Computer Simulation on the Vortex Lattice Melting in Type-II Superconductor

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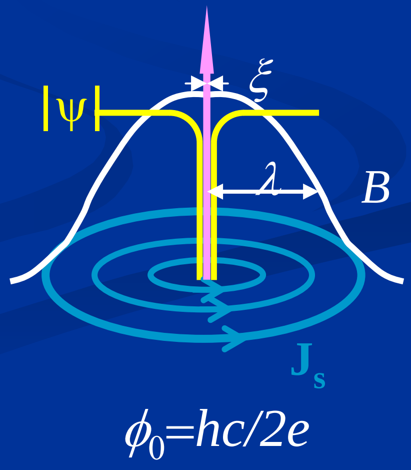


Ginzburg-Landau-Lawrence-Doniach model

- Gibbs free-energy functional for layered superconductors

$$G\left[\{\Psi_n\}\mathbf{A}\right] = \int d^2 R$$

$$\left\{ d\sum_n \left[\left(\alpha |\Psi_n|^2 + \frac{\beta}{2} |\Psi_n|^4 \right) + \frac{\hbar^2}{2m} \left| \left(\frac{\nabla^{(2)}}{i} + \frac{2\pi}{\phi_0} \mathbf{A}^{(2)} \right) \Psi_n \right|^2 \right. \right.$$

$$\left. \left. + \frac{\hbar^2}{2Md^2} \left| \Psi_{n+1} \exp\left(\frac{2\pi i}{\phi_0} \int_{nd}^{(n+1)d} dz A_z \right) - \Psi_n \right|^2 \right] + \int dz \left(\frac{B^2}{8\pi} - \frac{\mathbf{B}\cdot\mathbf{H}}{4\pi} \right) \right\}$$

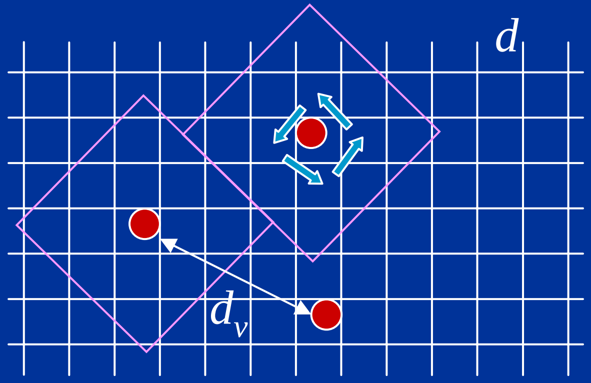
- Approximations:
  - constant B ⇐ $\xi_{ab} << d_v << \lambda_{ab}$
    ⇐ $\gamma d << \lambda_{ab}$ $\quad \gamma^2 = M/m$
  - constant $|\Psi|$ ⇐ $H << H_{c2}$
  - discretization in the *ab* plane ⇐ $\xi_{ab} << l_{ab}$

3D anisotropic XY model on phase variables

$$H = -J \sum_{\langle i,j\rangle \| \mathrm{ab-plane}} \cos\left(\varphi_i - \varphi_j - A_{ij}\right) - \frac{J}{\gamma^2} \sum_{\langle i,j\rangle \| \mathrm{c-axis}} \cos\left(\varphi_i - \varphi_j - A_{ij}\right)$$

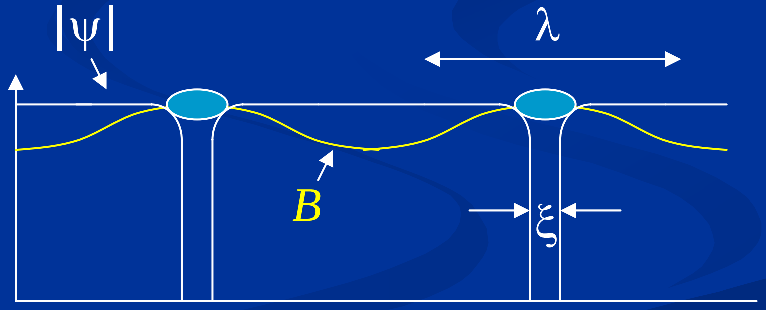
where $J = \frac{\hbar^2 |\psi|^2 d}{m} = \frac{\phi_0^2 d}{16\pi^3 \lambda_{ab}^2}$ $\quad \gamma = \frac{\lambda_c}{\lambda_{ab}}$ $\quad A_{ij} = \frac{2\pi}{\phi_0} \int_i^j \mathbf{A} \cdot d\mathbf{r}$

- Vortex:



$d_v \sim d/\sqrt{f}$

- A=(0, 0, -xB)
- $f = Bd^2/\phi_0$
- $\lambda \gg d_v \gg \xi$

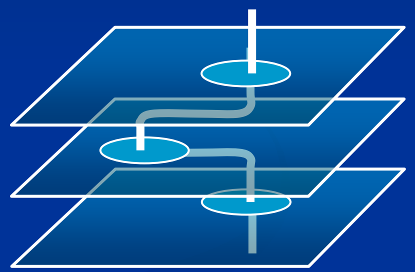


$$\sum_{cell} \left(\varphi_i - \varphi_j - A_{ij}\right)_{(-\pi,\pi)} = (n - f)2\pi$$

- advantages: (i) loop excitations (ii) short-range forces
- disadvantage: need a huge system of phases to support a few vortices

Monte Carlo simulations

- Typical process of MC simulations:
  - generate a random set of phases at a high *T*
  - cool system according to the Metropolis scheme
  - Measure *T* dependence of quantities
  - Search lattice structure



$\gamma^2=10$; f=1/25

- Parameters
  - System size: $L_{xy}=50$, $L_z=40$
  - Temp. skip: $\delta T=0.001J/k_B$
  - MC steps: $t\sim10^7$ sweeps
- relation to real material:

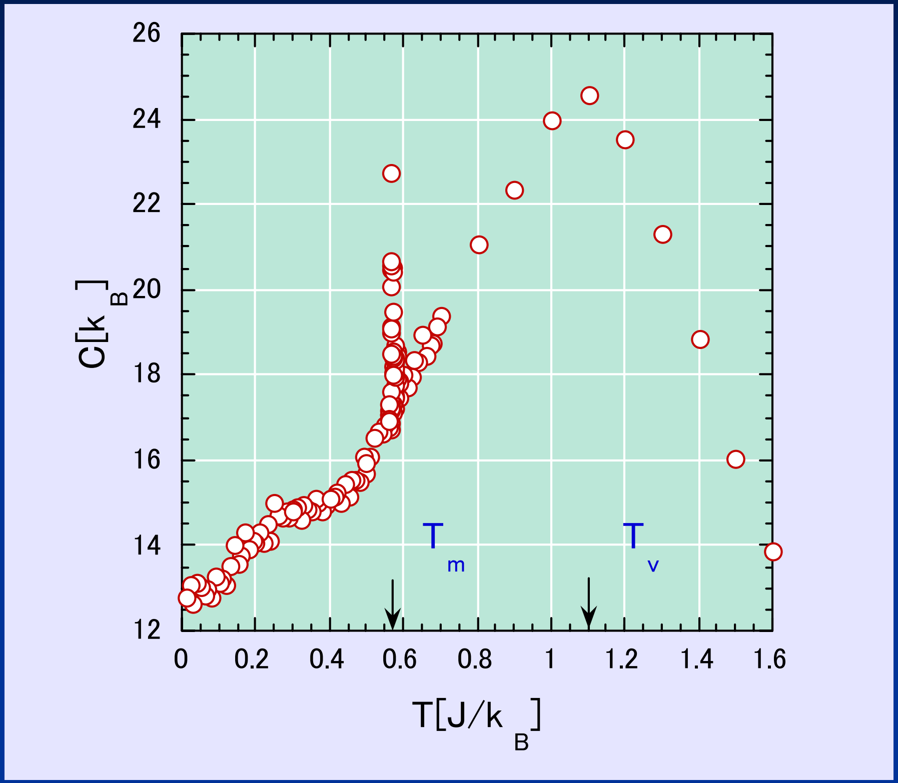
$$\gamma_{\text{model}} l_{ab} = \gamma_{\text{material}} d$$

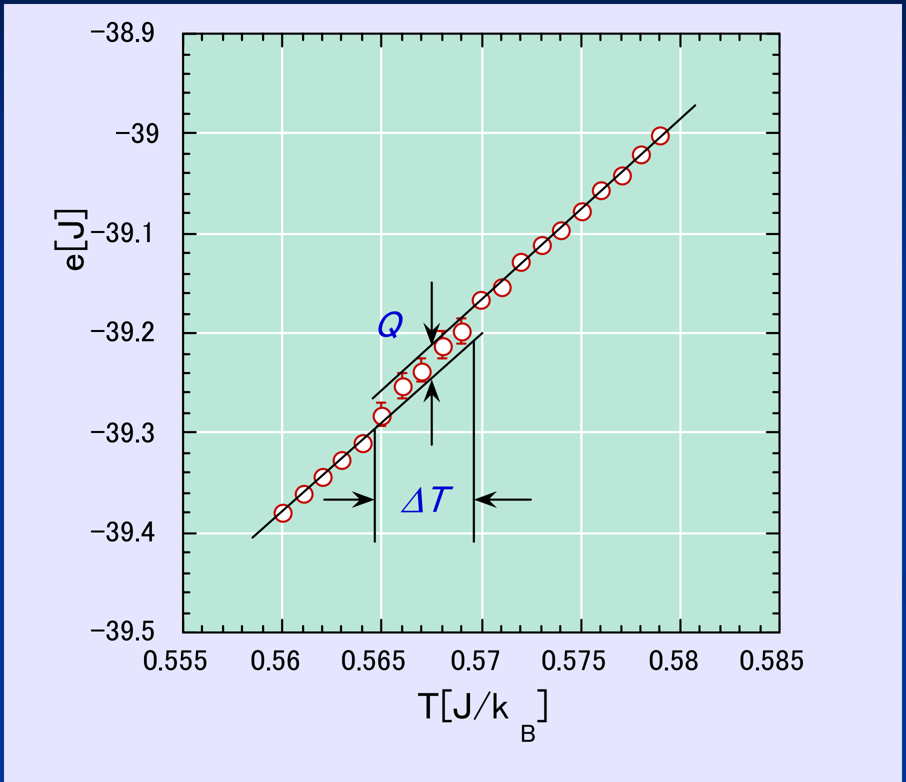
$$f=B\boldsymbol{l_{ab}}^2/\phi_0$$

$$J=\frac{\hbar^2|\psi|^2 d}{m}=\frac{\phi_0^2 d}{16\pi^3\lambda_{ab}^2}$$

- Difficulties: unknown spatial and temporal scales

First order thermodynamic phase transition





$C_+ \approx 18.5k_B$ $C_- \approx 17.5k_B$ $C_{max} \approx 23k_B$

$Q \approx 0.07k_BT_m$ $\Delta T \approx 0.008T_m$

- Finite size effects:

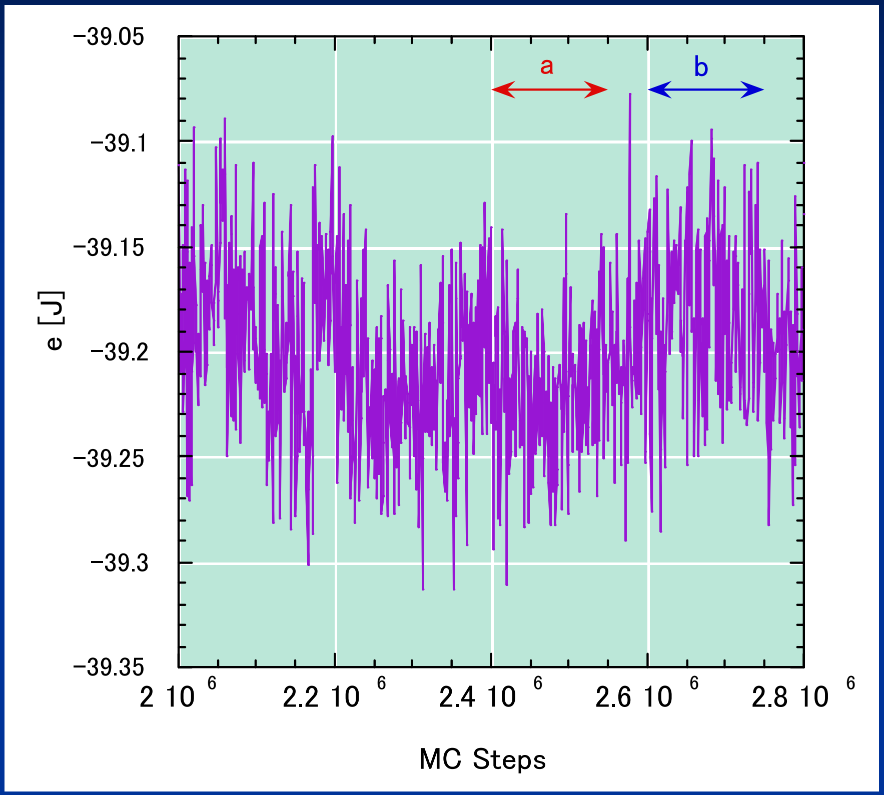
$$\Delta C = \frac{Q^2}{4k_BT_m^2}L_{xy}^2L_z f$$

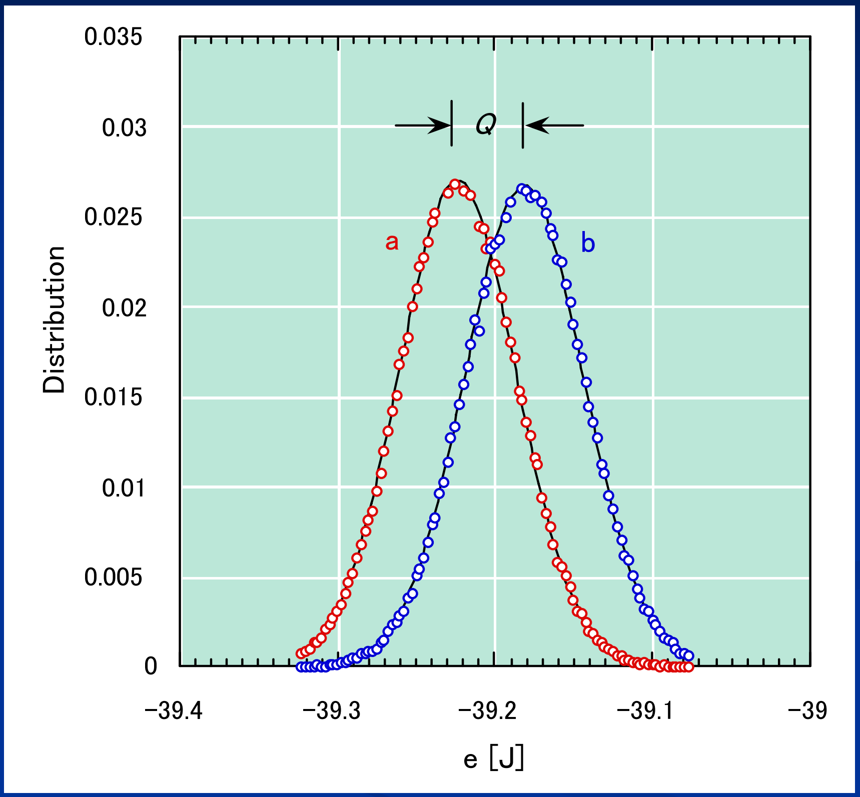
$$\Delta T = \frac{2k_BT_m^2}{QL_{xy}^2L_z f}$$

$\delta T = 0.001J/k_B$

$C = de/dT$

Fluctuation of internal energy at T_m





- $t_p \sim 3 \times 10^5$ MCS $t=10^7$ MCS
- Double Gaussian peaks
- Other method to differ 1st and 2nd order trs: $2/3 - V_L^{min} \sim Q^2/e^2$

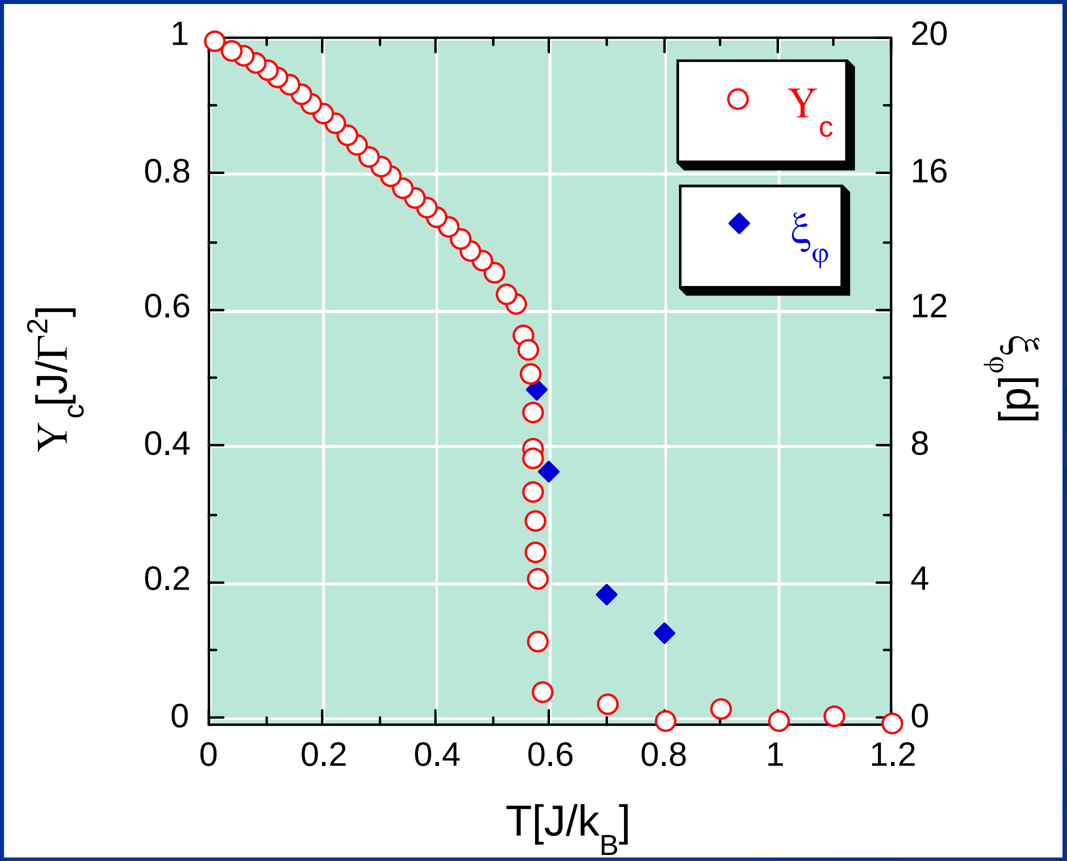
  $Q/e \approx 0.001$

Normal to superconductivity transition

- Helicity modulus

$$\varphi(z) \rightarrow \varphi(z) + \theta(z) \quad \text{where } \theta(z) = \theta \times (-1 + 2z/L)$$

$$\Upsilon = \lim_{\theta \rightarrow 0} \frac{F(\theta) - F(0)}{(\theta/L)^2 S}$$

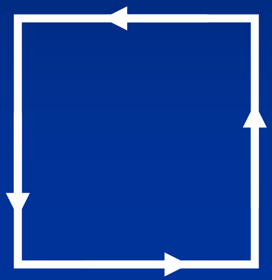


- U(1) Gauge symmetry broken at same point T_m
- long-range SC at $T<T_m$
- discontinuous jump in Υ_c
  ➔ first-order transition
- Υ_{ab} zero down to T~0
- $\xi_+ = 10d \sim L_c/4$
- $|\Psi|$ finite even for $T>T_m$

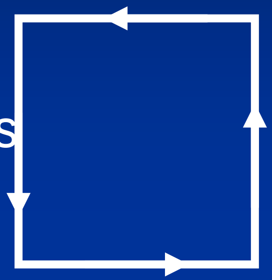
Y_{ab} in presence of vortex along c axis

Apply a phase twist

$\Delta\theta$

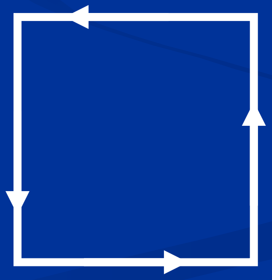


I increases



I decreases

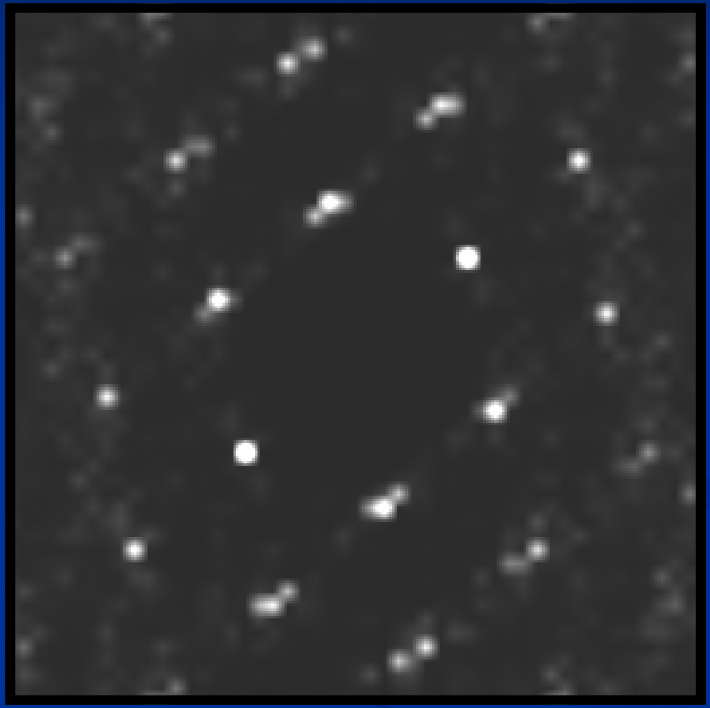
$$I_{j \to i} = \sin\left(\theta_j - \theta_i\right)$$



Slide the vortex to left side rightward

Melting of flux-line lattice

- structure factor
- ◇ correlation of density fluctuations

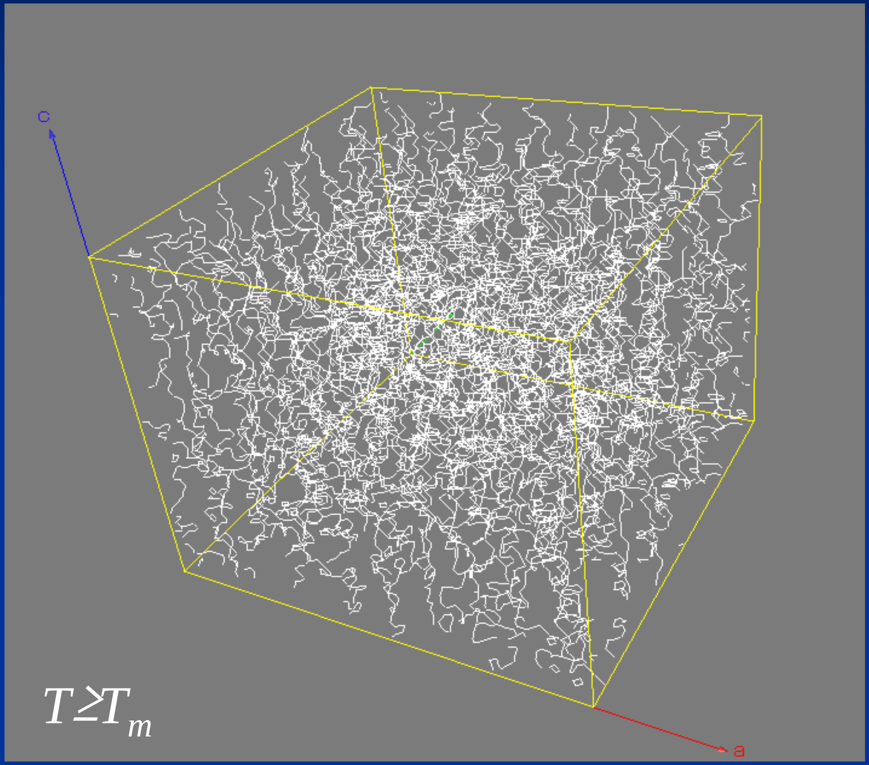


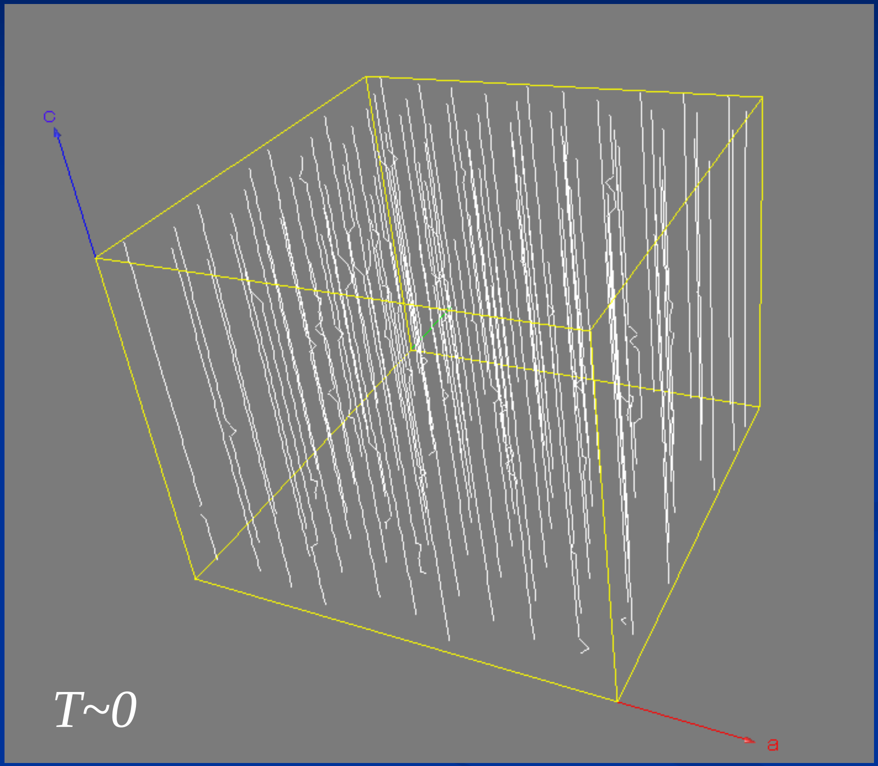
◇ T>T_{m}: flux line liquid

◇ T<T_{m}: flux line lattice

- translational & rotational symmetry broken at T_m
- simultaneous U(1) gauge and translational symmetry breakings

Real-space distribution of flux lines



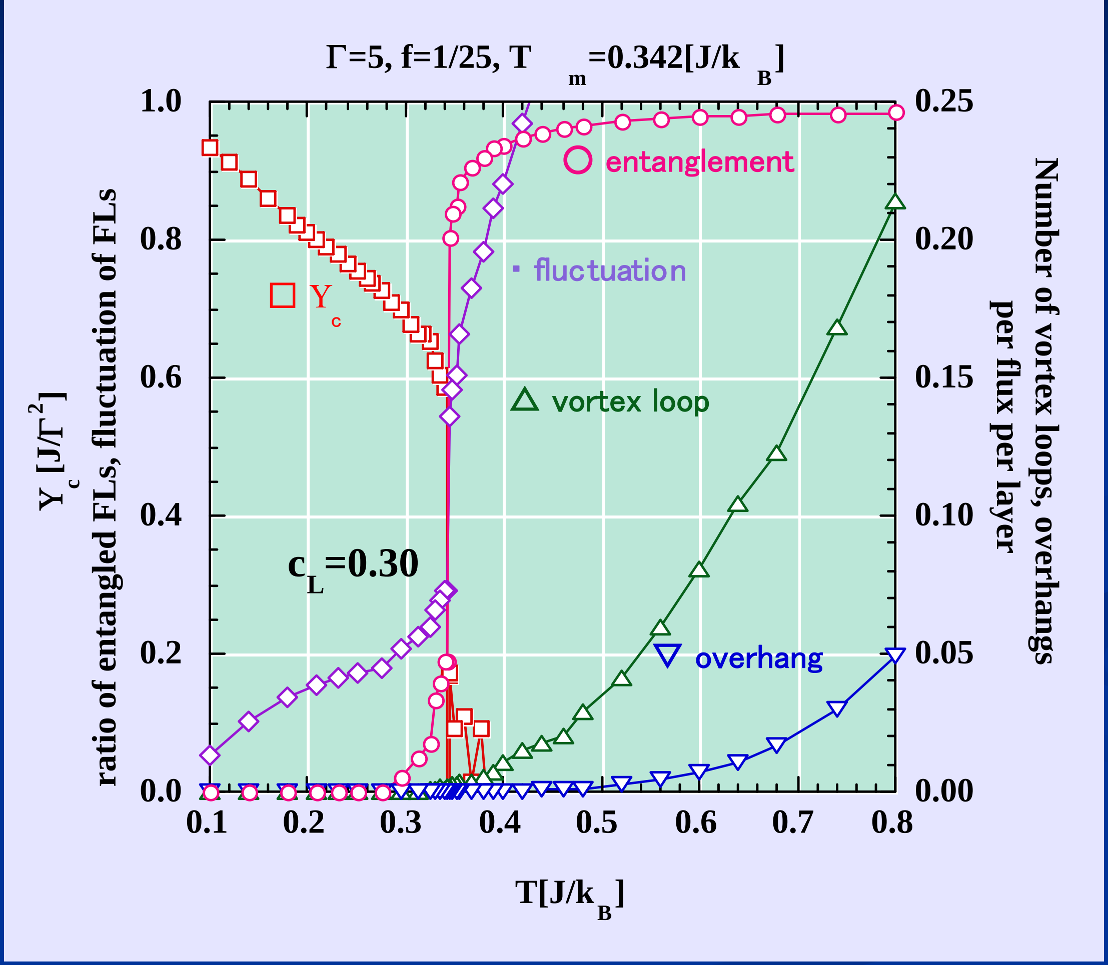


Flux-line liquid

Abrikosov flux-line lattice

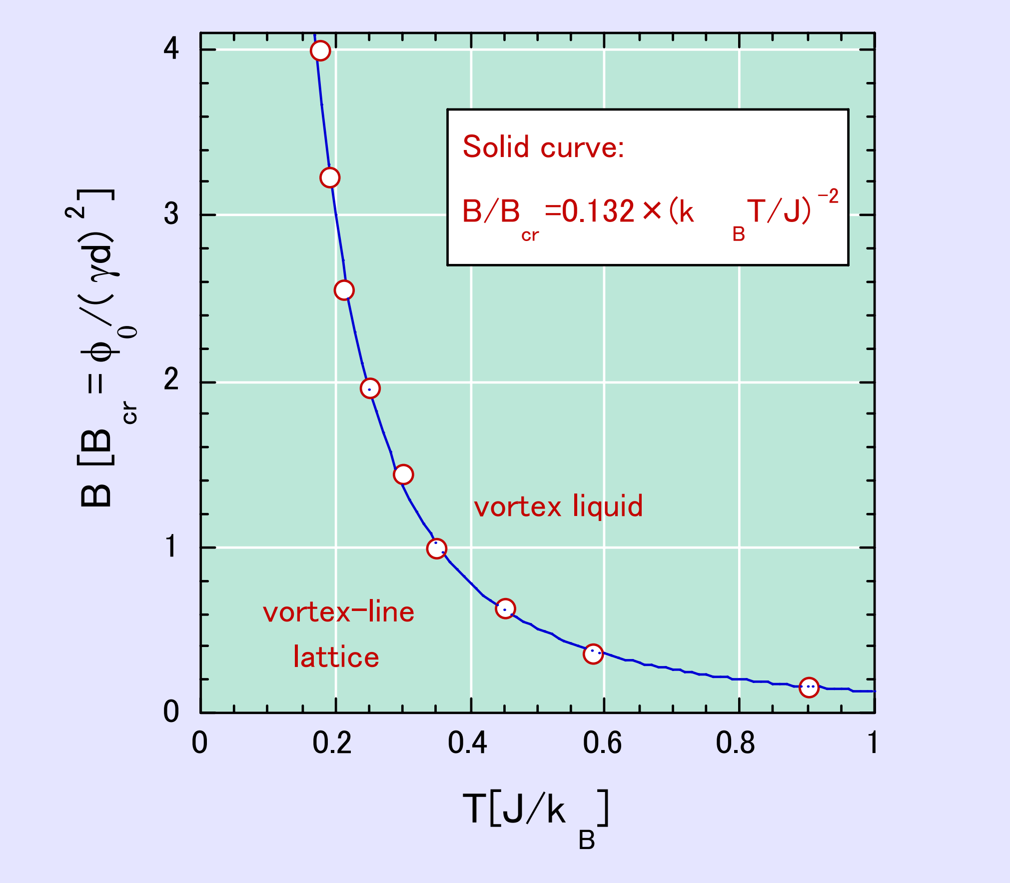
- Transition between flux line lattice to entangled line liquid

Mechanism of melting



- entanglement of flux lines

B-T phase diagram: melting line



□ $$B_m = 0.132 \times \frac{\phi_0}{(\gamma d)^2} \times (k_B T_m / J)^{-2}$$

□ Clausuis-Clapeyron relation:

$$\Delta B = -\frac{4\pi \Delta s}{dH_m / dT}$$

$B_{liquid} > B_{solid}$

Same as water!

□ Competition:

◇ Elastic energy

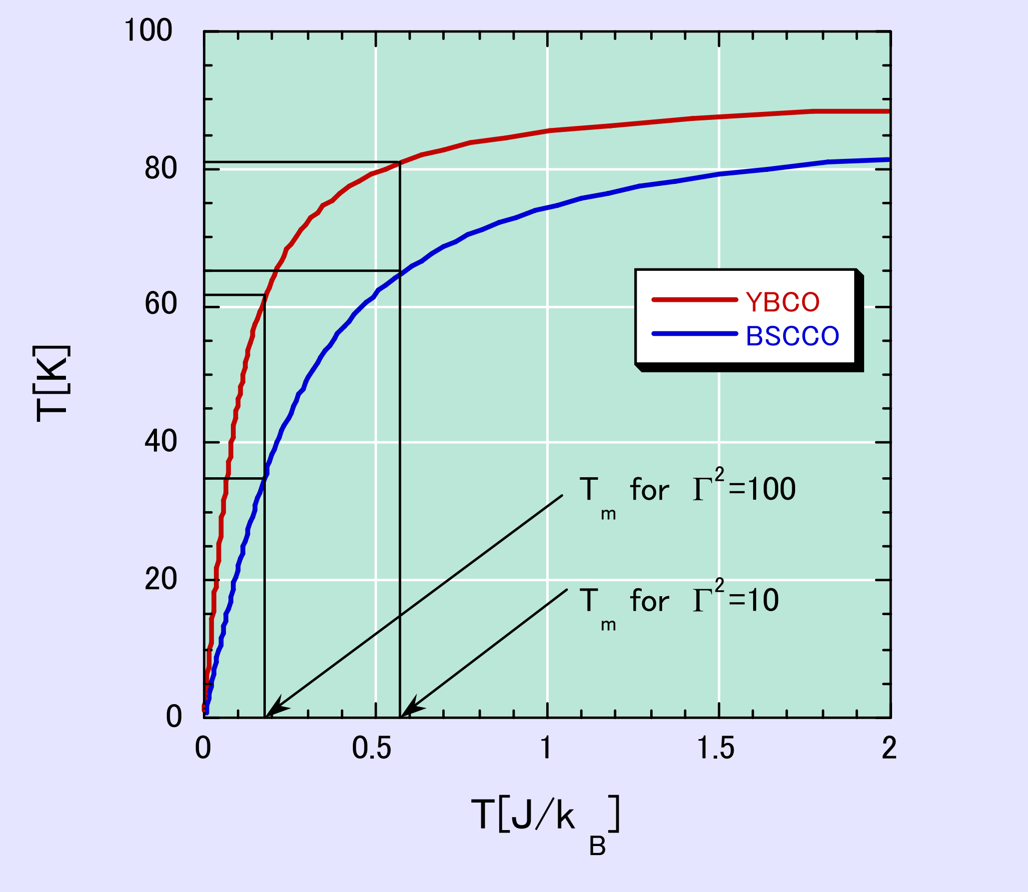
◇ Thermal fluctuation

◇Length scale in ab plane: γd

□ Lindemann number: $c_L = 0.18$ ⬄ Cage model

Temperature scale

- $$J = \frac{\phi_0^2 d}{16\pi^3 \lambda_{ab}^2(T)} = \frac{\phi_0^2 d}{16\pi^3 \lambda_{ab}^2(0)}\left(1-\left(\frac{T}{T_c}\right)^2\right)$$



Jump in entropy and magnetic induction

- T-dependent Hamiltonian
$$J=\frac{\phi_0^2 d}{16\pi^3\lambda_{ab}^2(0)}\left(1-\left(\frac{T}{T_c}\right)^2\right)$$

- Entropy
$$S=-\frac{\partial F}{\partial T}=\frac{\langle H\rangle - F}{T}-\left\langle\frac{\partial H}{\partial T}\right\rangle \quad \Rightarrow \quad \Delta S=\frac{1+(T_{\mathrm{m}}/T_{\mathrm{c}})^2}{1-(T_{\mathrm{m}}/T_{\mathrm{c}})^2}\times\frac{Q}{T_{\mathrm{m}}}$$

- Magnetic induction
  - Clausius-Clapeyron relation
  $$\Delta B=\frac{-4\pi}{dH_{\mathrm{m}}/dT}\times\Delta S\times\frac{B_{\mathrm{m}}}{d\phi_0}$$
  - shape of melting line
  $$\frac{dH_{\mathrm{m}}}{dT}\approx\frac{dB_{\mathrm{m}}}{dT}=\frac{-2B_{\mathrm{m}}}{T_{\mathrm{m}}}\times\frac{1+(T_{\mathrm{m}}/T_{\mathrm{c}})^2}{1-(T_{\mathrm{m}}/T_{\mathrm{c}})^2}$$

$$\Rightarrow \quad \Delta B=\frac{2\pi Q}{d\phi_0}$$

Comparison with experiments

- YBCO: $d=12\,Å$, $\lambda_{ab}(0)=1000\,Å$, $\gamma=8$, $T_c=92K$, $\kappa=100$ by Schilling et al.

B=8T	T_m[K]	$\Delta S[k_B/\text{vortex}]$	ΔB[G]
simulation	81	0.55	0.19
experiment	79	0.4	0.25

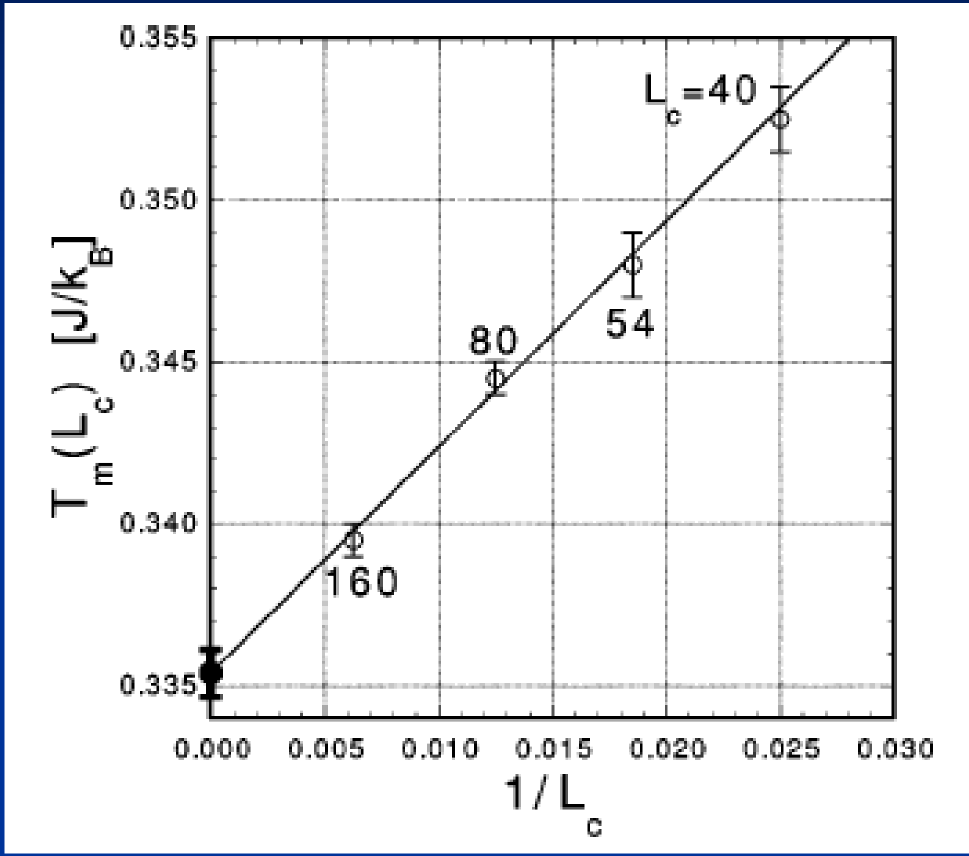
- BSCCO: $d=15\,Å$, $\lambda_{ab}(0)=2000\,Å$, $\gamma=150$, $T_c=90K$, $\kappa=100$ by Zeldov et al.

B=160G	T_m[K]	$\Delta S[k_B/\text{vortex}]$	ΔB[G]
simulation	65	0.22	0.12
experiment	65	0.4	0.35

- Condition for our model: $\xi << d_v << \lambda$

System size effect

f=1/25, Γ=5



$$T_m(L_c) = T_m(\infty) + A/L_c$$

Summary

- H. Nordborg and G. Blatter -- Phys. Rev. B, **58** p.14556-14571 (1998).

The absence of an analytical description of the vortex lattice melting transition has led a large interest in numerical simulations. A popular approach is to use the frustrated XY model or the closely related lattice London model. Unfortunately, many of the simulations have suffered from highly nontrivial finite-size effects and have indicated two transitions instead of one at low filling factors, whereas a first-order transition was seen at large filling factors. The problems have been overcome recently [Hu et al. 1997], and a picture with a single first-order transition is emerging.

X. Hu, S. Miyashita and M. Tachiki: Phys. Rev. Lett. vol. 79, p.3498 (1997)

- T. Schneider & J. M. Singer:

Phase transition approach to high temperature superconductivity: Universal properties of cuprate superconductors (Imperial College Press, 2000)

on p.224: Ten years after Abrikosov's classic prediction of a lattice of quantized vortices, the Abrikosov vortex lattice, as the ground state of type II superconductors when the magnetic field is tuned beyond a lower critical value, Eilenberger (1967) suggested that the lattice could melt close to the critical temperature of the system. The magnetic field versus temperature (H,T) phase diagram of the extremely type II superconductors has for some time been under intense investigation following suggestions that the melting transition of the vortex lattice in high temperature superconductors could be experimentally resolved [Gammel et al. (1987) and Nelson (1988)]. While it now appears well established that the vortex lattice in a clear limit of type II bulk superconductors melts in a first order phase transition, much less consensus has been reached on how to describe the state which the vortex lattice melts into, even in the clean limit. Recently, numerical simulations revealed, that the vortex liquid is incoherent, i.e. phase coherence is destroyed in all directions, including the direction of the applied magnetic field, as soon as the vortex lattice melts [Hu et al. (1997)…