Tutorial
BEC and quantized vortices in superfluidity and superconductivity
6-7 December 2007
Institute for Mathematical Sciences
National University of Singapore

Vortices in superconductors: I. Introduction

François Peeters

Universiteit Antwerpen

Literature

- Superconductivity of Metals and Alloys, P. G. De Gennes (Addison-Wesley, New York, 1989).
- Introduction to superconductivity, M. Tinkham (Mc. Graw Hill, New York, 1966).
- Vortices in unconventional superconductors and superfluids, Eds. R.P. Huebener, N. Schopohl and G.E. Volovik (Springer, Berlin, 2002).
- Fundamentals of the theory of metals, A. A. Abrikosov (North-Holland, Amsterdam, 1988).
- Quantum theory of solids, C. Kittel (John Wiley & Sons, N.Y., 1987).
- Theory of superconductivity, J.R. Schrieffer (Benjamin/Cummings Publ. Comp., London, 1964).

Overview

I. Introduction to superconductivity
1. **Historical introduction**
2. Basic properties & early phenomenological theories
3. Phase transitions and the GL theory
4. Type-I and type-II superconductors
5. Molecular dynamics: London approach
6. Numerical solution of GL-equations

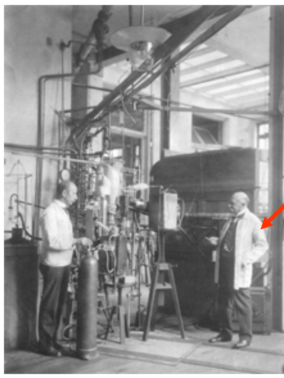
I.1. Historical survey

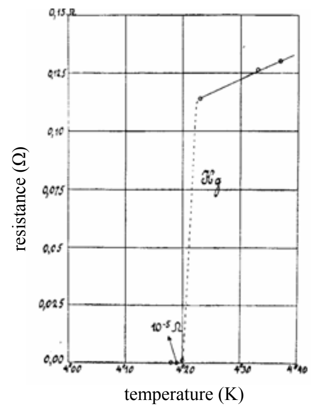
- 1911: Discovery of superconductivity
- 1933: Meissner effect
- 1935: London theory
- 1950: Ginzburg-Landau theory
- 1957: BCS theory
- 1986: Discovery of high T_c superconductors
- 1991: Superconducting fullerenes
- 2000: MgB_2

Discovery of superconductivity

1911: H. Kamerlingh Onnes (Leiden)

First basic property: “Perfect conductivity”

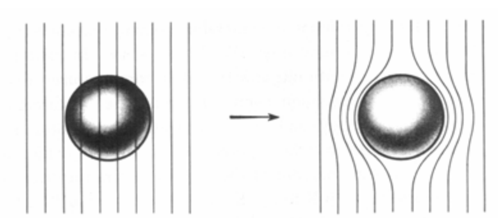




Nobel prize: 1913

Meissner effect

1933: Meissner and Ochsenfeld



Magnetic levitation

Second basic property: “Perfect diamagnetism”

London theory

F. London and H. London
Proc. R. Soc. London Ser. A **149**, 71 (1935).

First attempt to develop a theory to describe the electrodynamics of a superconductor:
- absence of resistance
- Meissner effect

Fritz London (1900–1954), for many years a professor at Duke University, was the first to suggest that both superconductivity and superfluid flow in liquid helium are manifestations of quantum effects operating on the scale of macroscopic objects.

Ginzburg-Landau theory

- 1950: Ginzburg and Landau
  They introduced the order parameter Ψ:
  $\Psi = 0$ when $T > T_c$
  $\Psi \neq 0$ when $T < T_c$
  Ψ is related to the density of superconducting electrons n_s as
  $$|\Psi|^2 = n_s/2$$
  Ψ is in general a spatial varying function
  GL theory was able to explain the distinction between type-I and type-II superconductors

BCS theory

- 1956: Cooper
  Superconducting electrons are coupled two by two and such a pair has a lower energy than two individual electrons.
  → “Cooper-pairs”
- 1957: Bardeen, Cooper and Schrieffer
  → Microscopic theory

Nobel prize: 1972

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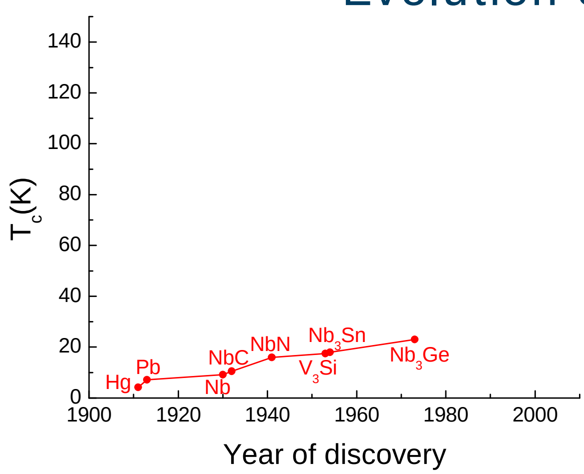
Evolution of T_c



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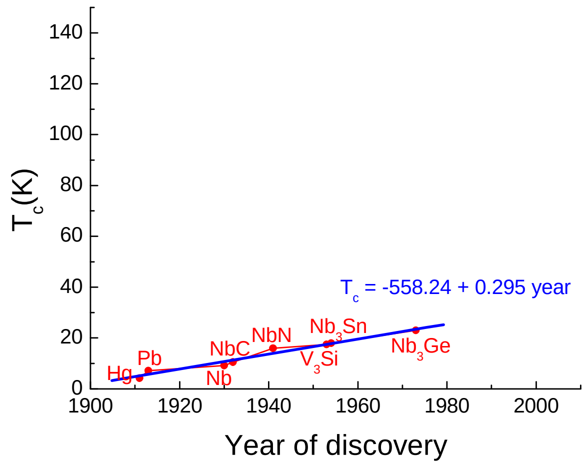
Evolution of T_c



High T_c superconductors

J.G. Bednorz and K.A. Müller,
Z. Phys. B **64**, 189 (1986)

IBM Zurich Research Laboratory,
Rüschlikon, Switzerland.

Nobel prize: 1987

High T_c superconductors

1973 : Nb_3Ge

T_c = 23.2K

Intermetallic material with A15 structure

Spring 1986 : La-Ba-Cu-O

Bednorz and Müller

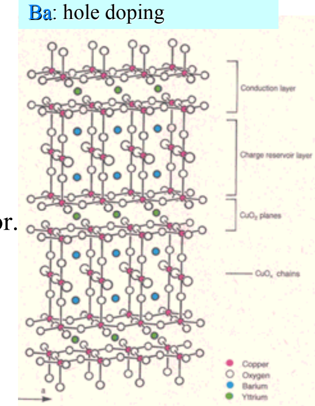
T_c = 36K; about 10K higher than any previously known superconductor.

November 1986 : Y-Ba-Cu-O

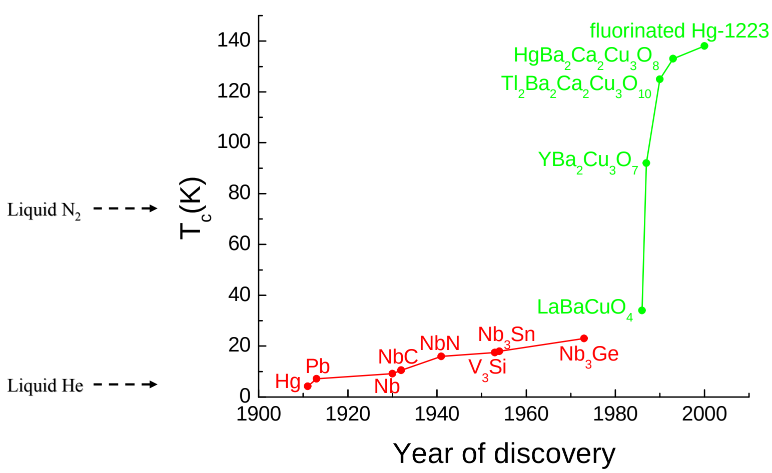
P.C.W. Chu (University of Houston)

T_c > 90K

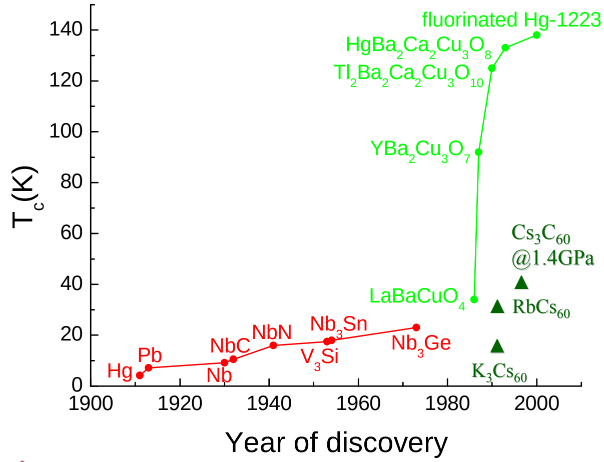
Y: separates the CuO-layers
Ba: hole doping



High T_c superconductors



Fullerenes



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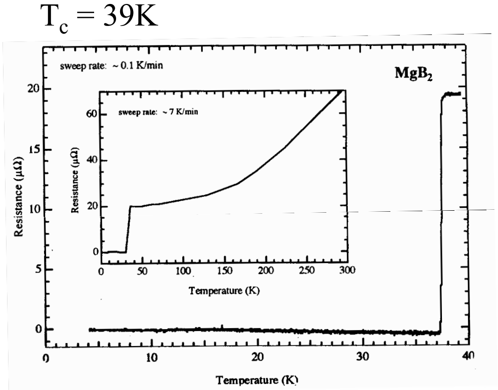
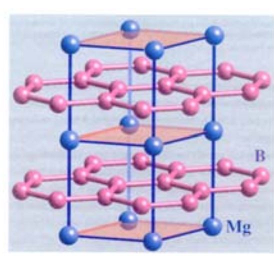
Discovery of MgB_2

I. Nagamatsu et al., Nature **410**, 63 (2001).

$T_c = 39K$





Hexagonal AlB_2-type crystal structure. B-atoms form graphite like sheets which are separated by hexagonals layers of Mg atoms.

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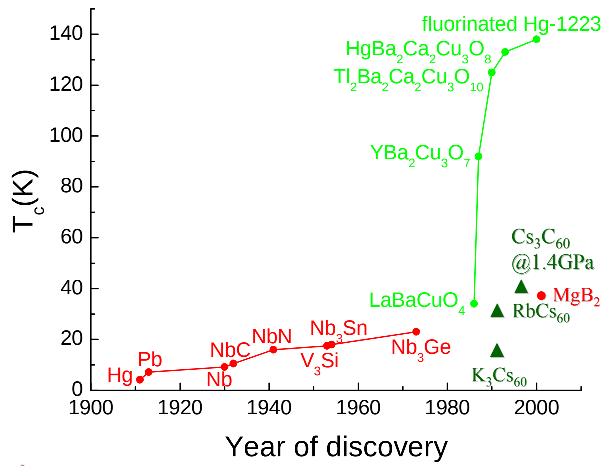
MgB_2



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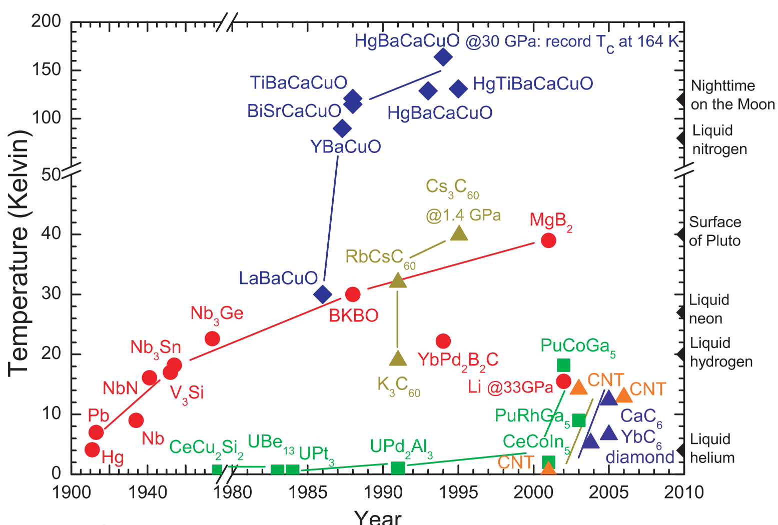
Transition temperatures



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Overview

I.2. Basic properties

- Perfect conductivity: zero resistance
- Meissner effect: perfect diamagnetism

London equation

F. London and H. London, Proc. R. Soc. London Ser. A **149**, 71 (1935).

First attempt to develop a theory to describe the electrodynamics of a superconductor: ➔ absence of resistance
➔ Meissner effect

A free electron in an electric field: $m\frac{d\vec{v}}{dt} = e\vec{E}.$

$\vec{j} = n_e e\vec{v}$ with n_e the electron density.

$$\frac{\partial}{\partial t}\left(\Lambda\vec{j}\right) = \vec{E} \quad \text{with} \quad \Lambda = \frac{m}{n_e e^2}$$

➔ Zero resistance!

$$\frac{\partial}{\partial t} rot\,\Lambda\vec{j} = \underbrace{rot\,\vec{E}}_{-\frac{1}{c}\frac{\partial\vec{B}}{\partial t}} \quad \text{(Maxwell eq.)} \qquad \Rightarrow \frac{\partial}{\partial t}\left(rot\,\Lambda\vec{j} + \frac{1}{c}\vec{B}\right) = 0$$

London equation:

$$rot\,\Lambda\vec{j} + \frac{1}{c}\vec{B} = 0 \qquad \text{or (because B=rotA):} \qquad \vec{j} = -\frac{1}{c\Lambda}\vec{A}$$

London equation

Next we will show that London's equation gives that inside a superconductor:

$$\vec{j} = 0 \quad \text{and} \quad \vec{B} = 0$$

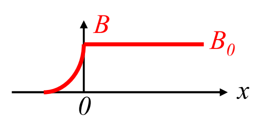
$$rot\,\vec{B} = \frac{4\pi}{c}\vec{j} \quad \text{(Maxwell equation)} \Rightarrow rot\,rot\,\vec{B} = \frac{4\pi}{c} rot\,\vec{j}$$
$$= grad\left(div\,\vec{B}\right) - \Delta\vec{B}$$

$rot\,\Lambda\vec{j} + \frac{1}{c}\vec{B} = 0$: London equation

$\Delta\vec{B} - \frac{1}{\lambda_L}\vec{B} = 0$ with $\lambda_L = \sqrt{\frac{mc^2}{4\pi n_e e^2}}$ the London penetration depth

This equation accounts for the **Meissner effect**.
Example: for a superconductor which occupies the half-space $x < 0$: $B(x) = B_0 e^{-|x|/\lambda_L}$
with B_0 the magnetic field at the surface.

From the London equation: $j_y(x) = \frac{cB_0}{4\pi\lambda_L} e^{-|x|/\lambda_L}$



London equation

It was assumed that all electrons participate in the superconducting current
➔ λ_L depends on temperature ➔ $n_e(T)$.

➲ Different form for London equation:

$$\vec{B} = rot\,\vec{A}$$

- $rot\left(\Lambda\vec{j}\right) + \frac{1}{c}\vec{B} = 0 \Rightarrow rot\left(\Lambda\vec{j} + \frac{1}{c}\vec{A}\right) = 0 \rightarrow \vec{j} = \frac{1}{\Lambda c}\vec{A}$
- $rot\,\vec{E} = -\frac{1}{c}\frac{\partial\vec{B}}{\partial t} \Rightarrow rot\left(\vec{E} + \frac{1}{c}\frac{\partial\vec{A}}{\partial t}\right) = 0 \rightarrow \vec{E} = -\frac{1}{c}\frac{\partial\vec{A}}{\partial t}$

Equalities are valid up to a gradient-term, i.e. rot (grad) = 0.
In fact it corresponds to the following gauge choice: $div\,\vec{A} = 0$

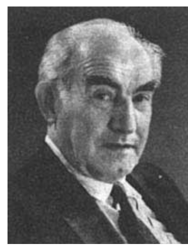
Theory is valid in the limit $\xi \rightarrow 0$ or extreme type-II materials.

Overview

Ginzburg-Landau theory

- Developed by Ginzburg and Landau in 1950.
- Based on the ideas of Landau's theory of second-order phase transitions.
- Gor'kov showed in 1959 that the GL equations can be derived from the BCS theory in the limit $T_c - T << T_c$.

V.L. Ginzburg



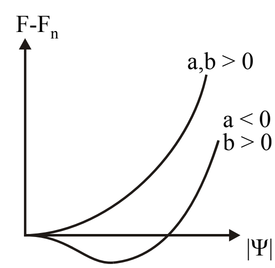
L.D. Landau

GL-theory: derivation

- Order parameter: wave function of Cooper-pairs in the Bose condensate
  $\Psi(\vec{r})$: characterizes all particles of the condensate
- Near the critical temperature $T \sim T_c \rightarrow \Psi(\vec{r})$ is small

$$F = F_n + a|\Psi|^2 + ½b|\Psi|^4 + ...$$

and a and b can be expanded in $\tau = (T-T_c)/T_c$.



For $T > T_c$: $|\Psi| = 0$ and thus we must have $a > 0$.
For $T < T_c$: $|\Psi| \# 0$ and consequently $a < 0$.
Therefore to first order in τ : $a = \alpha\tau$ with $\alpha > 0$.
$b > 0$ because $|\Psi|$ must be finite.

GL-theory: Equilibrium & Thermodynamics

Equilibrium: $\frac{\partial F}{\partial \Psi} = 0 \rightarrow \Psi\left(\alpha\tau + b|\Psi|^2\right) = 0$

$$\begin{cases} \Psi = 0 \quad ; \quad T > T_c \\ |\Psi|^2 = -\frac{\alpha\tau}{b} = |\Psi_0|^2 \quad ; \quad T < T_c \end{cases}$$

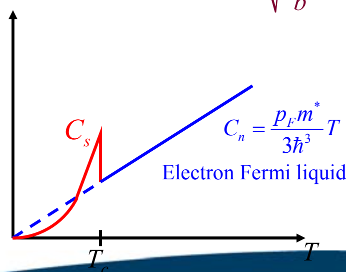
$$F_n - F_s = \frac{(\alpha\tau)^2}{2b} = \frac{H_c^2}{8\pi}$$

thermodynamic critical field of a bulk superconductor: $H_c = \sqrt{\frac{4\pi}{b}}\alpha\frac{T_c - T}{T_c}$

Thermodynamics:

specific heat: $C = -T\frac{\partial^2 F}{\partial T^2}$

$$C_n - C_s = -\frac{T}{T_c}\frac{\alpha^2}{b}$$



GL-theory: external magnetic field

When an external magnetic field is applied:

$H(\vec{r})$ → because of the Meissner effect.

$\Psi(\vec{r})$ → order parameter is a spatial varying function.

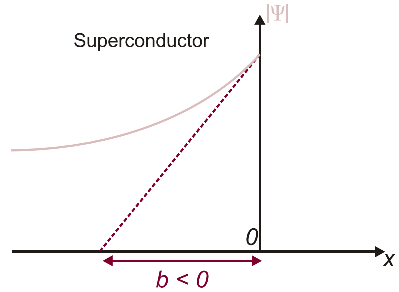
Energy:

- $\frac{H^2}{8\pi}$: energy of magnetic field per unit volume.
- $|\vec{\nabla}\Psi|^2$: energy due to spatial variation of Ψ (if variation is slow).
- $-i\hbar\vec{\nabla} \rightarrow -i\hbar\vec{\nabla} - \frac{2e}{c}\vec{A}$: because Ψ is wavefunction of Cooper-pairs.

$$F_s = F_n^{H=0} + \int dV\left[\alpha\tau|\Psi|^2 + \frac{b}{2}|\Psi|^4 + \frac{1}{4m}\left|\left(-i\hbar\vec{\nabla} - \frac{2e}{c}\vec{A}\right)\Psi\right|^2 + \frac{H^2}{8\pi}\right]$$

Boundary condition

$$\vec{n}\cdot\left(-i\vec{\nabla}-\vec{A}\right)\ \psi\Big|_{\text{boundary}}=\frac{i}{b}\psi\Big|_{\text{boundary}}$$



GL-theory: comments

All constants appearing in the GL theory have a microscopic interpretation (from the derivation from BCS):

- $\alpha/b=n_e$: total electron density
- $\alpha=\left(12\pi^2/7\zeta(3)\right)\left(mT_c^2/p_F^2\right)$
- $\Psi(\vec{r})=\left(7\zeta(3)n_e/8\pi^2\right)^{1/2}\left(\Delta(\vec{r})/T_c\right)$: $\Delta(\vec{r})$=superconducting gap

GL-theory: region of validity

pure superconductors:

$$1 \gg \left|\frac{T-T_c}{T_c}\right| \gg \left(\frac{T_c}{E_F}\right)^4$$

T_c/E_F: thermal fluctuations (~ 10^{-3})
Thus: GL theory is valid up to T_c.

dirty superconductors:

$$1 \gg \left|\frac{T-T_c}{T_c}\right| \gg \left(\frac{\hbar}{\tau_{tr}}\right)^3 \frac{T_c}{E_F}$$

This condition is less stringent, but it also practically rules out the fluctuation regime.

→ Thus, fluctuations are unimportant in the thermodynamics of bulk superconductors.

→ But in high-T_c ceramics the fluctuation regime is relatively large. This can be due to the small correlation length (~ 30Å) or the relatively large value of T_c/E_F.

→ In thin films and filaments the role of fluctuations increases.

Ginzburg-Landau formalism

condensation energy (<0) — interaction energy (>0) — internal magnetic field

$$F_s = F_n + \int d\vec{r} \left(\alpha |\Psi(\vec{r})|^2 + \frac{\beta}{2}|\Psi(\vec{r})|^4 + \frac{1}{2m^*}\Psi^*(\vec{r})\left\{-i\hbar\nabla - \frac{e^*}{c}\vec{A}(\vec{r})\right\}^2 \Psi(\vec{r}) + \frac{1}{8\pi}(h(\vec{r}) - H)^2 \right)$$

kinetic energy operator for Cooper pairs: m*=2m, e*=2e — applied magnetic field

$$\alpha = -\frac{\hbar^2}{2m\xi_o^2}\left(1-\frac{T}{T_o}\right)$$, length scales: $\xi = \hbar/\sqrt{-m^*\alpha}$ (coherence length), $\lambda = \frac{c}{4e}\sqrt{\frac{m}{\pi}}\sqrt{\frac{\beta}{-\alpha}}$ (penetration length)

Ginzburg Landau equations

$$F_s\left[\Psi,\vec{A}\right] \quad\rightarrow \frac{\delta F_s}{\delta\Psi}=0, \qquad \frac{\delta F_s}{\delta\vec{A}}=0$$

$$\frac{1}{2m}\left(-i\hbar\vec{\nabla}-\frac{2e}{c}\vec{A}\right)^2\Psi=-\alpha\Psi-\beta\Psi\left|\Psi\right|^2$$

$$\left(-i\hbar\vec{\nabla}-\frac{2e}{c}\vec{A}\right)_n\Psi=0$$

$$\vec{\nabla}\times\vec{\nabla}\times\vec{A}=\frac{4\pi}{c}\vec{j}$$

$$\vec{j}=\frac{e\hbar}{im}\left(\Psi^*\vec{\nabla}\Psi-\Psi\vec{\nabla}\Psi^*\right)-\frac{4e^2}{mc}\left|\Psi\right|^2\vec{A}$$

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Dual point of the GL equations

Dimensionless free energy: $F=\int dV\left[\frac{1}{2}B^2+\kappa^2\left(1-\left|\Psi\right|^2\right)^2+\left|\left(\vec{\nabla}-i\vec{A}\right)\Psi\right|^2\right]$

The GL equations are obtained by minimizing F with respect to Ψ and $\vec{B}=\vec{\nabla}\times\vec{A}$

$$\left(\vec{\nabla}-i\vec{A}\right)^2\Psi=2\kappa^2\Psi\left(1-\left|\Psi\right|^2\right) \qquad \& \qquad \vec{\nabla}\times\vec{B}=2\vec{j}$$

where the current is given by $\vec{j}=\mathrm{Im}\left(\Psi^*\vec{\nabla}\Psi\right)-\left|\Psi\right|^2\vec{A}$, and
the boundary condition at the superconducting/insulater interface: $\left(\vec{\nabla}-i\vec{A}\right)\Psi\Big|_n=0.$

The GL equations are coupled nonlinear second-order differential equations.

$\kappa=1/\sqrt{2}$ → Dual point of the GL equations.
→ Separates type-I and type-I superconductors.

It was identified by Bogomol'nyi [Sov. J. Nucl. Phys. **24**, 449 (1997)] in the general context of stability and integrability of classical solutions of some quantum field theories.

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Dual point

For $\kappa = 1/\sqrt{2}$ the GL equations can be reduced to first-order differential equations.

Introducing the operator $D = \partial_x + i\partial_y - i\left(A_x + iA_y\right)$ one can write the GL equations at $\kappa = 1/\sqrt{2}$ as the two Bogomol'nyi equations: $D\Psi = 0$

$B = 1 - |\Psi|^2$

These two equations can be decoupled and one obtains that |Ψ| is a solution of the second-order nonlinear equation $\nabla^2 \ln|\Psi|^2 = 2\left(|\Psi|^2 - 1\right)$.

Relation to other fields:

- the equation is related to the Liouville equation.
- it appears in other situations, eg. Higgs, Yang-Mills and Chern-Simons field theories.

It was proven that these equations admit families of vortex solutions.

See e.g. E. Akkermans and K. Mallick, J. Phys. A: Math Gen. **32**, 7133 (1999).

Gross-Pitaevskii equation

Nonlinear Schrödinger equation.

Bose-Einstein condensation of dilute gasses:

$$i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = H_0 \Psi(\vec{r},t) + \underbrace{N_0 U_0 \left|\Psi(\vec{r},t)\right|^2}_{} \Psi(\vec{r},t)$$

Potential due to the mean field of all the other atoms.

$\Psi(\vec{r},t)$: condensate wave function

N_0 : number of particles in the condensate

Interaction between the atoms → modeled by a zero-range potential whose strength is given by the s-wave scattering length a → $U_0 = 4\pi\hbar^2 a/m$.

$H_0 = H_{kin} + V_{trap}$

Overview

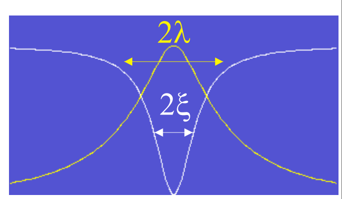
I. Introduction to superconductivity

Bulk superconductors

- Two characteristic length scales:
  - Coherence length ξ: typical length scale over which the size of the Cooper-pair density can vary.
  - Penetration depth λ: typical length scale over which the magnetic field can vary.
- Ginzburg-Landau parameter κ determines type of superconductivity:

$$\kappa = \frac{\lambda}{\xi} < \frac{1}{\sqrt{2}} \quad \text{Type-I}$$

$$\kappa = \frac{\lambda}{\xi} > \frac{1}{\sqrt{2}} \quad \text{Type-II}$$



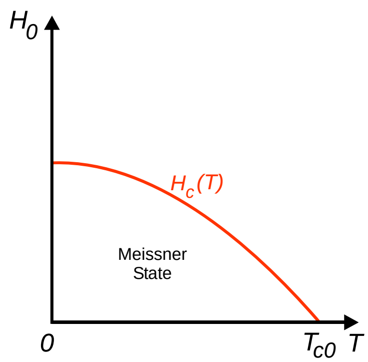
Properties of some superconductors

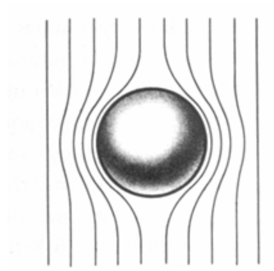
Superconductor	T_c (K)	B_{c2} (T)	ξ (nm)	λ (nm)	
Al	1.2	0.01	550	40	Type I
Nb	9.3	0.21	38	39	Type I
Sn	3.7	0.031	230	34	Type I
Pb	7.2	0.078	83	37	Type I
Nb_3Ge	23.2	39	3	90	
Nb_3Sn	17.9	24	3	65	
V_3Si	17	23	3	60	
$PbMo_6S_8$	15.2	60	2.2	215	
$LaMo_8Se_8$	11	5			
MgB_2	39	19-40	2-5	85-180	
UPd_2Al_3	2.0	$\sim$40			
UPt_3	0.46	1.9	12-14	600	
K_3C_{60}	19.3	17-32	$\sim$3	240	
Rb_3C_{60}	29.6	38	$\sim$2		
High T_c: $La_{2-x}Ba_xCuO_4$[1]; x=0.2	30		3.3	290	
High T_c: $YBa_2Cu_3O_{7-\delta}$[1]	93	115	2.5	150	
High T_c: $Bi_2Sr_2Ca_2Cu_3O_{10}$[1]	110	198	2.9		
High T_c: $TbBa_2Ca_2Cu_3O_9$[1]	123			173	
High T_c: $HgBa_2Ca_2Cu_3O_{8+\delta}$[1] at 30 GPa	164	190	1.3	130	

Type-I ⇔ type-II superconductors

The difference between the two types of superconductors refers to the way the superconducting state reacts to an applied magnetic field.

Type-I superconductors





Meissner State

Type-I

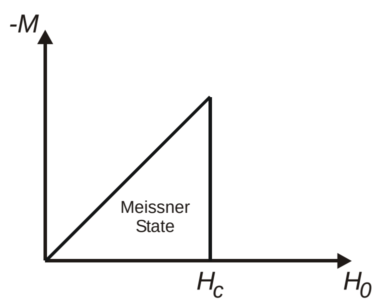
$$\vec{B} = \vec{H} + 4\pi \vec{M}$$

Inside the superconductor:

$$\vec{B} = 0 \Rightarrow \vec{M} = -\frac{1}{4\pi}\vec{H}$$

The superconductor is an ideal diamagnet:

$$\chi = -\frac{1}{4\pi}$$



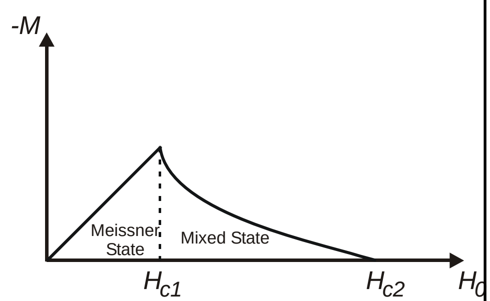
Type-II

Two critical magnetic fields.

$H < H_{c1}$: material behaves like a type-I superconductor.

$H > H_{c2}$: normal superconductor.

$H_{c1} < H < H_{c2}$: Mixed state: the magnetic field lines (i.e. vortices) penetrate the sample.
At the core of the vortices the material is in the normal state.



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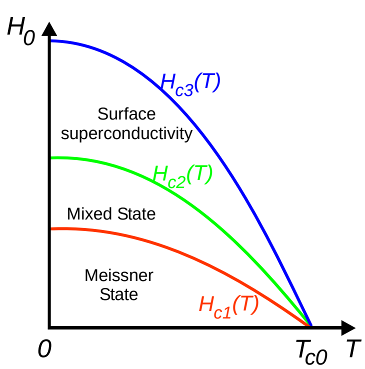
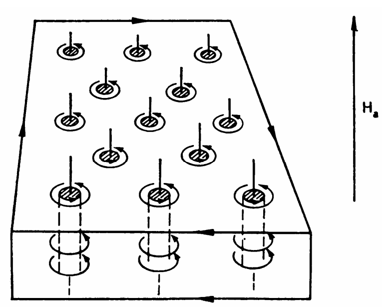
Type-II superconductors





Mixed state:
Abrikosov vortex lattice

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Type-II

First vortex creation ← first critical field

Magnetic field penetrates an area $\pi\lambda^2$.
Flux = flux quantum:
$$H_{c1}\pi\lambda^2 \approx \phi_0 \rightarrow H_{c1} \approx \frac{\phi_0}{\pi\lambda^2}$$

Maximum number of vortices ← second critical field

Vortices overlap → almost uniform penetration of magnetic field
Area of superconducting material between vortices ~ $\pi\xi^2$

$$H_{c2}\pi\xi^2 \approx \phi_0 \rightarrow H_{c2} \approx \frac{\phi_0}{\pi\xi^2}$$

Stabilization energy of a vortex.

$H_c^2/8\pi$ Thermodynamic condensation energy

$F_{core} \simeq \frac{H_c^2}{8\pi}\pi\xi^2$ Energy cost due to the decreased amount of superconducting phase.

$F_{mag} \simeq \frac{-B_a^2}{8\pi}\pi\lambda^2$ Energy gain because an amount of field does not have to be expelled.

$$F \simeq F_{core} + F_{mag} = \frac{1}{8\pi}\left(H_c^2\xi^2 - B_a^2\lambda^2\right)$$

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Type-II

$$F \simeq F_{core} + F_{mag} = \frac{1}{8\pi}\left(H_c^2\xi^2 - B_a^2\lambda^2\right)$$

The vortex is stable when $F < 0$.

$$F = 0 \rightarrow B_a \simeq H_c \underbrace{\frac{\xi}{\lambda}}_{\left(\frac{H_{c1}}{H_{c2}}\right)^2} = H_{c1}$$ First critical field

$H_{c2} \simeq \frac{H_c^2}{H_{c1}}$ Inverse relation between H_{c1} and H_{c2}.

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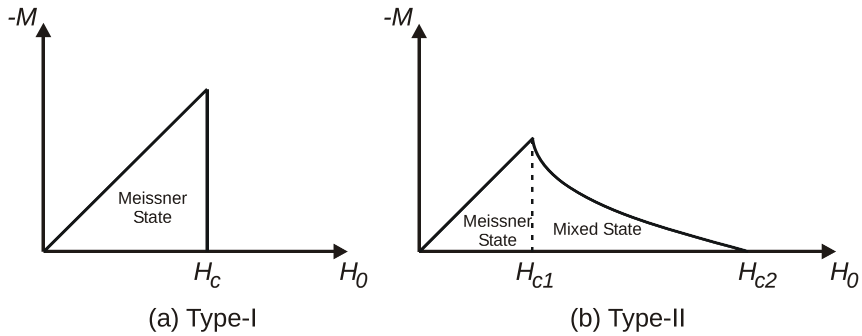
Magnetization

$$\vec{M} = \frac{1}{4\pi}\left(\vec{B} - \vec{H}_0\right)$$



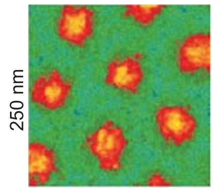
Mixed state: vortex lattice

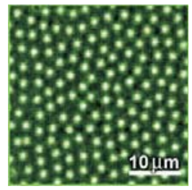
- **Abrikosov lattice in type II (hard) superconductors**
  A.A. Abrikosov, Soviet Phys. JETP **5**, 1174 (1957)
- **First experimental observation:**
  D. Cribier *et al*, Phys. Lett. **9**, 106 (1964)
  using neutron diffraction
- **Earliest visualization:**
  U. Essmann and H. Träube, Phys. Lett. A **24**, 526 (1967)
  using Bitter patterning

Imaging of vortices

STM image of Abrikosov vortices in MgB_2

M.R. Eskildsen et al,
Phys. Rev. Lett. **89**, 187003 (2002)





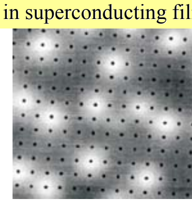
Magneto-optical image of vortex lattice in $NbSe_2$

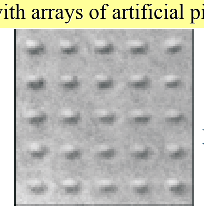
P.E. Goa et al, Supercond. Sci. Technol. **14**, 729 (2001)

Vortices in superconducting films with arrays of artificial pinning sites

Scanning Hall microscopy

S.B. Field et al,
Phys. Rev. Lett. **88**, 067003 (2002)





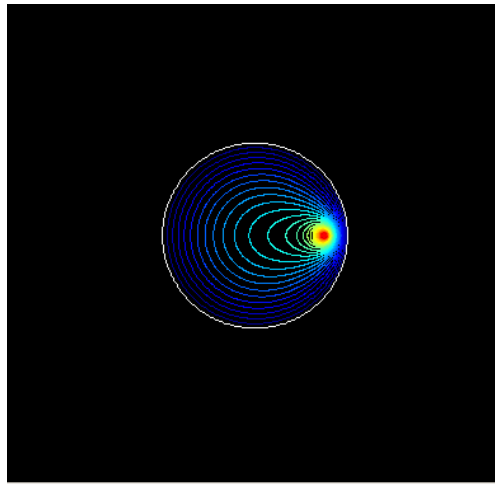
Lorentz microscopy

K. Harada et al,
Science **274**, 1167 (1996)

Overview

I. Introduction to superconductivity
   1. Historical introduction
   2. Basic properties & early phenomenological theories
   3. Phase transitions and the GL theory
   4. Type-I and type-II superconductors
   5. Molecular dynamics: London approach
   6. Numerical solution of GL-equations

Vortices in Confined Systems



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Vortices in confined systems

London approximation

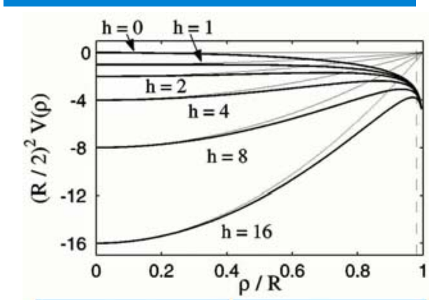
$$\mathcal{G} = \sum_{i=1}^{L}\left(\epsilon_i^{\text{self}} + \epsilon_i^{\text{shield}} + \sum_{j=1}^{i-1}\epsilon_{ij}\right)$$

$$\epsilon_{ij} = \left(\frac{2}{R}\right)^2 \ln\left[\frac{(r_i r_j)^2 - 2\boldsymbol{r}_i\cdot\boldsymbol{r}_j + 1}{r_i^2 - 2\boldsymbol{r}_i\cdot\boldsymbol{r}_j + r_j^2}\right]$$

$$\epsilon_i^{\text{self}} = \left(\frac{2}{R}\right)^2 \ln\left(1 - r_i^2\right)$$

$$r = \rho/R$$

$$\epsilon_i^{\text{shield}} = -2H_0\left(1 - r_i^2\right)$$



$$V = \varepsilon^{\text{self}} + \varepsilon^{\text{shield}}$$

$$h = R^2 H_0 / 2$$

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Theoretical model

- Dimensionless Ginzburg-Landau equations:

$$\left(-i\vec{\nabla} - \vec{A}\right)^2 \psi = \psi - |\psi|^2 \psi$$

$$\vec{\nabla} \times \left(\vec{\nabla} \times \vec{A}\right) = \frac{1}{\kappa^2}\left[\frac{1}{2i}\left(\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^*\right) - |\psi|^2 \vec{A}\right]$$

- Boundary conditions:

$$\vec{A}\Big|_{\infty} = \vec{A}_0$$

$$\vec{n} \cdot \left(-i\vec{\nabla} - \vec{A}\right) \psi\Big|_{\text{boundary}} = \frac{i}{b}\psi\Big|_{\text{boundary}}$$

length scale: $\xi = \hbar / \sqrt{-m^* \alpha}$

order parameter: $\psi_0 = \sqrt{-\alpha / \beta}$

vector potential: $c\hbar / 2e\xi$

magnetic field scale:
$H_{c2} = \kappa \sqrt{2} H_c = c\hbar / 2e\xi^2$

2D formalism

- axial symmetry and fixed vorticity *L*:

$$\Psi(\rho,\phi) = f(\rho)e^{iL\phi}$$

- Restriction to thin disks: *d* < ξ
- GL equations:

$$-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial F}{\partial\rho}+\left\langle\left(\frac{L}{\rho}-A\right)^2\right\rangle f = f\left(1-f^2\right) \qquad 1D$$

$$-\kappa^2\left(\frac{\partial}{\partial\rho}\frac{1}{\rho}\frac{\partial\rho A}{\partial\rho}+\frac{\partial^2 A}{\partial z^2}\right)=\left(\frac{L}{\rho}-A\right)f^2\theta\left(\frac{\rho}{R}\right)\theta\left(\frac{2|z|}{d}\right) \qquad 2D$$

2D formalism

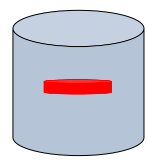
- Boundary conditions:
  - Vector potential: $\left.\vec{A}\right|_{\vec{r}\to\infty} = \frac{1}{2}\vec{e}_\phi H_0\rho$
  - Order parameter: $\left.\frac{\partial f}{\partial\rho}\right|_{\rho=R} = 0 \qquad \left.\rho\frac{\partial f}{\partial\rho}\right|_{\rho=0} = 0$

2D formalism

- Magnetic field created by supercurrents has a $H \approx 1/r^3$ dependence.

→ finite simulation region with size R_s and thickness d_s.

→ $$\begin{cases} A(z, \rho = R_s) = \frac{1}{2} H_0 R_s \\ A(|z| = d_s, \rho) = \frac{1}{2} H_0 \rho \end{cases}$$



2D formalism

- Finite difference representation:
  - Non-uniform space grid ρ_i, z_j
  - In every grid point *(i,j)*:
    - Order parameter: f_i
    - Vector potential: $A_{i,j}$
  - Iteration step *k*

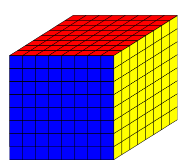
2D formalism

$$\eta_f f_i^k - \frac{2}{\rho_{i+1/2}^2 - \rho_{i-1/2}^2}\left(\rho_{i+1/2}\frac{f_{i+1}^k - f_i^k}{\rho_{i+1} - \rho_i} - \rho_{i-1/2}\frac{f_i^k - f_{i-1}^k}{\rho_i - \rho_{i-1}}\right)$$
$$+\left\langle\left(\frac{L}{\rho} - A\right)^2\right\rangle_i f_i^k - f_i^k + 3\left(f_i^{k-1}\right)^2 f_i^k = \eta_f f_i^{k-1} + 2\left(f_i^{k-1}\right)^3$$

$$\eta_a A_{j,i}^k - \frac{2\kappa^2}{\rho_{i+1/2} - \rho_{i-1/2}}\left(\frac{\rho_{i+1}A_{j,i+1}^k - \rho_i A_{j,i}^k}{\rho_{i+1}^2 - \rho_i^2} - \frac{\rho_i A_{j,i}^k - \rho_{i-1}A_{j,i-1}^k}{\rho_i^2 - \rho_{i-1}^2}\right)$$
$$-\frac{2\kappa^2}{z_{j+1/2} - z_{j-1/2}}\left(\frac{A_{j+1,i}^k - A_{j,i}^k}{z_{j+1} - z_j} - \frac{A_{j,i}^k - A_{j-1,i}^k}{z_j - z_{j-1}}\right) - \left(\frac{L}{\rho_i} - A_{j,i}^k\right)\left(f_i^k\right)^2 = \eta_a A_{j,i}^{k-1}$$

3D formalism

- General solution
- Restriction to thin disks d < λ and ξ
- GL equations:



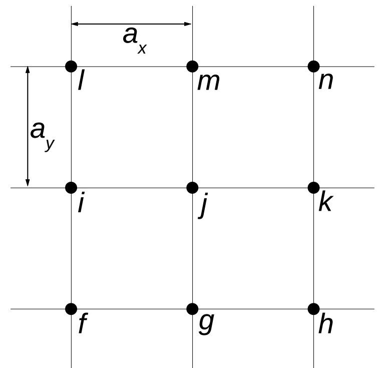
$$\left(-i\vec{\nabla} - \vec{A}\right)^2 \psi = \psi - |\psi|^2 \psi$$

$$-\Delta_{3D}\vec{A} = \frac{d}{\kappa^2}\delta(z)\vec{j}_{2D}$$

$$\text{where} \quad -\vec{j}_{2D} = \frac{1}{2i}\left(\psi^*\vec{\nabla}_{2D}\psi - \psi\vec{\nabla}_{2D}\psi^*\right) - |\psi|^2\vec{A}$$

3D formalism

- Finite difference representation:
  - Cartesian grid *(x,y)*
  - In grid point *j*:
    - Order parameter Ψ_j
    - Vector potential A_j
  - "Link variable approach"
  - Time derivatives to find steady-state solutions of the GL equations



3D formalism

- First GL equation:

$$\frac{\partial \Psi}{\partial t} = -\frac{1}{12}\left[\frac{U^{kj}\Psi_k}{a_x^2} + \frac{U^{ij}\Psi_i}{a_x^2} + \frac{U^{mj}\Psi_m}{a_x^2} + \frac{U^{gj}\Psi_g}{a_x^2} - \frac{4\Psi_j}{a_x^2} + (1-T)\left(\left|\Psi_j\right|^2 - 1\right)\Psi_j\right] + \tilde{f}_j(t)$$

where U is the link variable:

$$U_\mu^{r_1,r_2} = \exp\left[\int_{r_1}^{r_2} \vec{A}_\mu(\vec{r}) \cdot d\vec{\mu}\right] \quad (\mu = x, y)$$

3D formalism

- Second GL equation

$$j_{x,y} = \frac{1}{2}\left[\Psi^*\left(\frac{1}{i}\frac{\partial}{\partial x, y} - A_{x,y}\right)\Psi + \Psi\left(\frac{1}{i}\frac{\partial}{\partial x, y} - A_{x,y}\right)^*\Psi^*\right]$$

where the link variable is used: $\left(\frac{1}{i}\frac{\partial}{\partial x} - A_x\right)\Psi \rightarrow -i\frac{U_x^{kj}\Psi_k - \Psi_j}{a_x}$

From the supercurrents one calculates the vector potential:

$$-\Delta_{3D}\vec{A} = \frac{d}{\kappa^2}\delta(z)\vec{j}_{2D}$$

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Expansion method

- GL functional: $G = G_n + \int d\vec{r}\left(\alpha|\Psi|^2 + \frac{\beta}{2}|\Psi|^4 + \Psi^*\hat{L}\Psi\right)$

$\hat{L} = \frac{1}{2m^*}\left(-i\hbar\vec{\nabla} - \frac{e^*}{c}\vec{A}\right)^2$ → Kinetic energy operator with $e^* = 2e; \quad m^* = 2m$

- Orthonormal eigenfunctions of the kinetic energy operator $\hat{L}_i\psi_i = \varepsilon_i\psi_i$
- Expansion of the order parameter: $\Psi = \sum_i^N C_i\Psi_i$

→ GL functional: $G - G_n = (\alpha + \varepsilon_i)C_iC_i^* + \frac{\beta}{2}A_{kl}^{ij}C_i^*C_j^*C_kC_l$

with matrix elements $A_{kl}^{ij} = \int d\vec{r}\,\psi_i^*\psi_j^*\psi_k\psi_l$ → numerically calculated

See: V.A. Schweigert and F.M. Peeters, Phys. Rev. Lett. **83**, 2409 (1999)

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Expansion method

- The sample geometry enters in the calculations only through the eigenenergies ε_i and the eigenfunctions ψ_i, through the boundary condition.
- Circular symmetry: $\psi_{i=(l,n)} = \exp(il\phi) f_n(\rho)$ l: angular momentum, n: Landau level
- Expansion of order parameter over all eigenfunctions with $\varepsilon_i < \varepsilon_*$ (cut-off).
- Thus, the superconducting state is mapped in a 2D cluster of N particles (x,y) → (Re(C), Im(C)), which is governed by the Hamiltonian

$$G - G_n = (\alpha + \varepsilon_i) C_i C_i^* + \frac{\beta}{2} A_{kl}^{ij} C_i^* C_j^* C_k C_l.$$

- No distortion of the magnetic field:
  - → No second GL equation.
  - → Magnetic field = externel field everywhere (λ-large, i.e. κ=λ/ξ>>1)
  - → Improve by: solve LGL with effective H_{eff} which is taken as a varational parameter

See: J.J. Palacios, F.M. Peeters and B.J. Baelus, Phys. Rev. B **64**, 134514 (2001)

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The end – part I

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