DFT Approach for Melting Transition of Josephson Vortex Lattice in HTSC

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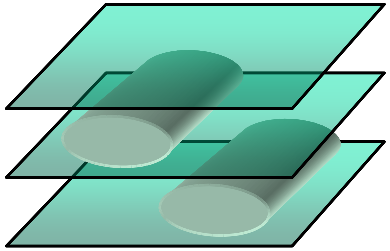


Correlation in liquid state: structure factor

- Structure factor: S(Q)

$$\int d\vec{r} = V, \ \rho V = N$$

$$S(\vec{Q}) = \frac{1}{N}\left\langle \sum_i \sum_j \exp[-i\vec{Q}\cdot(\vec{r}_i - \vec{r}_j)] \right\rangle$$

$$= \frac{1}{N}\left\langle \sum_{i=j} \exp[-i\vec{Q}\cdot(\vec{r}_i - \vec{r}_j)] \right\rangle + \frac{1}{N}\left\langle \sum_{i\neq j} \exp[-i\vec{Q}\cdot(\vec{r}_i - \vec{r}_j)] \right\rangle$$

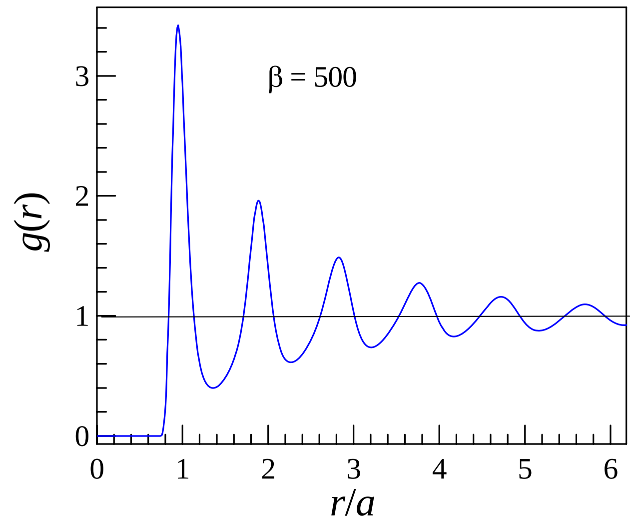
$$= 1 + \frac{1}{N}\left\langle \sum_{i\neq j} \exp[-i\vec{Q}\cdot(\vec{r}_i - \vec{r}_j)] \right\rangle$$

- pair distribution function: g(r)

$$S(\vec{Q}) = 1 + \frac{1}{N}\rho^2 \int d\vec{r}_i \int d\vec{r}_j e^{-i\vec{Q}\cdot(\vec{r}_i - \vec{r}_j)} g(\vec{r}_i - \vec{r}_j)$$

$$= 1 + \frac{1}{N}\rho^2 \int d\vec{r}_i \int d\vec{r} e^{-i\vec{Q}\cdot\vec{r}} g(\vec{r})$$

$$= 1 + \rho \int d\vec{r} e^{-i\vec{Q}\cdot\vec{r}} g(r) = 1 + \rho g(\vec{Q})$$



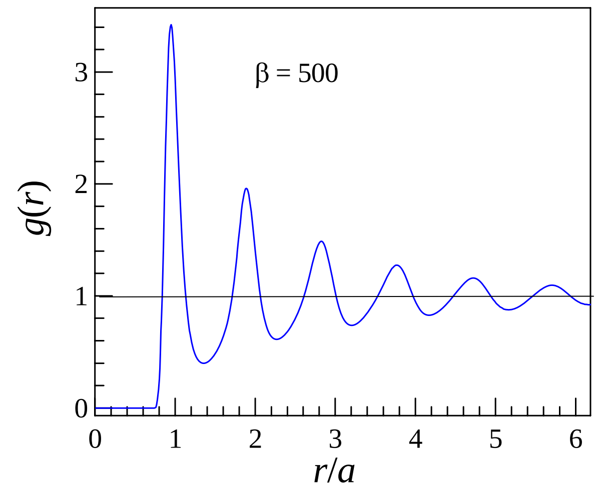
Ornstein-Zernike (OZ) approach

- Pair direct correlation function: c(r)

$$h(\vec{r}) = c(\vec{r}) + \rho \int d\vec{r}\,' c(r')h(\vec{r} - \vec{r}\,')$$

where $h(\vec{r}) = g(\vec{r}) - 1$

$$S(\vec{Q}) = 1 + \rho g(\vec{Q})$$



in Fourier transform

$$h(\vec{Q}) = c(\vec{Q}) + \rho c(\vec{Q})h(\vec{Q})$$

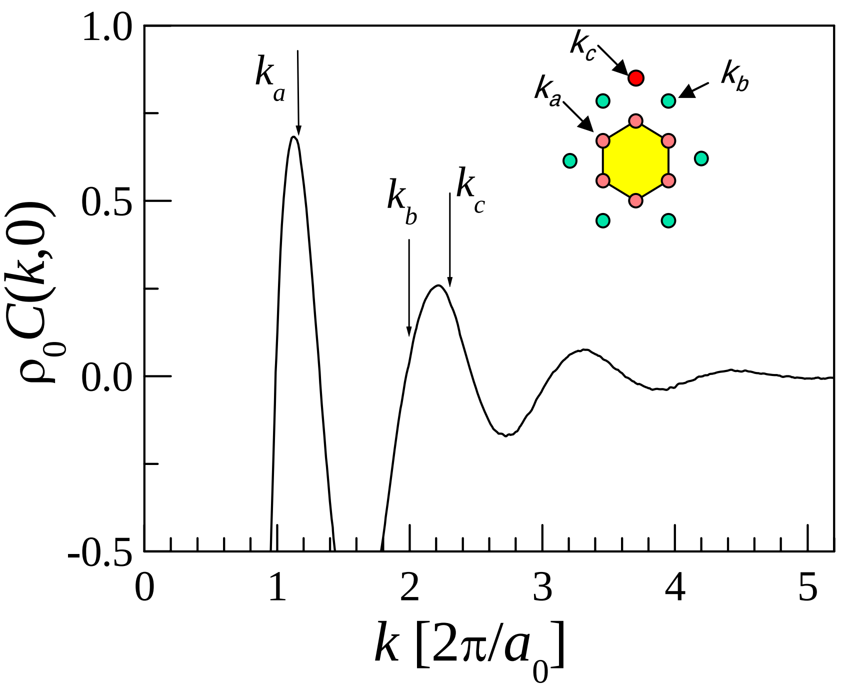
$$= \frac{c(\vec{Q})}{1 - \rho c(\vec{Q})}$$

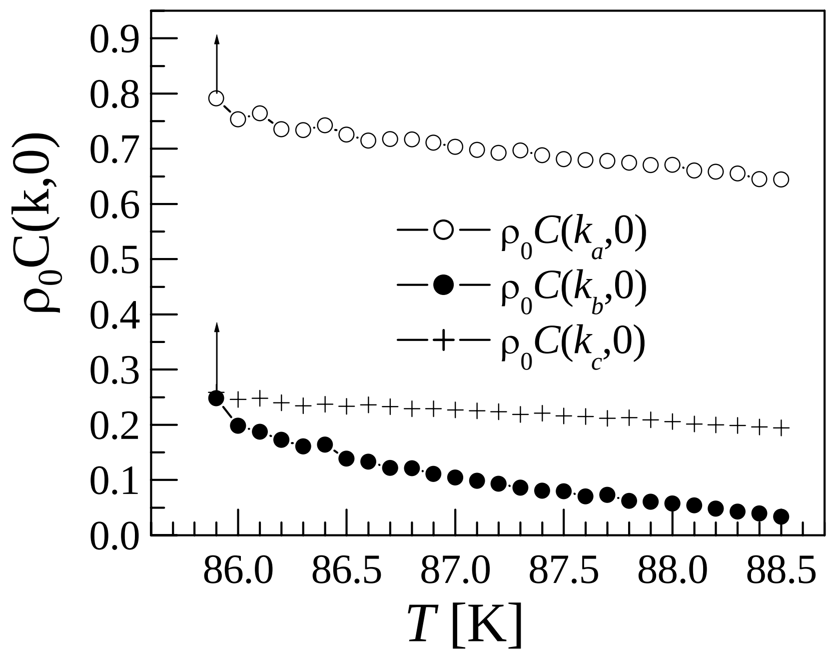
with $h(\vec{Q}) = g(\vec{Q}) - \delta(\vec{Q})$

$$S(\vec{Q}) = 1 + \rho g(\vec{Q}) = 1 + \frac{\rho c(\vec{Q})}{1 - \rho c(\vec{Q})} = \frac{1}{1 - \rho c(\vec{Q})}$$

Direct pair correlation function C(**k**)

- k and T dependence at a typical B





- sharp peaks at a series of wave numbers ← strong liquid correlations
- C(k,0) decreases quickly as k increases ← thermal fluctuations
- C(k,0) at given k increases linearly upon cooling

Introduction to DFT

- free energy of ideal gas: uniform density ρ_0

$$f = k_B T \rho_0 \left(\ln\left(\rho_0 \lambda^3 \right) - 1 \right) \qquad \lambda = 1 \Big/ \sqrt{2\pi m k_B T}$$

- free energy of ideal gas: non-uniform density ρ

$$\beta \Delta F\left[T, \{\rho(\mathbf{r})\}, \rho_0 \right] = \int d^d r \left[\rho \ln \frac{\rho}{\rho_0} + (A-1)\left(\rho - \rho_0 \right) \right]$$

$$A = \ln\left(\rho_0 \lambda^3 \right) \qquad \text{chemical potential}$$

Introduction to DFT

Ramakrishnan and Yussouff (1979)

- free-energy functional:

$$\beta F\left[T,\{\rho(\mathbf{r})\},\rho_0\right]=\int d^d r\left[\rho(\mathbf{r})\ln\frac{\rho(\mathbf{r})}{\rho_0}+(A-1)\left(\rho(\mathbf{r})-\rho_0\right)\right]$$

$$-\frac{1}{2}\iint d^d r d^d r'\left[\rho(\mathbf{r})-\rho_0\right]\left[\rho(\mathbf{r}')-\rho_0\right]C(\mathbf{r}-\mathbf{r}')$$

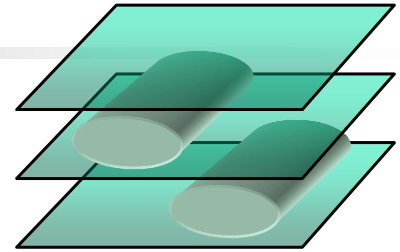
- Ursell function $S_{nn}(\mathbf{r}\text{-}\mathbf{r}')$: $S_{nn}(\mathbf{r}-\mathbf{r}')=\langle\rho(\mathbf{r})\rho(\mathbf{r}')\rangle-\langle\rho(\mathbf{r})\rangle\langle\rho(\mathbf{r}')\rangle$

$$S_{nn}^{-1}(\mathbf{r}-\mathbf{r}')=\frac{\delta^2\beta F}{\delta\rho(\mathbf{r})\delta\rho(\mathbf{r}')}=\frac{\delta(\mathbf{r}-\mathbf{r}')}{\rho_0}-C(\mathbf{r}-\mathbf{r}')$$

$$S_{nn}(\mathbf{q})=S(\mathbf{q})=\frac{1}{1-\rho_0 C(\mathbf{q})}$$ for $\mathbf{q}\neq\mathbf{0}$, with S($\mathbf{q}$) structure factor

→ C($\mathbf{q}$) the Orenstein-Zernike direct pair correlation function

Study on interlayer Josephson vortices

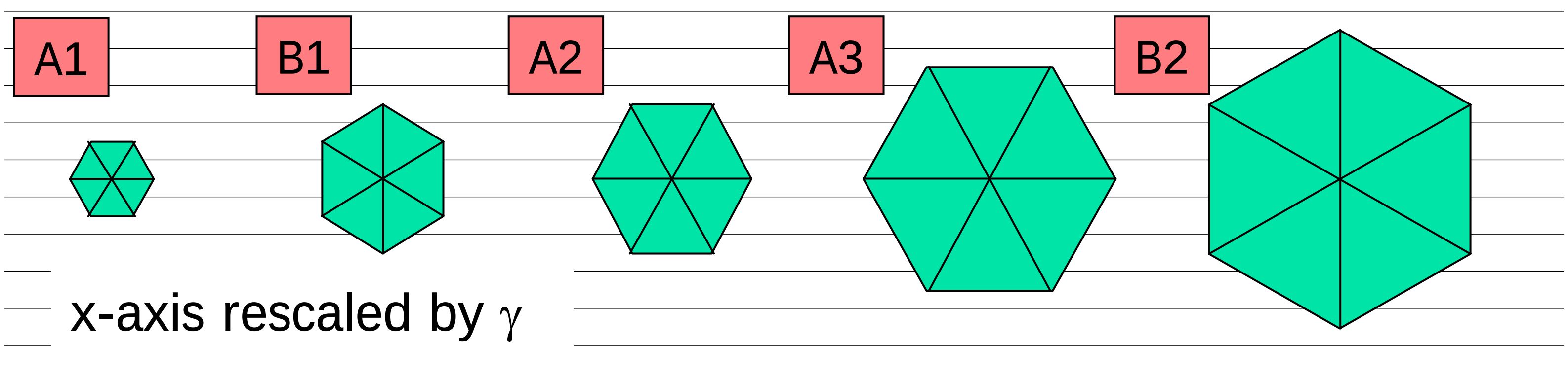


- high-T_c cuprate SC: profound layered structure
  - interlayer Josephson vortex in B || ab
  - intrinsic pinning → fluctuations suppressed

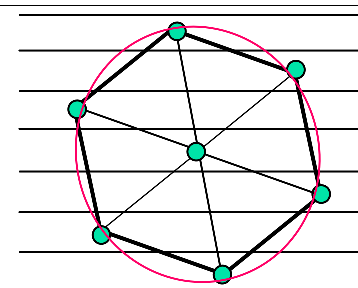
Tachiki & Takahashi

→ minimal c-axis vortex separation: s ~ 1.2nm

- Commensurate magnetic fields

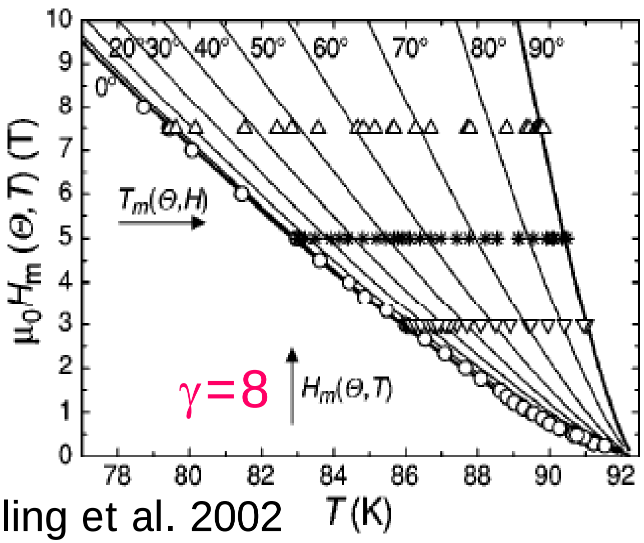


- for other magnetic fields:
  - x-axis stretched or squeezed
  - shear-distorted
  - rotated

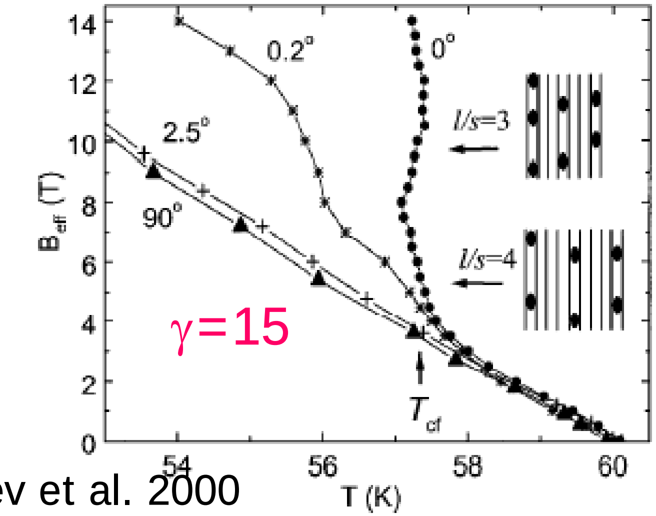


Experimental phase diagrams

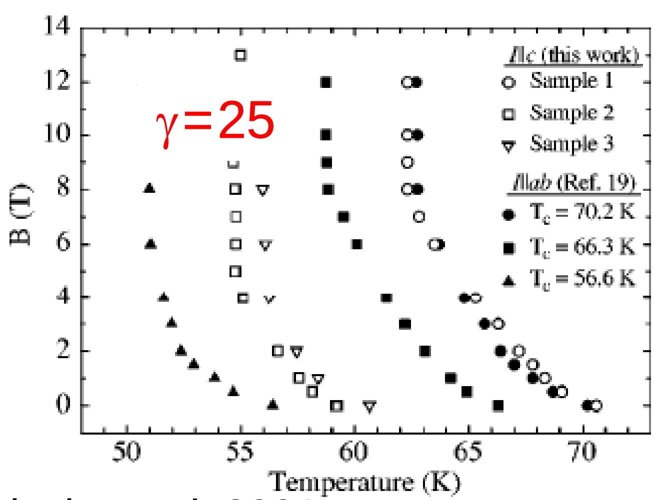
- Why so different beyond scaling theory $B \sim \phi_0/\gamma s^2$?



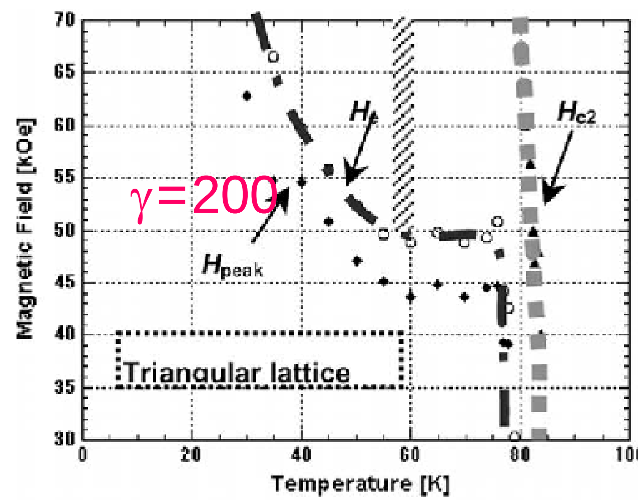
Schilling et al. 2002



Gordeev et al. 2000



Lundqvist et al. 2001

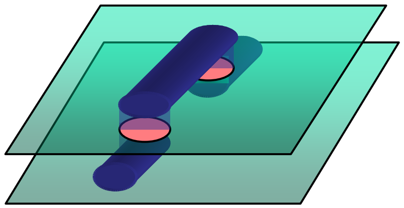


Hirata et al. 2004

Possibility of smectic: purterbative RG analysis

- 2D elastic hamiltonian $F = \sum_n \frac{1}{2} \int \frac{d^2\mathbf{q}_\perp}{(2\pi)^2} \left(K_x q_x^2 + K_y q_y^2\right) \left|u_n(\mathbf{q}_\perp)\right|^2$ in plane QLRO
- interlayer coupling $F_{\text{int}} = -\sum_n \int dxdy v_{IL} \cos\left(2\pi\left(u_{n+1} - u_n\right)/a\right)$
- dislocations ⇔ hopping $\oint \nabla u_k \cdot dl = a\left(\delta_{k,n} - \delta_{k,n+1}\right)$
  - fugacity of dislocation pair $y_d = \exp\left(-E_{lk}/k_B T\right)$ $E_{lk} \approx \sqrt{\varepsilon_0 \gamma U_p} ms$
- perturbative RG equations

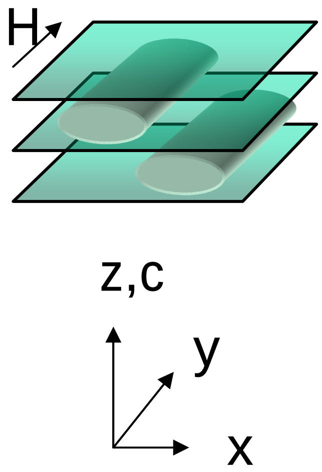
$$\frac{dv_{IL}}{dl} = \left(2 - \frac{2\pi k_B T}{Ka^2}\right) v_{IL} \qquad \frac{dy_d}{dl} = \left(2 - \frac{Ka^2}{2\pi k_B T}\right) y_d$$



- possible orders
  - low T regime: $k_B T < Ka^2/4\pi$
  - high T regime: $k_B T > Ka^2/\pi$
  - intermediate T regime $Ka^2/4\pi < k_B T < Ka^2/\pi$ → Smectic phase ?!
- drawback: 3D lattice (stable fixed point at low T) not considered

Density functional theory: layer pinning

- free-energy functional: ○ $\rho(\mathbf{r})$ areal vortex density



$$\beta F = \int d^3r \left[\rho(\mathbf{r}) \ln \frac{\rho(\mathbf{r})}{\rho_0} + (A-1)\delta\rho(\mathbf{r}) \right]$$

$$-\frac{1}{2}\iint d^3r d^3r' \delta\rho(\mathbf{r})\delta\rho(\mathbf{r}')C(\mathbf{r}-\mathbf{r}') - \int d^3r \delta\rho(\mathbf{r}) \beta V_p \cos(2\pi z/s)$$

$$\delta\rho(\mathbf{r}) = \rho(\mathbf{r}) - \rho_0$$

ρ_0: uniform liquid

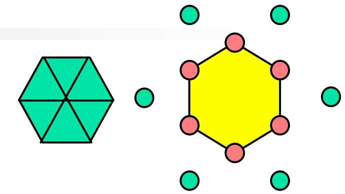
○ A: lagrangian multiplier   A ⇔ μ chemical potential

○ V_p: layer pinning energy

- Variational calculus → condition for free-energy minima

$$\ln \frac{\rho(\mathbf{r})}{\rho_0} + A = \int d^3r' \delta\rho(\mathbf{r}')C(\mathbf{r}-\mathbf{r}') + \beta V_p(\mathbf{r})$$

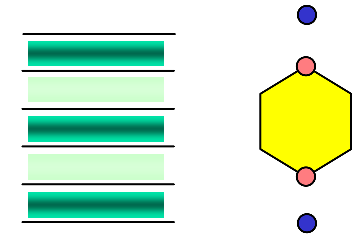
DFT



- trial states: reciprocal lattice vectors **K**=(K_x,K_z)

$$\rho(\mathbf{x}) = \rho_0 + \sum_K \rho_K \exp(i\mathbf{K}\cdot\mathbf{x})$$

x=(x,z)



- ρ_K=0 ⇔ liquid
- whole set ρ_K>0 ⇔ lattice
- subset ρ_K>0 ⇔ smectic

- task: finding solution to the following constraint $C(\mathbf{K},0) = \int d^3 r C(\mathbf{r}) e^{i\mathbf{K}\cdot\mathbf{x}}$

$$\left[1 + \sum_{\mathbf{K}} \frac{\rho_{\mathbf{K}}}{\rho_0} \exp(i\mathbf{K}\cdot\mathbf{x})\right] \exp A = \exp\left[\sum_{\mathbf{K}} \frac{\rho_{\mathbf{K}}}{\rho_0} \rho_0 C(\mathbf{K},0) \exp(i\mathbf{K}\cdot\mathbf{x}) + \beta V_p \cos\left(\frac{2\pi z}{s}\right)\right]$$

- an equivalent process: finding free-energy minimum wrt {ρ_K}

$$\beta f = -\ln \int_{u.c.} dx dz \rho_0 \exp\left[\sum_{\mathbf{K}} \frac{\rho_{\mathbf{K}}}{\rho_0} \rho_0 C(\mathbf{K},0) \exp(i\mathbf{K}\cdot\mathbf{x}) + \beta V_p \cos\left(\frac{2\pi z}{s}\right)\right] + \frac{1}{2} \sum_{\mathbf{K}} \left(\frac{\rho_{\mathbf{K}}}{\rho_0}\right)^2 \rho_0 C(\mathbf{K},0)$$

A

- per unit cell in xz plane and unit length in y axis

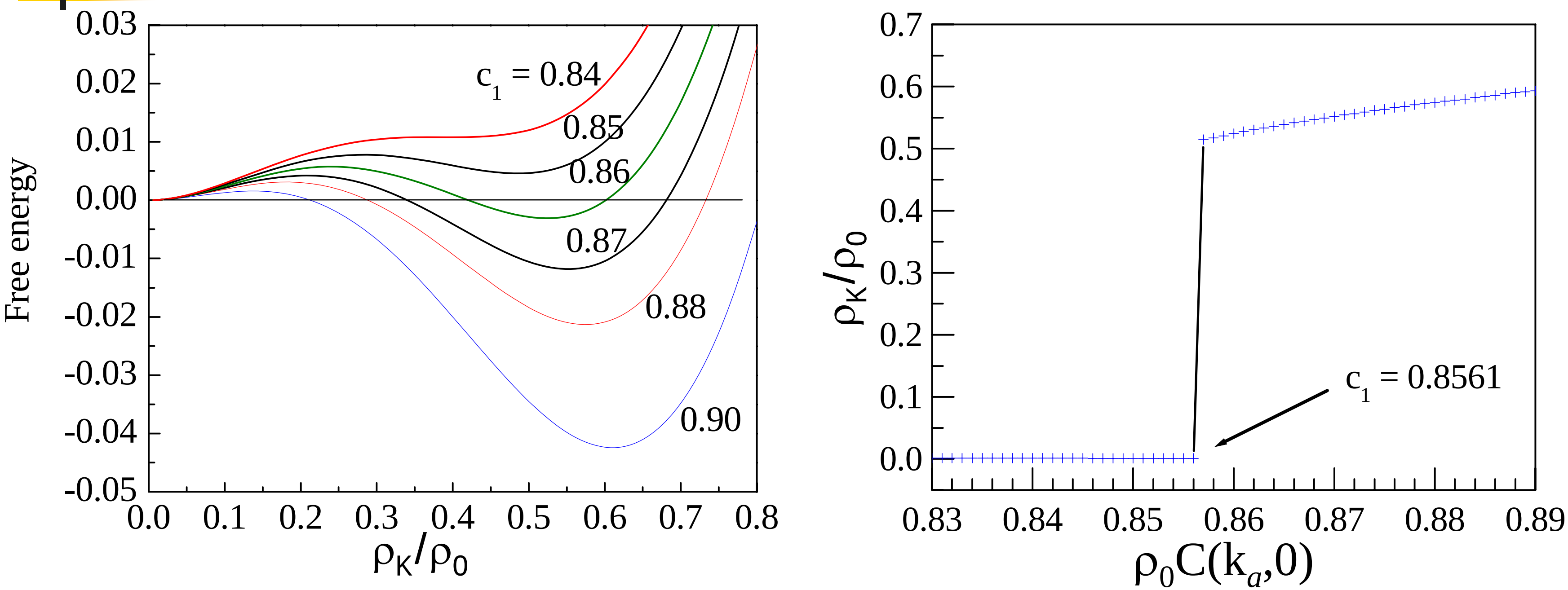
DFT

- Physical insights

$$\beta f = -\ln \int_{u.c.} dxdz\rho_0 \exp\left[\sum_{\mathbf{K}} \frac{\rho_{\mathbf{K}}}{\rho_0}\rho_0 C(\mathbf{K},0)\exp(i\mathbf{K}\cdot\mathbf{x}) + \beta V_p \cos\left(\frac{2\pi z}{s}\right)\right] + \frac{1}{2}\sum_{\mathbf{K}}\left(\frac{\rho_{\mathbf{K}}}{\rho_0}\right)^2 \rho_0 C(\mathbf{K},0)$$

  - liquid always presumes a free-energy minimum
  - crystallization can reduce free-energy if correlation strong enough
  - interference between lattice order and layer pinning

Crystallization for zero layer pinning



- First order freezing at $\rho_0 C(k_a,0) = 0.8561$
  - Debye-Waller factor: $\exp(-2W)=(\rho_K/\rho_0)^2=0.25$
  - Lindemann number: $c_L=0.21$

Sengupta et al. (1991); Menon et al. (1996)

- C(K,0) increases linearly with decreasing T

Characteristic vortex-line length

Barone, Larkin and Ovchinnikov: J. of Super. Vol.3, p.155 (1990)

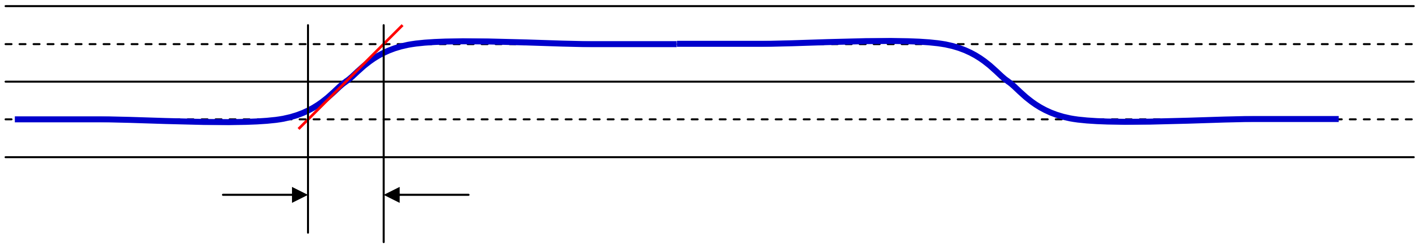
- Layer pinning energy per unit length

$$U_p = 5.23\times10^2 \frac{\varepsilon_0}{\gamma}\left(\frac{\xi_c}{s}\right)^{5/2} \exp(-15.8\,\xi_c/s)$$

$\varepsilon_0=(\phi_0/4\pi\lambda_{ab})^2$

- A single vortex line in layer pinning potential

$$f = \int dy\left[\frac{\varepsilon}{2}\left(\frac{\partial z}{\partial y}\right)^2 - U_p \cos\left(\frac{2\pi z}{s}\right)\right] \qquad z=0 \quad for \quad y=\pm\infty$$



- Meta-stable configuration:

$$\frac{\partial}{\partial y}\left[-\frac{\varepsilon}{2}\left(\frac{\partial z}{\partial y}\right)^2 - U_p \cos\left(\frac{2\pi z}{s}\right)\right] = 0 \qquad -\frac{\varepsilon}{2}\left(\frac{\partial z}{\partial y}\right)^2 - U_p \cos\left(\frac{2\pi z}{s}\right) = -U_p$$

Layer pinning and kink length

- wall thickness

$$L_{wall} = s\sqrt{\varepsilon / 4U_p} \Leftarrow \frac{\partial z}{\partial y} = \sqrt{\frac{2U_p}{\varepsilon}\left[1-\cos\left(\frac{2\pi z}{s}\right)\right]} = \sqrt{\frac{4U_p}{\varepsilon}} \quad \text{at } z=s/2$$

- elastic energy and pinning energy for one cross

$$E_{elas.} = V_p = s\sqrt{\varepsilon U_p}$$

- kink length:

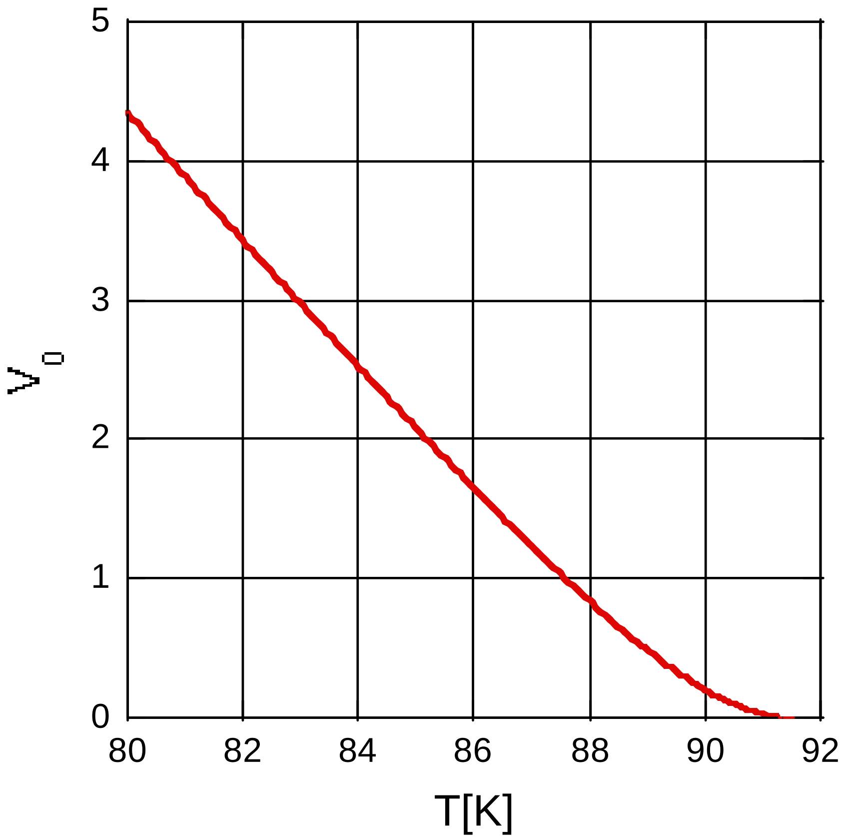
$$\frac{L_{kink}}{L_{wall}} \exp\left[-(E_{elas.}+V_p)/k_B T\right] = 1 \qquad L_{kink} = s\sqrt{\frac{\varepsilon}{4U_p}} \exp\left(2s\sqrt{\varepsilon U_p}/k_B T\right)$$

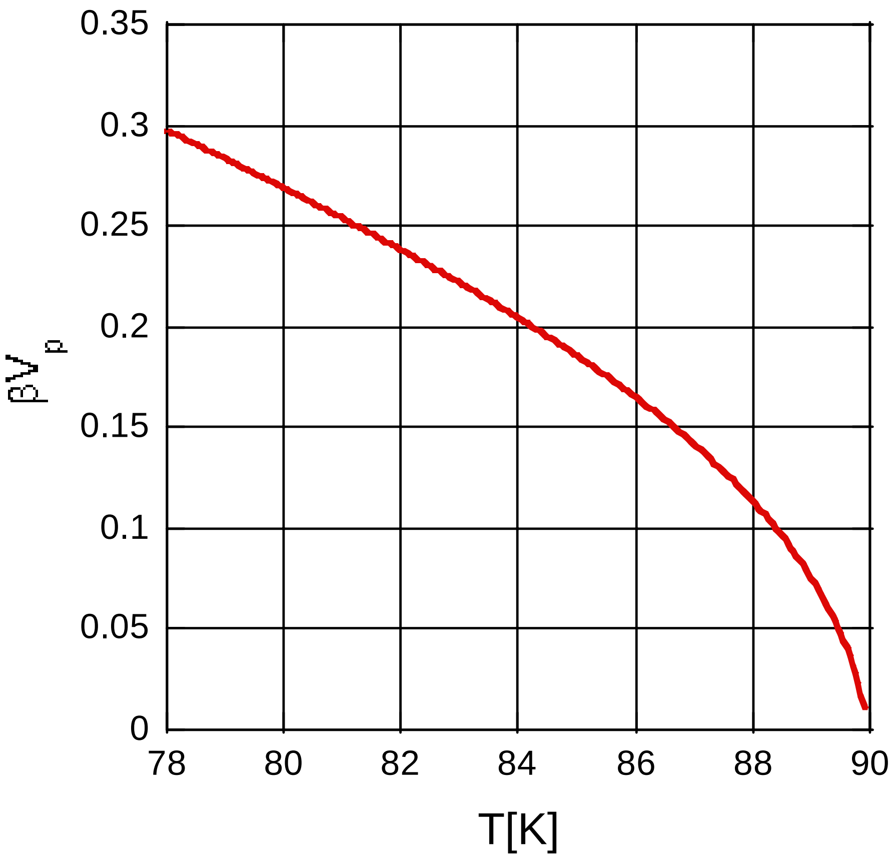
- L_{kink}: the characteristic length of vortex lines in periodic layer pinning

unit length: L_{kink} pinning energy: V_p

Layer pinning

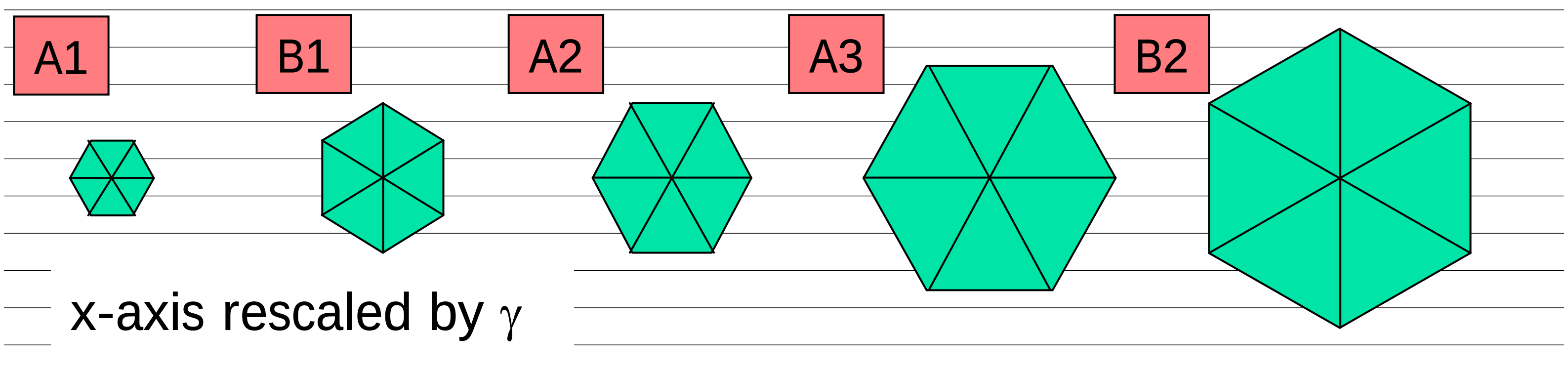
- YBCO: d=12 Å, $\lambda_{ab}(0)$=1000 Å, γ=8, T_c=92K, κ=100
- BSCCO: d=15 Å, $\lambda_{ab}(0)$=2000 Å, γ=150, T_c=90K, κ=100



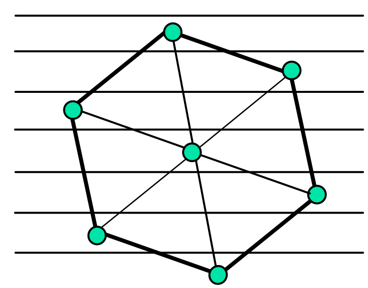


Lattice structure

- vortex lattice commensurate with layer structure: justified in HTSC
- *naturally* commensurate vortex lattice:
  - those by anisotropic GL theory coinciding with layer structure
- two series of magnetic fields $H_{Am} = \dfrac{\sqrt{3}\phi_0}{2\gamma(ms)^2}$ $H_{Bm} = \dfrac{\phi_0}{2\sqrt{3}\gamma(ms)^2}$

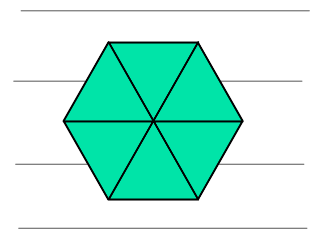


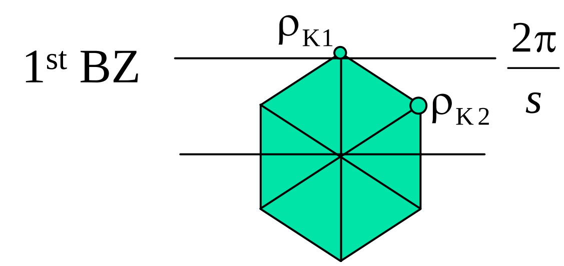
- for other magnetic fields:
  - x-axis stretched or squeezed
  - shear-distorted
  - rotated



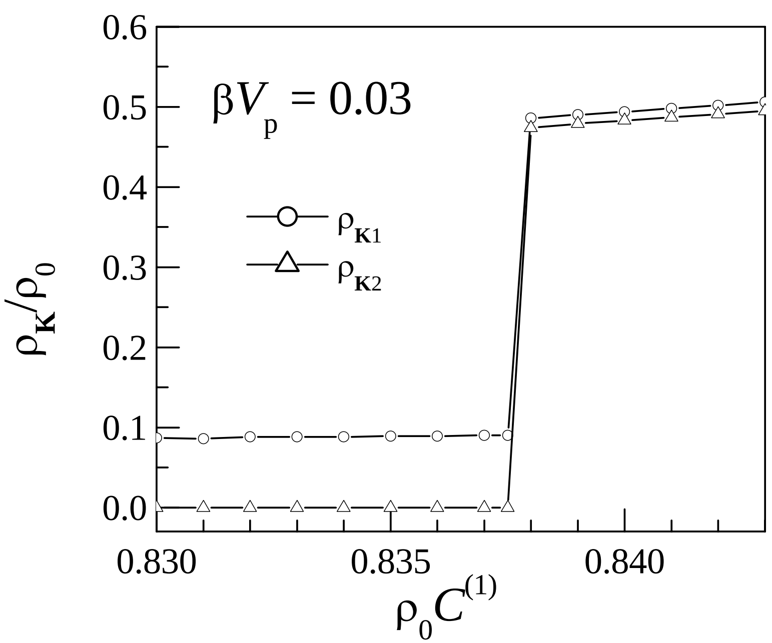
Phase transition for unit cell A1

- unit cell and order parameters:

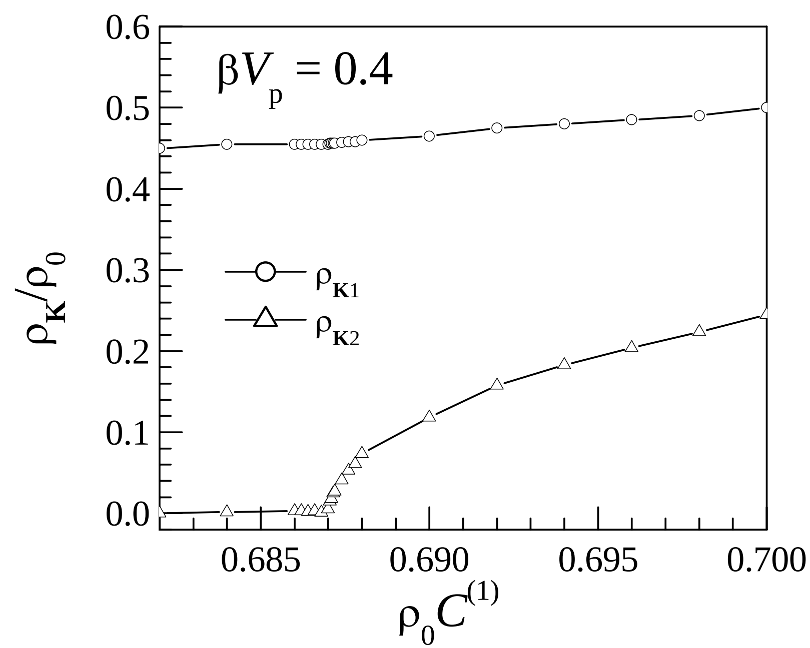




- crystallization



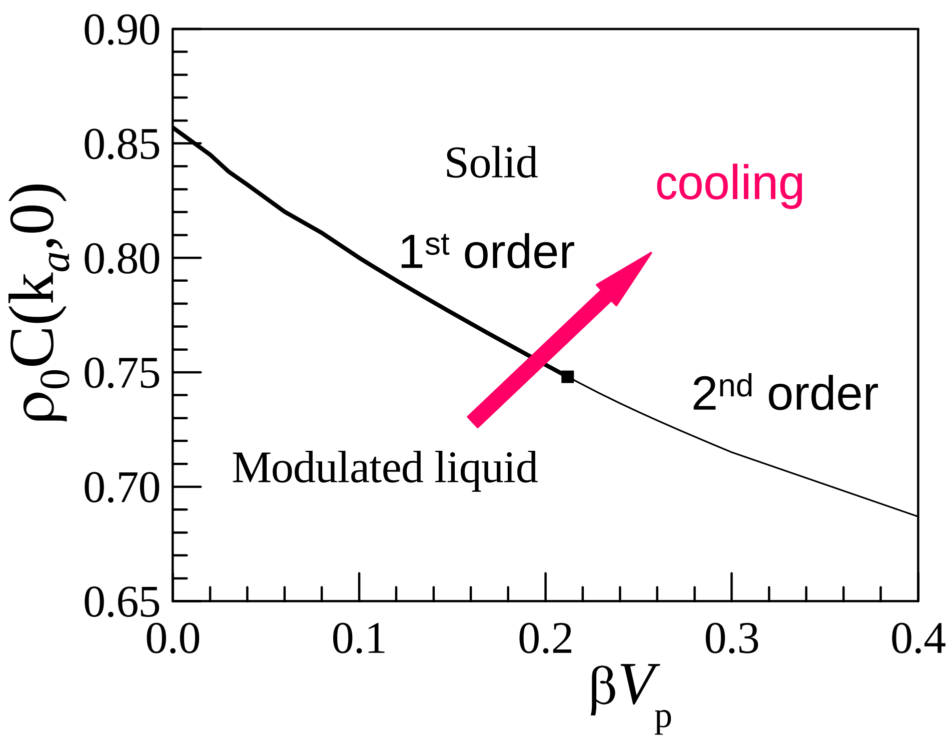
1st order transition

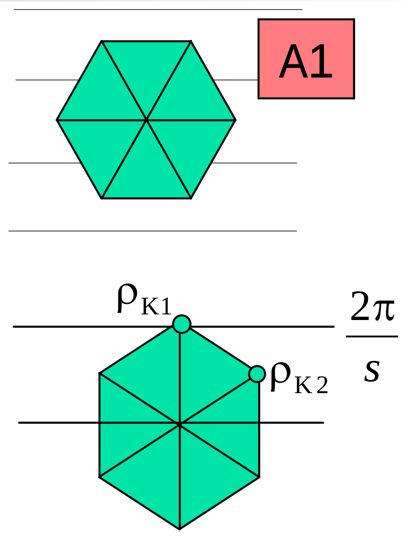


2nd order transition

Freezing transitions into A1-type lattice

- $\rho_0 C(k_a,0)$-βV_p phase diagram $\quad H = \sqrt{3}\phi_0 / 2\gamma s^2$





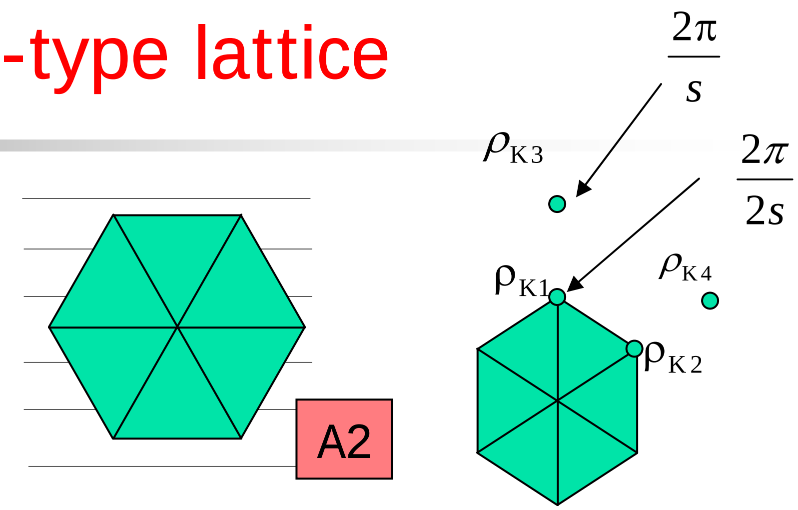
- tricritical point

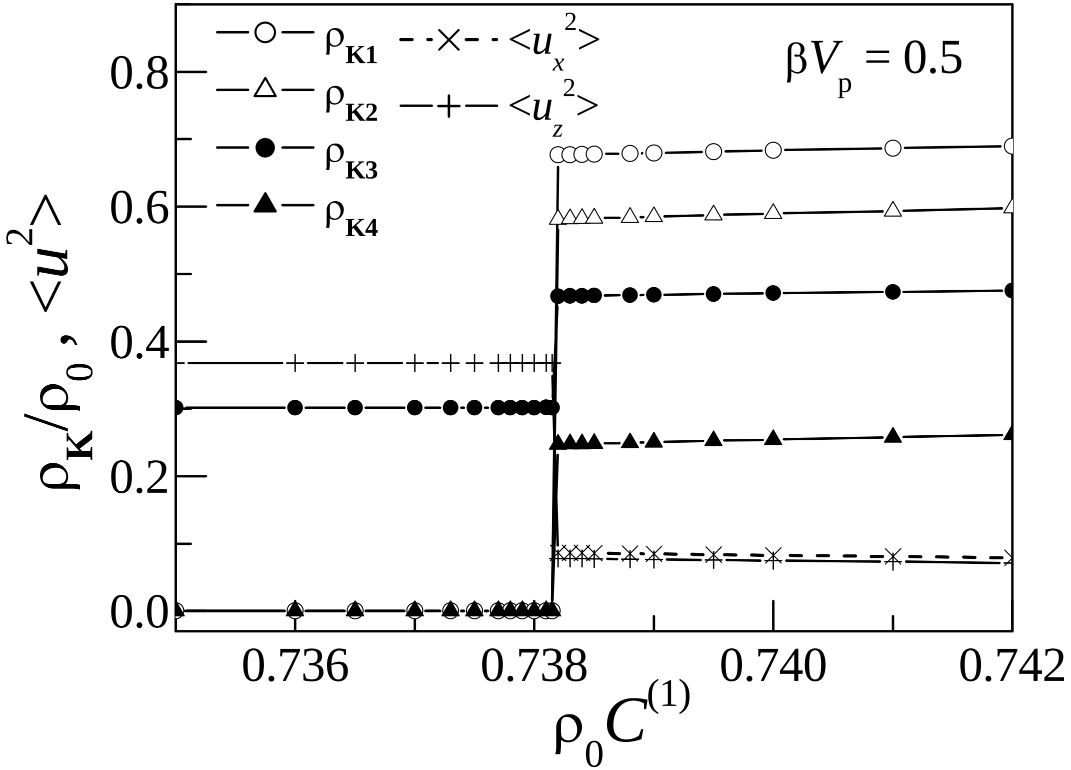
$$\left(\rho_0 C(k_a,0), \beta V_p\right) = \left(0.748, 0.212\right)$$

- free energy expansions: even order of ρ_{K2}
  - T_2 crossing 0 at $T_4<0$ and $T_6>0$ → 1st order
  - T_2 crossing 0 at $T_4>0$ → 2nd order

Freezing transition into A2-type lattice

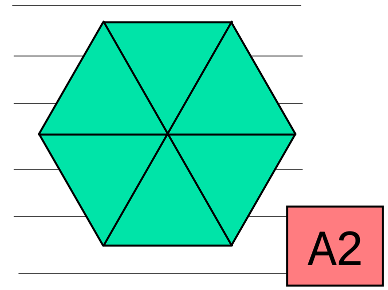
- $H = \sqrt{3}\phi_0 / 2\gamma(ms)^2$ with m=2
  - unit cell and order parameters
- freezing process: βV_p=0.5

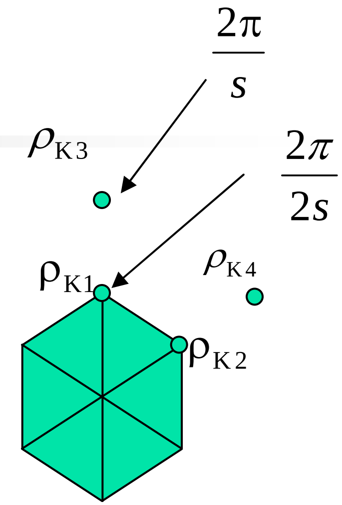


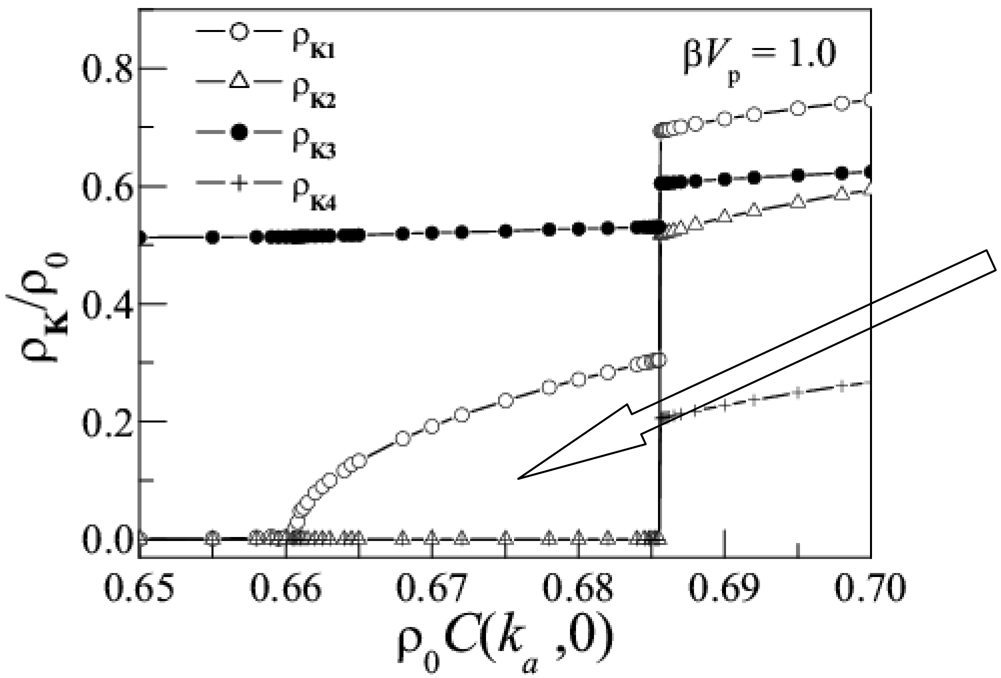


Freezing transition into A2-type lattice

- $H = \sqrt{3}\phi_0 / 2\gamma (ms)^2$ with m=2
  - unit cell and order parameters
- freezing process: $\beta V_p=1$

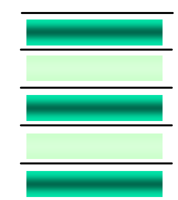






◇ smectic phase ⇔

$\rho_{K1}>0$, $\rho_{K2}=\rho_{K4}=0$



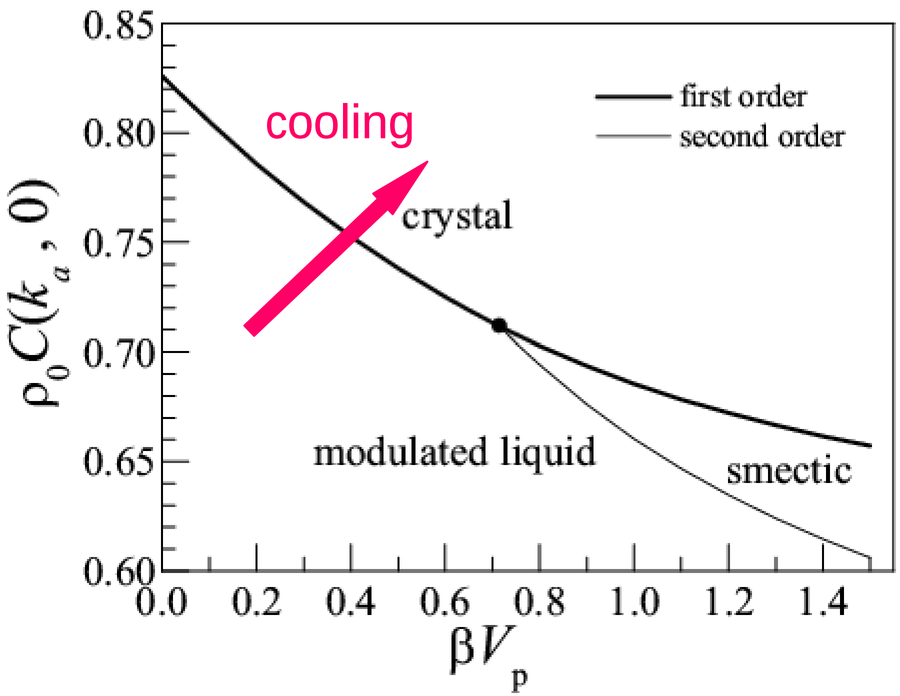
◇ absence of LP instability

- two-step freezing

◇ liquid-smectic: 2nd order in 2D Ising class ◇ smectic-crystal: 1st order

Freezing transition into A2-type lattice

- $\rho_0 C(k_a,0)$-βV_p phase diagram for $H = \sqrt{3}\phi_0 / 8\gamma s^2$

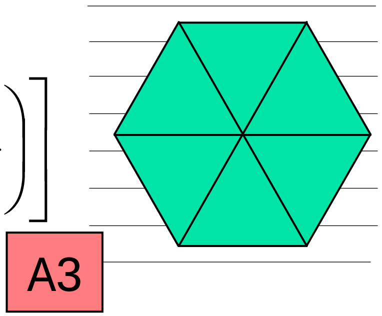


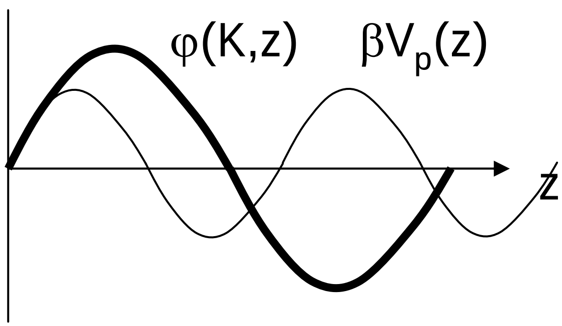
- critical endpoint: $\left(\rho_0 C(k_a,0), \beta V_p\right) = \left(0.714, 0.712\right)$
- smectic expected at H~40 Tesla for YBCO; not available in BSCCO

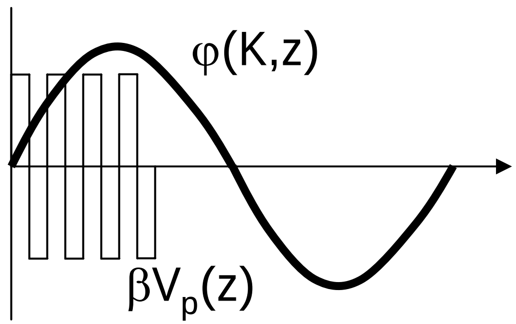
Single 1st order freezing into Am lattice: m≥3

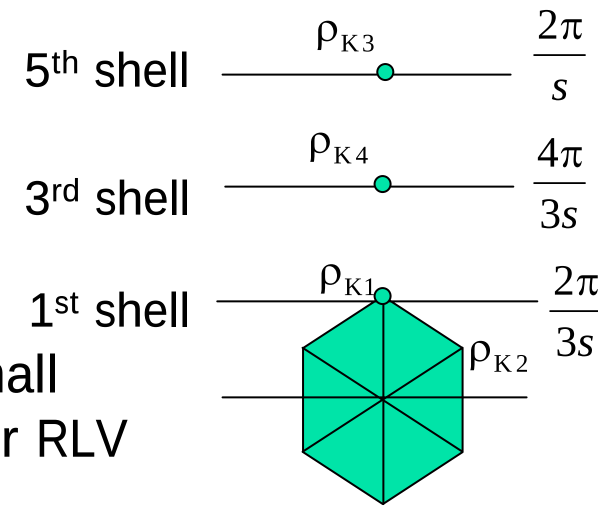
- effective potential:

$$A = \ln \int_{u.c.} dxdz \rho_0 \exp\left[\sum_{\mathbf{K}} \frac{\rho_{\mathbf{K}}}{\rho_0} \rho_0 C(\mathbf{K},0) \exp(i\mathbf{K}\cdot\mathbf{x}) + \beta V_p \cos\left(\frac{2\pi z}{s}\right) \right]$$









◇ resonance occurs when two wave vectors match

➔ for low magnetic field with large unit cell and small principle RLV K1, layer pinning works via high-order RLV on (2m-1)-th shell: C(0,mK1=2π/s,0) with m≫1

◇ C(K,0) decreases quickly with K: C(K3,0)≈C(K1,0)/10

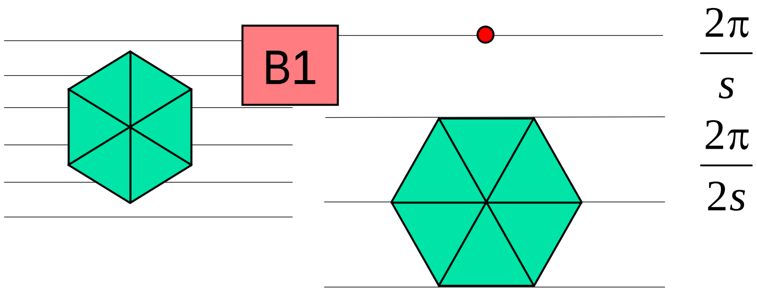
Pinning of small period not effective to fluctuations of long wave length !

- For $H \le \sqrt{3}\phi_0 / 2\gamma (3s)^2$ layer pinning plays no role ➔ γ scalable

Single 1st order freezing other lattices

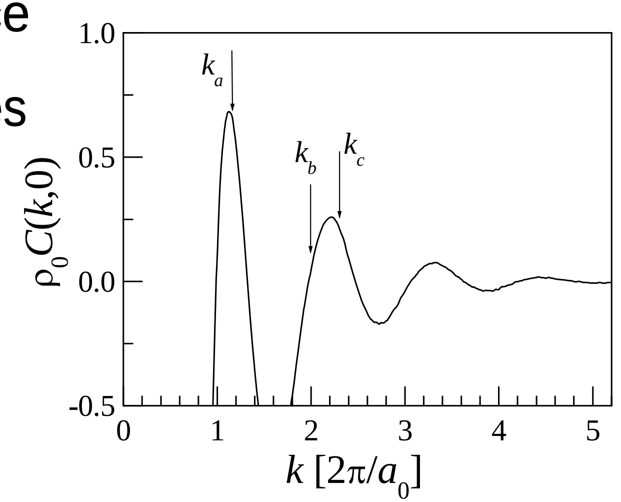
- For magnetic fields $B=\phi_0/2\sqrt{3}\gamma(ms)^2$
  - layer pinning induces the 6 primitive RLVs simultaneously

  ➔ a single first-order freezing



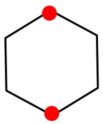
  - same for other fields where a rotated lattice is naturally commensurate
- For magnetic fields which are not naturally commensurate with layers
  - vortex lattice realized via stretching, squeezing, and shearing from those of naturally commensurate vortex lattice
  - additionally to the above property, peak values of C(K,0) not available because of distortion

  ➔ a single first-order freezing



Critical behaviors

- 2nd-order smectic transition at $H=\sqrt{3}\phi_0/2\gamma(ms)^2$ with m=2
- DFT



|K|=π/s

$$\frac{\beta F}{N_{xz}L_y}=-A+\frac{1}{2}\sum_{\mathbf{K}}\left(\frac{\rho_{\mathbf{K}}}{\rho_0}\right)^2\rho_0 C(\mathbf{K},0)$$

where $$A=\ln\int_{u.c.}dxdz\rho_0\exp\left[\sum_{\mathbf{K}}\frac{\rho_{\mathbf{K}}}{\rho_0}\rho_0 C(\mathbf{K},0)\exp(i\mathbf{K}\cdot\mathbf{x})+\beta V_p\cos\left(\frac{2\pi z}{s}\right)\right]$$

$$f=-\ln p_0+\left(\frac{\rho_K}{\rho_0}\right)^2\rho_0 C(K,0)\left(1-\frac{2p_2}{p_0}\rho_0 C(K,0)\right)+\left(\frac{\rho_K}{\rho_0}\right)^4(\rho_0 C(K,0))^4\left(2\left(\frac{p_2}{p_0}\right)^2-\frac{2p_4}{3p_0}\right)$$

where $$p_n=\int_0^{2s}\frac{dz}{2s}\cos^n(\pi z/s)\exp[\beta V_p\cos(2\pi z/s)]$$

- Critical point: $1-\frac{2p_2}{p_0}\rho_0 C(K,0)=0$
- renormalized correlation functions

Critical behaviors (cont.)

- order parameter and symmetry:

$\rho(\mathbf{r})-\rho_0=\rho_{\mathbf{K}1}e^{-i\mathbf{K}1\cdot\mathbf{u}}e^{-i\mathbf{K}1\cdot\mathbf{r}}+c.c.$ $\mathbf{K1}=(0,0,\pi/s)$

  - layer structure → $\mathbf{u}=u_z(y,z)\,\hat{z}$ with $u_z(y,z)=0$ or ns

→ $e^{-i\mathbf{K}1\cdot\mathbf{u}}=\mp1$ → real-number order parameter: $\mp\rho_K$ → Ising symmetry

  - layer structure kills the Landau-Peierls instability → LR smectic order

- Landau free energy: gradient terms included additionally

$F=1/2\int d^3r[\,h(\nabla_{yz}\Psi)^2+r\Psi^2+w\Psi^4]$

no LR correlation in x direction

  - *r* and *w* given explicitly by DFT, *r* changes sign at critical point

→ Correlation length diverges in y and z directions

$$\xi_{yz}=\sqrt{h/-r}\sim1\Big/\sqrt{1-T_{sm}/T}$$

2D critical behavior

- 2D Ising universality class: logarithmic divergence of the specific heat

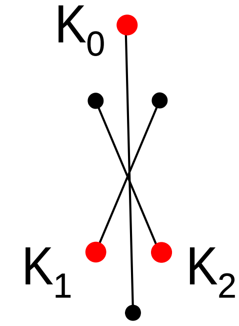
Freezing into A1-type lattice $H=\sqrt{3}\phi_0/2\gamma(ms)^2$ with m=1

- order parameter and symmetry

  $\rho(r)-\rho_0=\rho_{K0}e^{-i\mathbf{K}_0\cdot\mathbf{r}}+\Psi_1(r)e^{-i\mathbf{K}_1\cdot\mathbf{r}}+\Psi_2(r)e^{-i\mathbf{K}_2\cdot\mathbf{r}}$ +c.c.

  - strong layer pinning → $\rho_{K0}\sim 1$
  - $\Psi_{1,2}=|\Psi|\,e^{-i\mathbf{K}_{1,2}\cdot\mathbf{u}}=|\Psi|\,e^{\mp i2f\pi u_x/s}$ ← $\mathbf{u}=u_x(x,y,z)\,\hat{x}$

  u_x: period of s/f ⇔ Ψ: period 2π U(1) symmetry



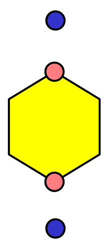
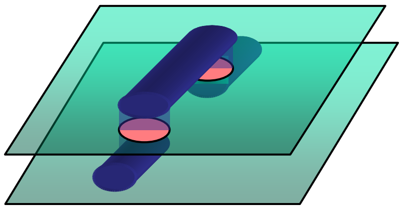
- dimensionality of critical fluctuations: two possibilities
  - long-range correlation of $u_x(\mathbf{r})$ in x & z & y directions: 3D XY class
  - long-range correlation of $u_x(\mathbf{r})$ in x & y directions: 2D XY ⇔ KT

QLRO

- Breakdown of MF theory:
  phase transition by MF theory (DFT) based on $|\Psi|$, is suppressed to crossover by thermal fluctuations and the true phase transitions take place at lower T, where $|\Psi|>0$.

- See the results by computer simulations

Summary

- First calculation of the B-T phase diagram of interlayer Josephson vortex state of the high-Tc superconductors using DFT
- First derivation of the thermodynamic stability of a smectic phase
  - smectic: (i) at H=40T for YBCO, scaled down with $1/\gamma$
    (ii) not in BSCCO
  - supersolid (i)  (ii) fugacity of dislocations 
- Effect of nano periodic pinning

Creating supersolid and Mott insulating phases of vortices