic size regulating the threshold among mesoscopic and macroscopic behavior. The following discussion depicts the reasoning that led us to stipulate this norm. It is well known that vortices nucleate at the central portions of the surface (i.e., not at the corners). Their complete development is preceded by a progressive deformation of the screening current mainstream which, otherwise, while the sample is in the Meissner phase, is parallel to the faces. As the applied field H is raised, this deformation proliferates into the sample until a vortex is completed. At this point, what was just a twist at the inception of the penetration process, becomes a curled screening current, enclosing the ingoing vortex. Thus, the pursuit for the threshold of the genuine mesoscopic behavior is equivalent to the search for the range of the interaction among vortices, which are just nucleating at the surfaces. Since this interaction is mediated by the superconducting regions, it should be detectable through all relevant superconducting properties (e.g., the order parameter, the magnitude and shape of the screening currents, and even the sample magnetization M).

Figure 1 illustrates this correlation for two samples of different sizes. As will become clear throughout this discussion, the largest among them ($L = 76$) has a macroscopic behavior, while the other ($L = 26$) exhibits mesoscopic superconductivity. The magnetization versus field curves shown in Fig. 1(a) for both samples exhibit clear jumps at the field H_j , corresponding to the first entrance of vortices into the sample. Noticeably, $M(H)$ for sample $L = 26$ develops a local minimum at H_m , nonexistent for sample $L = 76$. This minimum reflects a delay (in field) of vortex invasion, due to the repulsive interaction between the entities, which are nucleating at the borders [see Fig. 1(b), upper $L = 26$ panel]. Differently from the case for the larger sample [Fig. 1(b), upper $L = 76$ panel], the excessive proximity of the surfaces in sample $L = 26$ causes a strong repulsion between each vortex and its counterparts, even while embryonic at the other surfaces, which causes a non-negligible degradation on the screening capability, due to the extra repulsive barrier. This degradation is clearly manifested on $M(H)$ curves, whose deviation from the Meissner response for a bulk sample ($-4\pi M = H$) increases with decreasing L . The upper $L = 26$ and $L = 76$ panels in Fig. 1(b) also capture the situation, delineating the order parameter at the field H_j . The color code is such that dark red regions are fully screened, while dark blue tones represent strongly suppressed superconductivity. While four vortices³⁰ are being generated at the surfaces of both samples, the order parameter at the very center of the macroscopic sample ($L = 76$) is preserved, even though vortices are just about to enter; contrarily, the tones

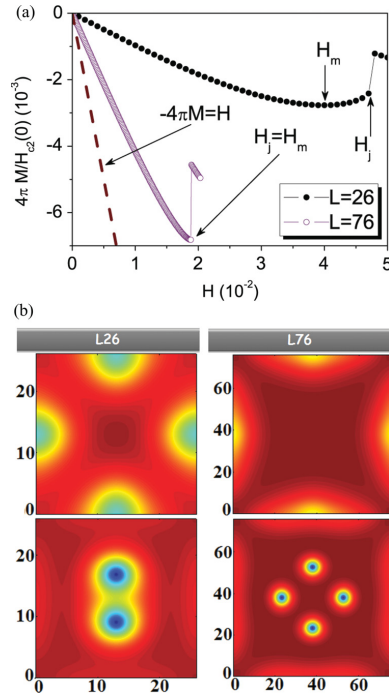


FIG. 1. (Color online) (a) Magnetization versus field curves for samples $L = 26$ and $L = 76$ at $T = 0.875$. As L increases, H_j and H_m (seen for $L = 26$) tend to approach each other and the minimum on the magnetization curve, coincident with H_j for $L = 76$, disappears for $L > 76$. On the magnetization curve disappears. (b) Upper and lower $L = 26$ panels show the order parameter for this sample, immediately before and after the first entrance of vortices (H_j and $H_j + 10^{-4}$, respectively). The same applies for the upper and lower $L = 76$ panels. Noticeably, as discussed in the text, only two vortices appear for $L = 26$. Notice also that the sample sizes are represented as equal, although their side ratio is $76/26 \approx 3$.

at the central portion of the mesoscopic sample ($L = 26$) are somewhat lighter, indicating that screening currents are already circulating in that region, and the nucleating vortices do interact with each other. The lower $L = 26$ and $L = 76$ panels in Fig. 1(b) depict the situation immediately after vortex entrance (i.e., at $H = H_j + 10^{-4}$) further emphasizing the repulsion among the entities that are being formed. While for the larger sample, all nucleating vortices manage to enter at H_j , the mesoscopic sample is not able to host all four at once and, as they would not fit along, only two vortices enter.

Even though one can visualize such differences and, accordingly, infer the existence of a limiting frontier among both regimes, it is not an easy task to assign a specific value of L for the threshold size. As will be further discussed in this paper, the meso-to-macroscopic frontier separates a region of pure macroscopic behavior from another where mesoscopic and macroscopic characteristics coexist. Based on our simulations for a large number of samples with different sizes, we came

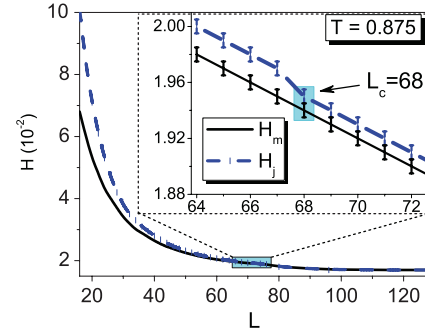


FIG. 2. (Color online) Size dependence of H_j and H_m , indicating that both superimpose (within the precision bar of the simulations) above the threshold value L_c . The zoomed area highlights the saturation point.

to the conclusion that the occurrence of local minima on the magnetization curves is due solely to the additional repulsion among vortices, which become important when the sample dimensions are sufficiently small, a feature that we take as the guiding line to quantify the meso-macro threshold criterion for such a rather subtle crossover. Thus, for a fixed temperature, we take the critical size L_c as that for which $H_m = H_j$. This means that, for sizes greater than L_c , the sample behaves as a macroscopic superconductor, in the sense that vortices nucleating at opposite sides do not interact before entering; below L_c , the mesoscopic regime dominates, as a consequence of the size of the sample being smaller than the interaction range. Figure 2 shows the size dependence of H_m and H_j for $T = 0.875$. The zoomed up box emphasizes the difference among both quantities; the vertical bars correspond to the width of the field step in our simulations, $\Delta H = 10^{-4}$. Taking the critical size as that above which the vertical bars start to overlap, we determined $L_c = 68$ for this temperature.

We have also investigated the surface contribution to the magnetic free energy of the system in the whole range of values of L studied here. At the jump, this energy term is proportional to the difference among two field integrals, between zero and H_j , of the magnetization: the bulk (i.e., surface-free) case, exhibiting a perfect Meissner response ($-4\pi M = H$), and the finite sample, for which the magnetization is affected by repulsion among nucleating vortices. To illustrate this point, the energy of the state of the sample immediately before the first penetration is shown in Fig. 3, as a function of the sample size. As can be seen, such energy decreases monotonically with L and its derivative saturates, within a certain precision indicated by the error bars, at a length scale that is quite close to $L_c(T)$ found by the criterion described previously. Our search for other evidences of this regime transformation included the size dependence of the initial slope of $M(H)$, which also exhibits a smooth variation with respect to L .

The following remarkable characteristics of this meso-to-macroscopic crossover were observed: (i) for $L > L_c$, at any temperature, the symmetry of the vortex lattice is hexagonal, as shown in the upper $L = 96$ panel of Fig. 4, which also indicates that it is destroyed upon increase of the field, from $H = 0.126$

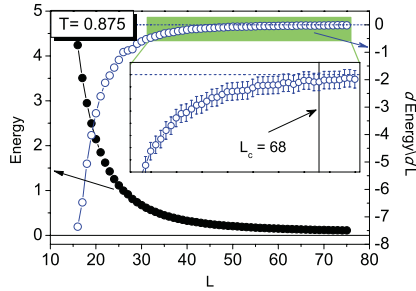


FIG. 3. (Color online) Black circles: energy as a function of L ; blue circles: derivative of the energy with respect to L . The energy was calculated as $\int_0^{H_j} B dH$, where B is the induction, and H_j is the field right before the first entrance of vortices; in this calculation, only the magnetic field energy inside the superconductor is accounted for. The temperature is $T = 0.875$.

to $H = 0.127$, and that superconductivity remains only at the borders. Notice that there is a quite close coincidence between this field and $H_{c2}(T = 0.875) = 1 - 0.875 = 0.125$, which represents the applied field sufficient to destroy the vortex lattice for a bulk superconductor. We will comment further about it later on. (ii) For $L \ll L_c$ the vortex lattice most predominantly has square symmetry; depending on T and L , one can also have giant vortex states coexisting with single vortices.^{20,21} Such behavior can be seen in the lower $L = 20$ panel of Fig. 4; for $H = 0.110$, two vortices penetrate the sample and a giant vortex with two flux quanta is formed at the center. Nonetheless, for $H = 0.126$, two more vortices enter into the sample and the giant vortex splits in four separate entities, following the fourfold symmetry of the problem. (iii) The most interesting characteristic of the meso-to-macro occurs for $L \lesssim L_c$; for high external applied fields, that is, close to the Abrikosov upper critical field $H_{c2}(T)$, when the density of vortices is large, the lattice develops a progressive crossover from hexagonal to square symmetry. We illustrate this scenario in the $L = 64$ panels of Fig. 4 for $T = 0.875$. As shown in this figure, for applied fields still low but sufficient to form a vortex lattice ($H = 0.110$) the symmetry is hexagonal. As we increase the field, the symmetry is somewhat mixed, with hexagons at the central portions of the sample and squares closer to the edges, as illustrated for $H = 0.113$ and $H = 0.123$. For even higher fields ($H = 0.127$), the lattice is eventually destroyed and surface superconductivity survives only at the surface.

We have also studied the system for lower temperatures, as exemplified in Fig. 5 for $T = 0.3125$, at which $L_c = 38$. To describe the vortex configurations around L_c , two samples were chosen, one right below ($L = 36$) and the other right above ($L = 40$) the crossover value. For $H = 0.600$, vortices are displayed in hexagonal lattices for both samples. However, at $H = 0.620$ and $H = 0.694$, triangular and square vortex lattices coexist for sample $L = 36$, whereas for these same values of the applied field, the vortex lattice remains triangular for sample $L = 40$. Eventually, at sufficiently high applied fields, the vortex lattice is entirely destroyed on both samples; for $T = 0.3125$ the suppression of the vortex

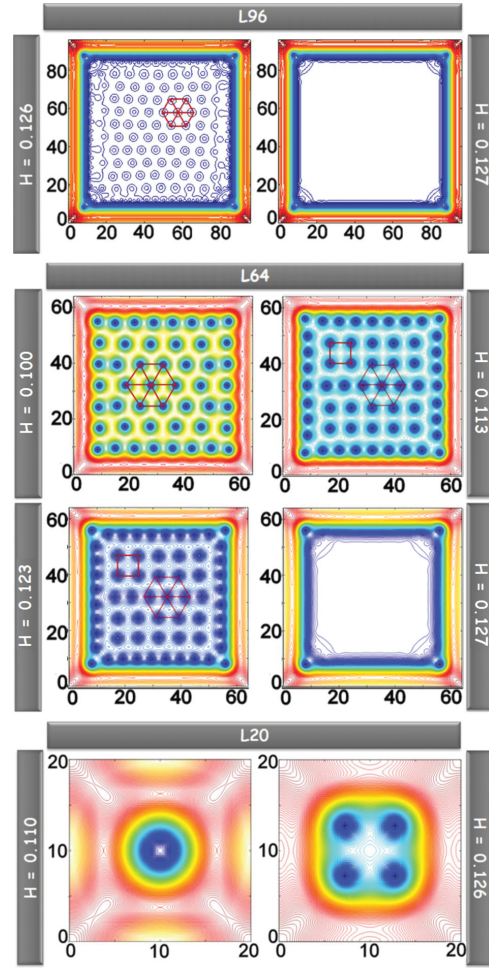


FIG. 4. (Color online) Vortex lattice for samples $L = 96$, $L = 64$, and $L = 20$ for several values of the external field at temperature $T = 0.8750$. The upper panel shows that a hexagonal vortex lattice is maintained until the suppression of superconductivity in the center of the sample $L = 96$. In the middle panel, the crossover of the vortex lattice, that takes place below the threshold line, is shown for sample $L = 64$. The lower panel shows that, far below the threshold line L_c (in this case $L = 20$), the vortices follow the symmetry of the sample due to size effects.

lattice occurs at $H = 0.695$. Again, notice that this field, as already seen for $T = 0.875$, is very close to the upper critical field $H_{c2}(T = 0.3125) = 1 - 0.3125 = 0.6875$. We see thus that, for different temperatures, the value of the applied field sufficient to destroy the lattice, but not superconductivity at the surface, is quite close to the Abrikosov field $H_{c2}(T)$ for bulk samples. We take this as a robust evidence of the accuracy of our simulations. At $T = 0.875$, only surface superconductivity remains on sample $L = 64$ for $H \geq 0.127$ (Fig. 4); the same

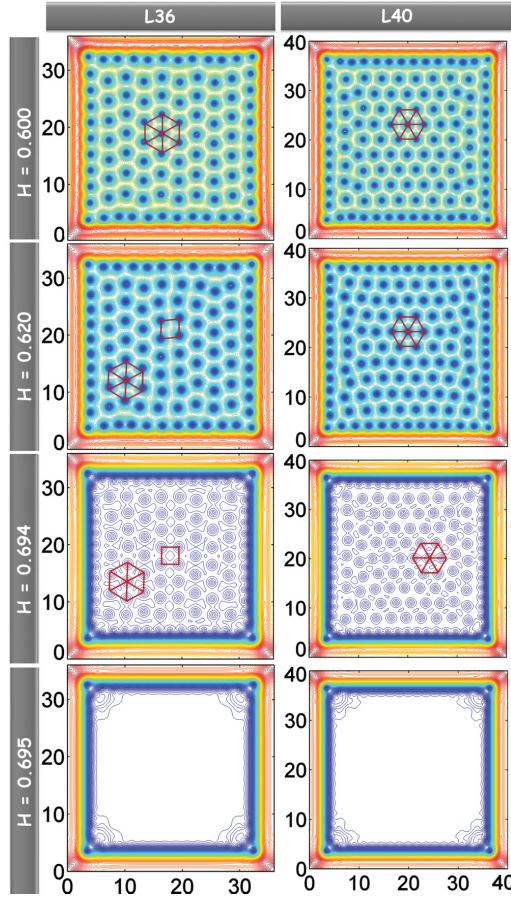


FIG. 5. (Color online) Vortex lattice for samples $L = 36$ and $L = 40$ for several values of the external field, at $T = 0.3125$. Notice that, for the macro sample ($L = 40$), vortices always form a hexagonal lattice. A crossover between hexagonal and square lattices takes place for the mesoscopic sample ($L = 36$). Right below L_c , the system starts developing a hexagonal lattice for low densities of vortices, but still carries vestiges of the mesoscopic regime as this density increases, developing a mixture of square and hexagonal vortex lattice.

at $T = 0.3125$ (Fig. 5) feature occurs for samples $L = 36$ and $L = 40$ for $H \geq 0.695$.

As stressed before, the vortex lattice always displays hexagonal symmetry for sample dimensions above L_c . A quantitative evidence, that the picture that comes out from the simulations indeed corresponds to a triangular lattice, can be obtained from the structure factor of the system. Figure 6 shows contour plots of the order parameter [Figs. 6(a) and 6(c)] and the corresponding structure factors of the vortex lattice for sample $L = 128$ at $H = 0.126$ [Fig. 6(b)] and $H = 0.127$ [Fig. 6(d)]. Considering the peak values of the structure factor in Fig. 6(b), we obtained the vector basis oriented

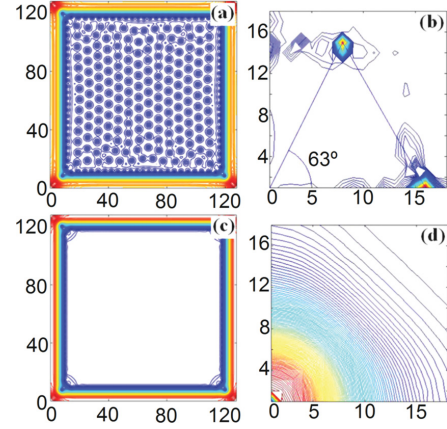


FIG. 6. (Color online) Topology of the superconducting density of the Cooper pairs $|\psi|^2$, and its corresponding structure factors, for sample $L = 128$. Top: $H = 0.126$, bottom: $H = 0.127$. Notice that the vortex lattice disappears abruptly at $H = 0.127$ [panels (c) and (d)], close to the Abrikosov bulk upper critical field $H_{c2}(T = 0.875) = 0.125$. The structure factor was calculated as the absolute value of the fast Fourier transform of $|\psi|$.

as approximately an equilateral triangle, as expected for an Abrikosov type-II superconductor. Notice that just a small increase in the applied field destroys the vortex lattice and the peaks in the structure factor disappear [Figs. 6(c) and 6(d)]. It is therefore clear that, for $L = 128$, the system is already in the macroscopic regime, exhibiting a genuine Abrikosov lattice, which disappears along with volume superconductivity.

In order to construct an L - T phase diagram, we repeated, for several temperatures, the procedure employed to determine L_c , as discussed above and exemplified in Figs. 1 and 2. The resulting phase diagram is shown in Fig. 7. Such diagram separates the region where the superconductor behaves predominantly as a macroscopic sample from that where a mesoscopic behavior takes place. We have used the expression $L_c(T) = L_0(1 - T)^n$ to fit the data, considering L_0 and n as free adjustable parameters. The value of L_0 corresponds to the length scale for which the mesoscopic-macroscopic transformation occurs at zero temperature; n is the critical exponent. The best fit, shown in Fig. 7 along with the data, gives $L_0 = 36.5$ and $n = -0.292 \approx -2/7$. Thus, it is clear that the length scale for the crossover between both regimes is much larger than the London penetration depth $\lambda(T) = \kappa/\sqrt{1 - T}$. A comparison between $L_c(T)$ and $\lambda(T)$ can be seen in Fig. 7. In real units, if we take $\xi(0) = 10$ nm, which is a typical size of low T_c type-II superconductors, then the value of $L_c(T)$ would range from 365 to 1150 nm as T varies from zero to 0.9375. This is of the same order of magnitude where size effects disappear in nanoparticle systems.³¹

The threshold line changes very little for different materials, as one can infer from the two curves shown in Fig. 7, for $\kappa = 5$ and $\kappa = \infty$. Not only the values for the infinity κ limit of the TDGL equations differ only a few percent from those obtained for $\kappa = 5$, but also the overall tendency of the two curves is similar, to an extent that the fitting exponent for both

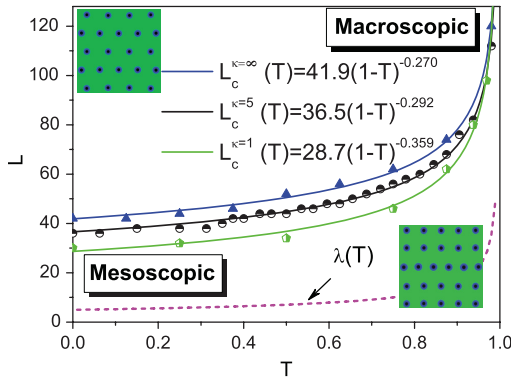


FIG. 7. (Color online) The L_c - T phase diagram; above the critical line the superconductor behaves as a macroscopic sample; below it, a mesoscopic behavior takes place. The insets indicate that for $L > L_c$ the lattice is always hexagonal, whereas for $L < L_c$ the system may develop other types of symmetries (see text). $\lambda(T)$ for $\kappa = 5$ is also shown for comparison.

is virtually the same ($\sim -2/7$), as evidenced in Fig. 7. It is not surprising that there is no significant differences between the characteristics of the $L_c(T)$ curves, since the vortex states are indistinguishable for $\kappa \geq 5$, as it was demonstrated in Ref. 32. For low values of κ the $L_c(T)$ curve presents the same dependence with T , however, if such curve is compared with that one for $\kappa = 5$, significant changes can be observed in the value of the n exponent, which is approximately $-5/14$, and the value of L_0 .

Recently, Connolly *et al.*³³ have made a similar study in order to find the meso-to-macro crossover for a superconducting disk. They used a criterion based in the competition between Abrikosov vortex lattice and shell-like ordering. As a result, they obtained that the crossover occurs in the diameter range of $[20\lambda(T), 40\lambda(T)]$ [in our units, $(20\kappa/\sqrt{1-T}, 40\kappa/\sqrt{1-T})$], which differs from our results for large κ .

As a final remark, we can surely say that our mapping of the frontier between the mesoscopic and macroscopic length scale could be an important guide for the fabrication of samples with desirable dimensions for which one can observe mesoscopic effects in superconductivity.

IV. CONCLUSION

In short, based on the physical evidence that, in the mesoscopic regime, vortices nucleating at the sample surface interact with each other even at the very early stages of their inception, we have developed a systematic procedure to determine the crossover between mesoscopic and macroscopic regimes of superconductivity in small samples. The progressive change of symmetry of the vortex lattice, from square to hexagonal, is intimately related to the meso-to-macro crossover and further emphasizes the robustness of our criterion.

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