Vacancies-Excitons Mechanism of Supersolidity (in helium?)

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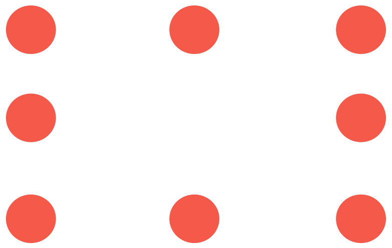
Intriguing possibility for quantum crystal:

- $\rho(r) = \rho_0 \cos(G \cdot r)$
- *but* atoms mobile
- mobile atoms (bosons) can Bose condense
- exhibit superfluidity
- SUPERSOLID

- NCRI observed in solid He4 by 3 groups
- Bulk, equilibrium property?

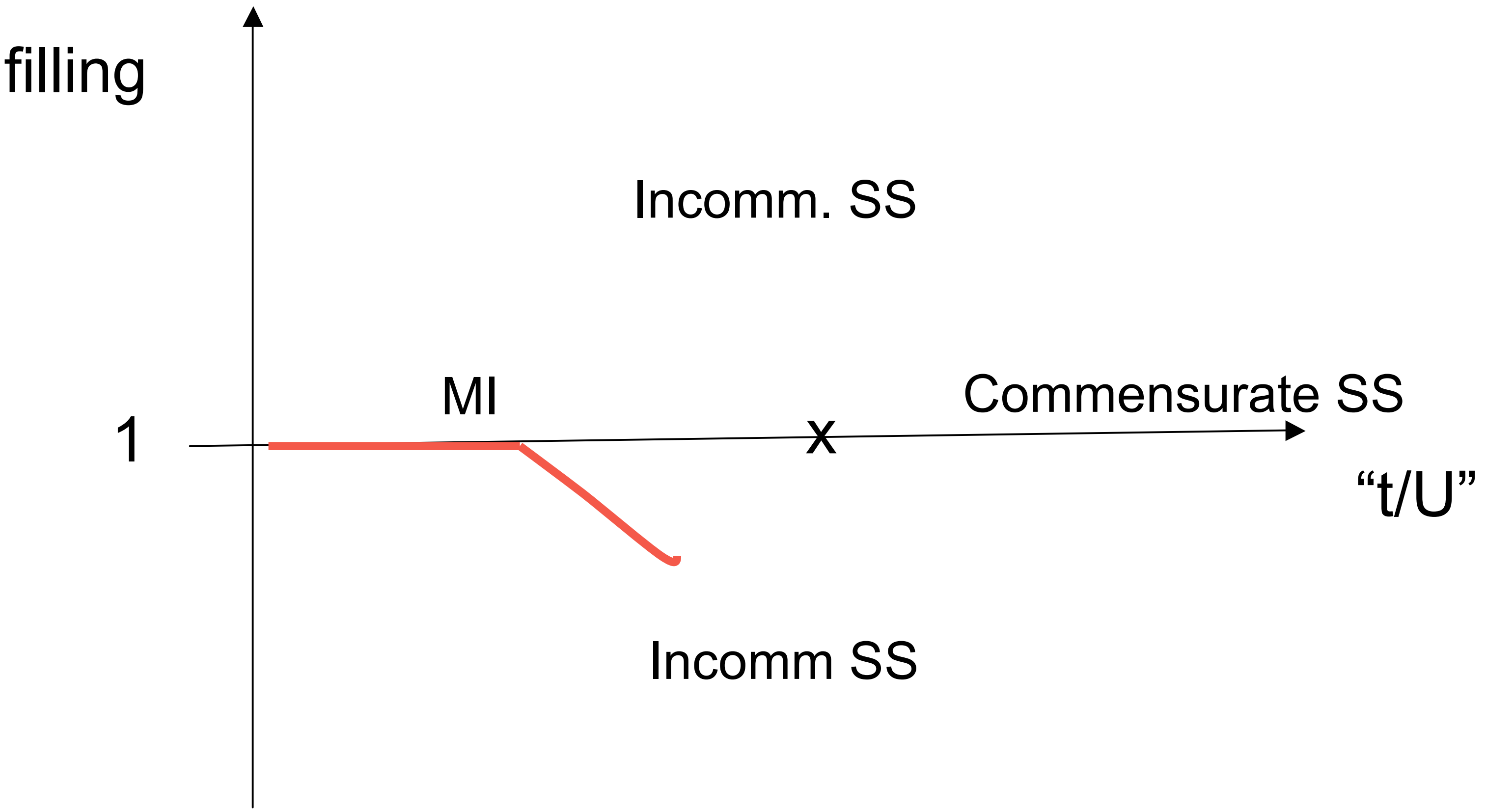
Vacancy mechanism of supersolid



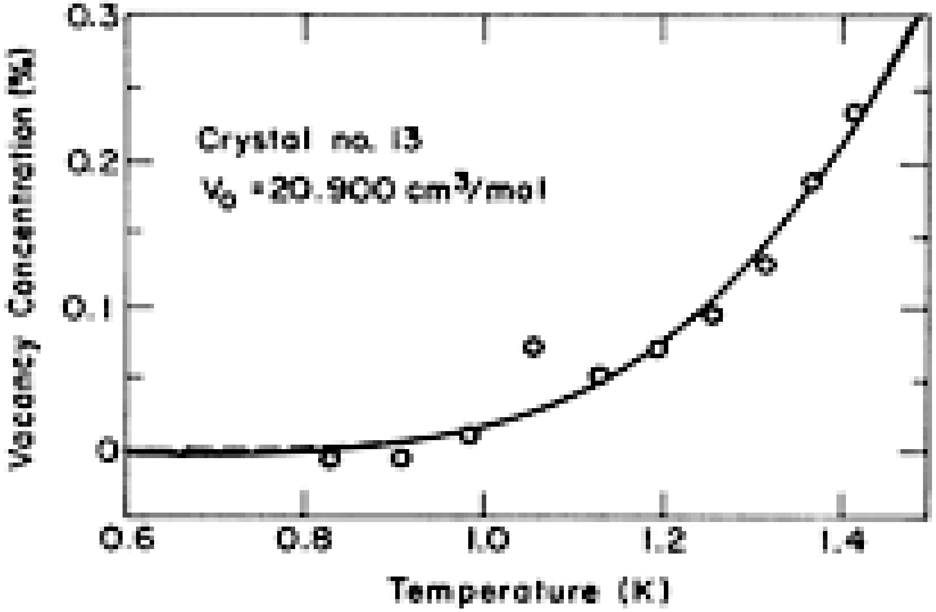
- Andreev and Lifshitz - quantum fluctuations favor finite density of vacancies even at T=0. Vacancies are mobile and can Bose condense.

- Chester - Jastrow wavefunctions generally have ODLRO, including ones describing solid order. Speculate due to vacancy condensation.

- Presence of vacancies in supersolids necessary provided there is no vacancy-interstitial symmetry, shown by Prokofev and Svistunov recently.


filling
Incomm. SS
MI
Commensurate SS
1
x
"t/U"
Incomm SS

But expt => vacancies activated



X-ray data
Simmons

data fit to c(T) ~ exp -(f/kT)

E_v ~ 10 K

- Supersolid He4 not observed until Kim and Chan’s expt

- Previous expts and theoretical calculations place strict limit on vacancy density in normal solid

- High activation energies for defects
  $E_v \sim 10 - 15$ K $E_i \sim 50$ K

Quandary:
How can defects of such high activation energies condense at low temperature, $T_c \sim 0.2$ K?

We provide one resolution to this quandary.
New mechanism for vacancy condensation.

Proposed Resolution

- First order transition

  At T=0, n_v = 0 in normal solid
  finite in supersolid

- “Vacuum” switching

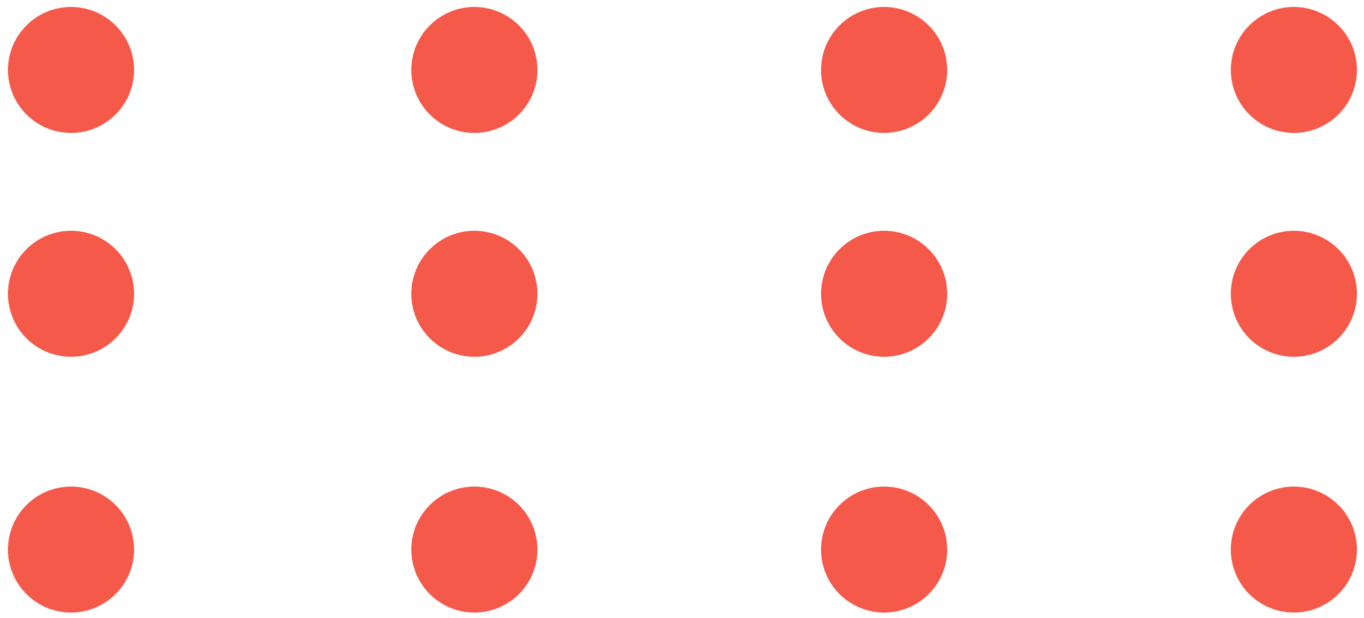
  vacancies condense in background of another type of defectons called **“excitons”**

- Normal-Supersolid transition accompanied by

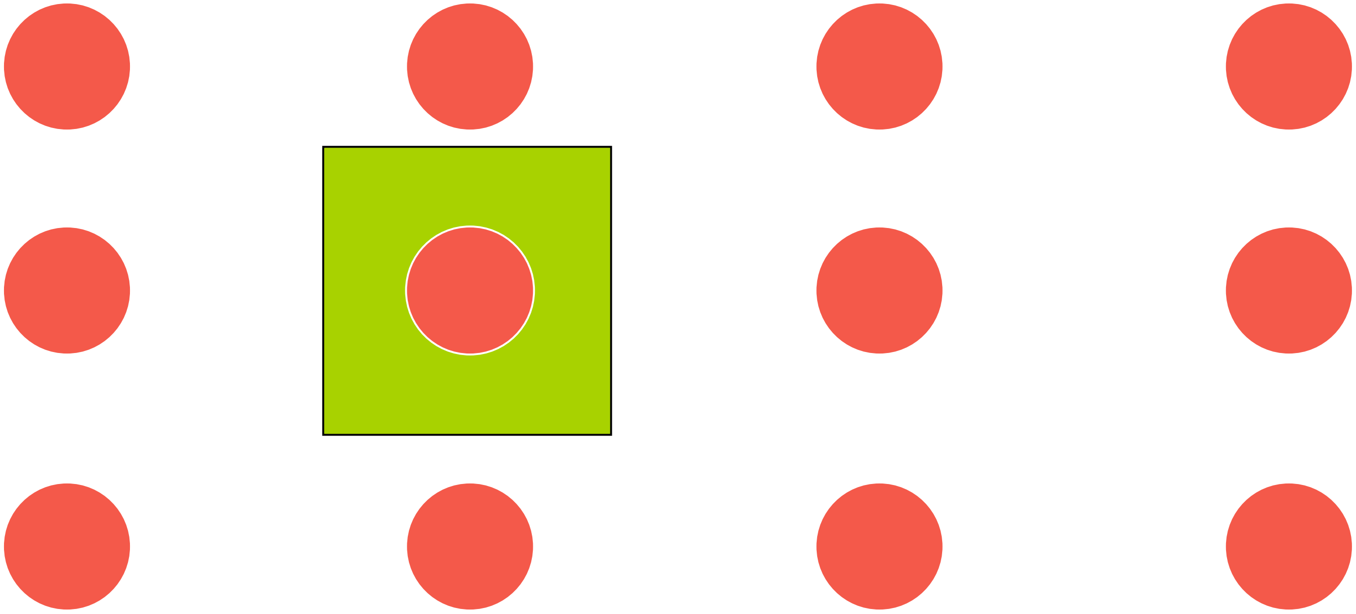
  Commensurate-incommensurate transition
  Change in local density profile

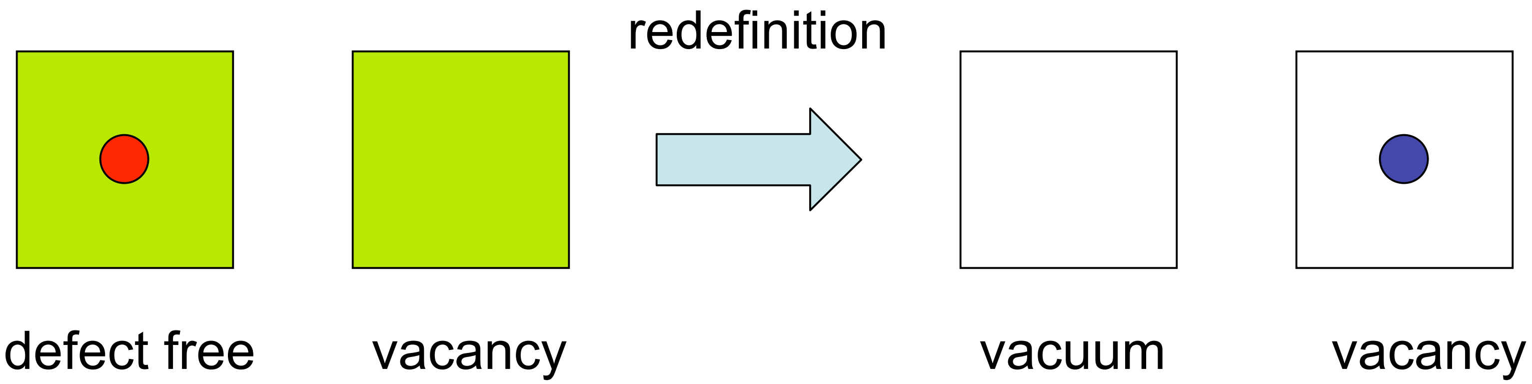
Andreev-Lifshitz Vacancy Model

Defect free solid - Mott insulator



Andreev-Lifshitz Vacancy Model





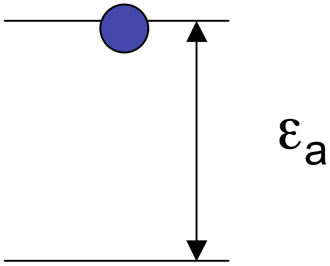
redefinition

defect free

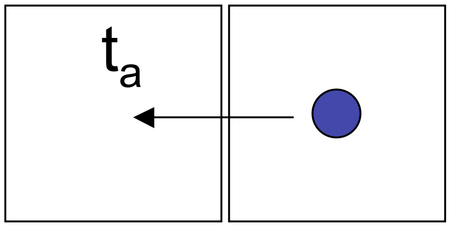
vacancy

vacuum

vacancy



ε_a



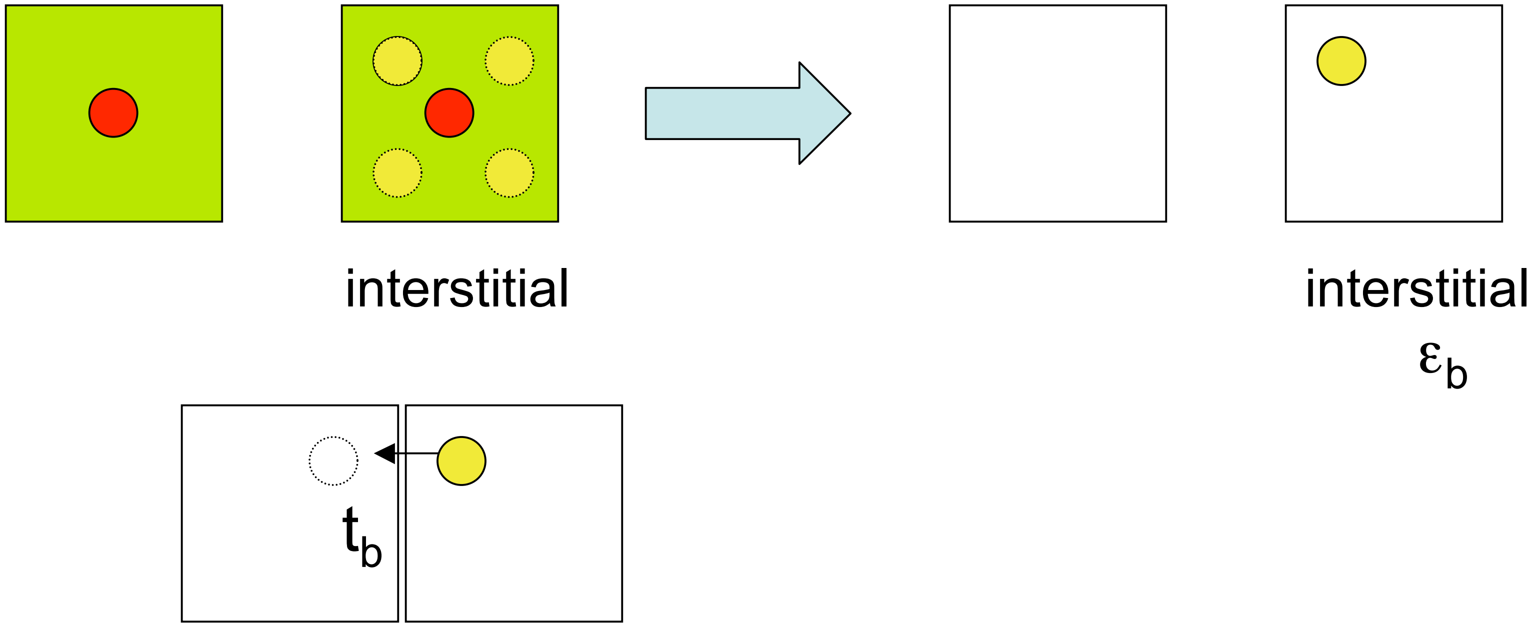
t_a

$$E_v = \varepsilon_a - zt_a$$

If $E_v < 0$, spontaneous creation of vacancies at $T = 0$
Such vacancies will Bose condense

$E_v < 0$ not supported by expts or theories

Interstitial Model



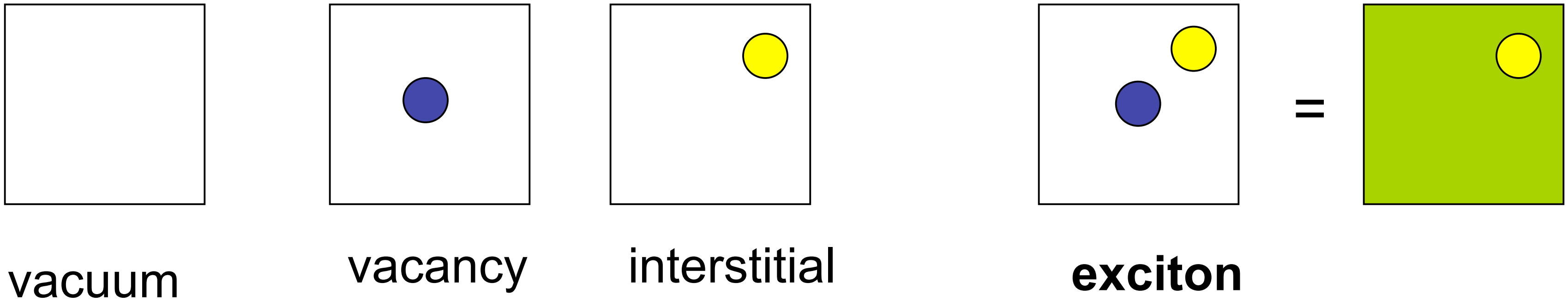
$E_b = \varepsilon_b - zt_b$

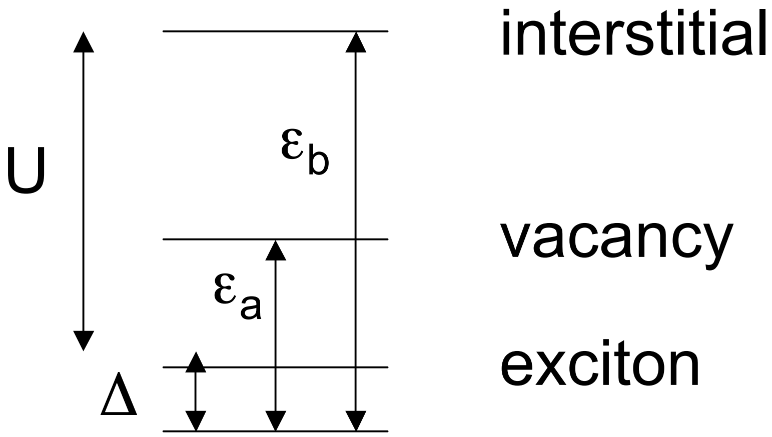
$t_b > t_a$, but $\varepsilon_b >> \varepsilon_a$, so $E_b > E_a$

Interstitial condensation even more unfavorable.

Have Your Cake and Eat it Too Model

Third type of defect : bound vacancy-interstitial or “exciton”

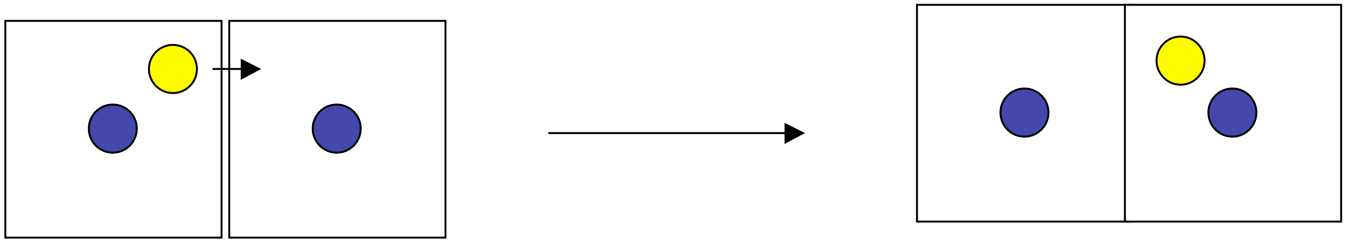




$$\varepsilon_b >> \varepsilon_a > \Delta$$

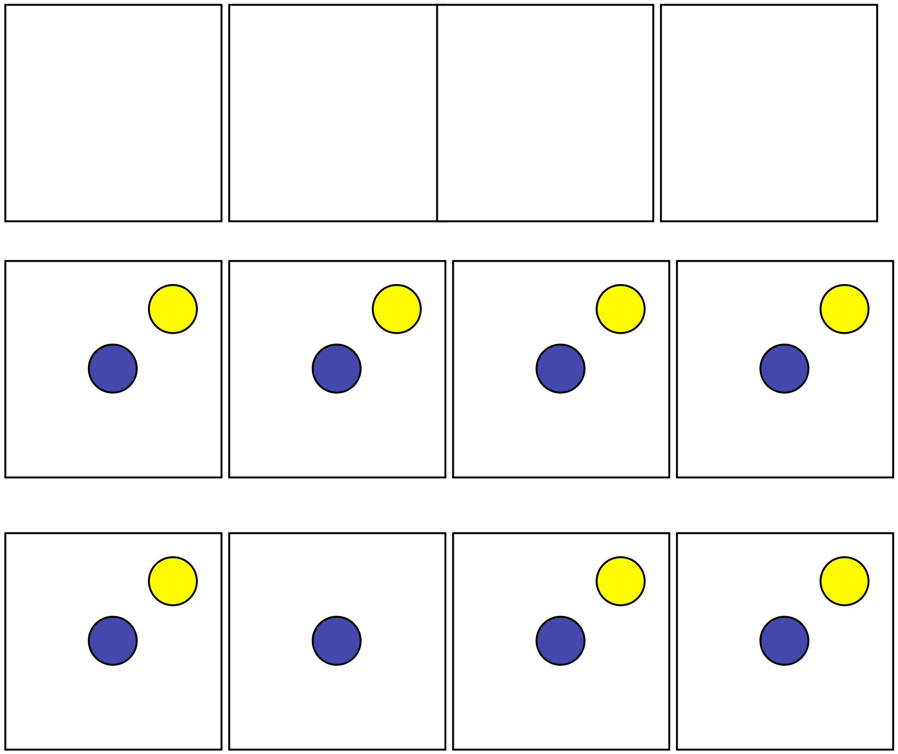
Key physics:
Vacancies can Bose condense easier over exciton background than over defect free background

- activation energy $\varepsilon_a - \Delta < \varepsilon_a$
- vacancy hops with t_b , not t_a



Instability criteria $\varepsilon_a - \Delta - zt_b$

If condensation amplitude sufficiently large,
condensation energy $> \Delta$
vacancies Bose condense



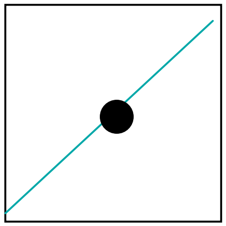
stable normal solid
defect free
$n_{ex} = n_v = 0$

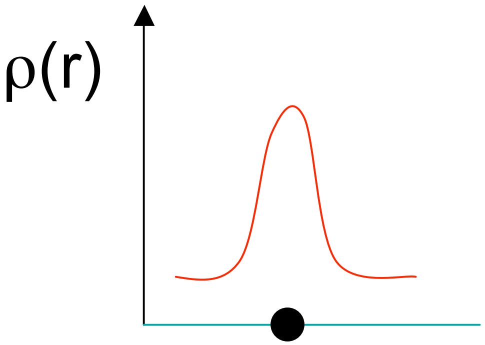
unstable normal solid
defect rich
$n_{ex} \neq 0, n_v = 0$

stable supersolid
defect rich
$n_{ex} \neq 0, n_v \neq 0$

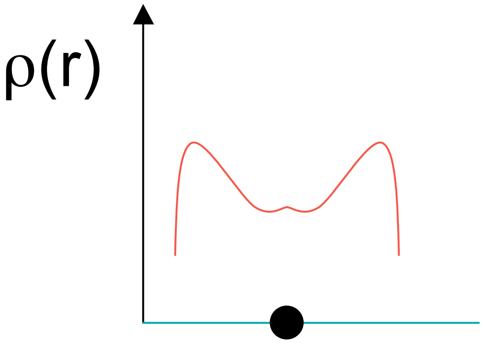
- T = 0 transition first order
- normal - supersolid transition
  commensurate - incommensurate transition
  change in local density profile

Change in Local Density Profile



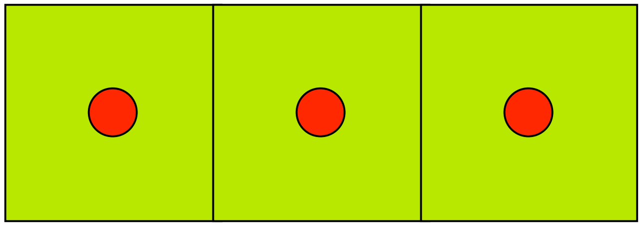


Normal Solid



Supersolid

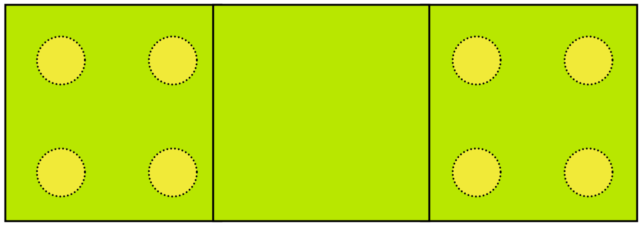
Microscopic Wavefunction



Normal solid $\psi = \prod_{i=1}^{N} b_i^{+} |vacuum\rangle$

b_i^+ creates a He atom in localized state $\phi_i = \phi(r-R_i)$

commensurate
ϕ has single peak



Supersolid $\psi_{SS} = \prod_{i=1}^{N_0} (u + v a_i^{+}) |vacuum\rangle$

a_i^+ creates a He atom in localized state $\chi_i = \chi(r-R_i)$
$|u^2|$ = vacancy fraction

$N < N_0$, incommensurate
χ less localized than ϕ, perhaps even multiipeak

Equivalence between Jastrow and Nosanow-Jastrow wavefunctions with vacancies

$$\psi_{SS} = \prod_{i=1}^{N_0} (u + v a_i^{+}) \left| vacuum \right\rangle$$

$$\equiv P_G \left(\sum_{i=1}^{N_0} \frac{v}{u} a_i^{+} \right)^N \left| vacuum \right\rangle$$

$$\sim P_G \left(\int dr \sum_{i=1}^{N_0} \chi(r - R_i) \psi^{+}(r) \right)^N \left| vacuum \right\rangle$$

$$= P_G \prod_{\alpha} \left(\sum_{i=1}^{N_0} \chi(r_\alpha - R_i) \right)$$

Single-Site Mean Field Theory

- Decouple K.E.

  $ta^{+}a \rightarrow t\langle a^{+}\rangle a + ta^{+}\langle a\rangle - t\langle a^{+}\rangle\langle a\rangle$

  $\langle a\rangle$ solved self-consistenty to give Bose condensed amplitude

- $E = E_{MF}$ + elastic energy for change in lattice constant

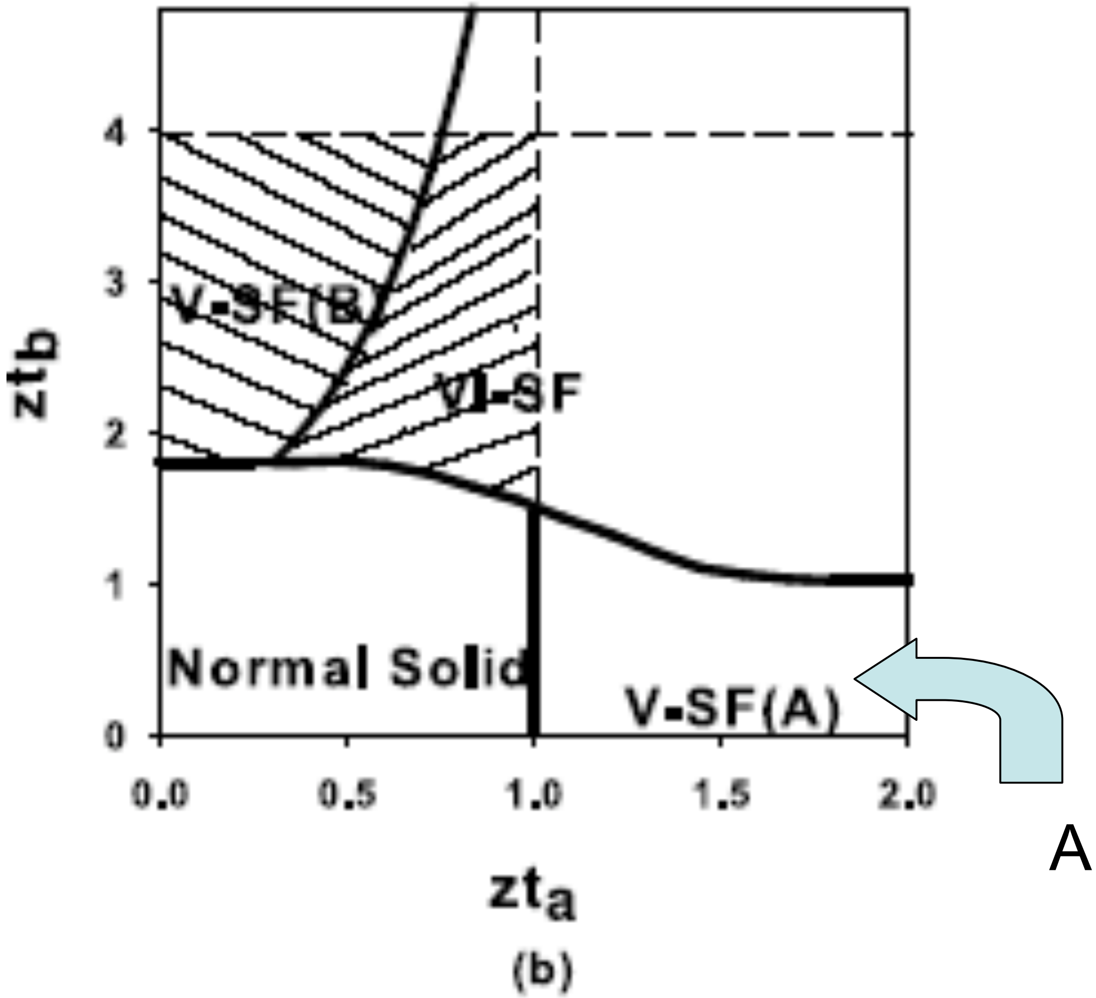
- Respect strong on-site correlations (hard core)

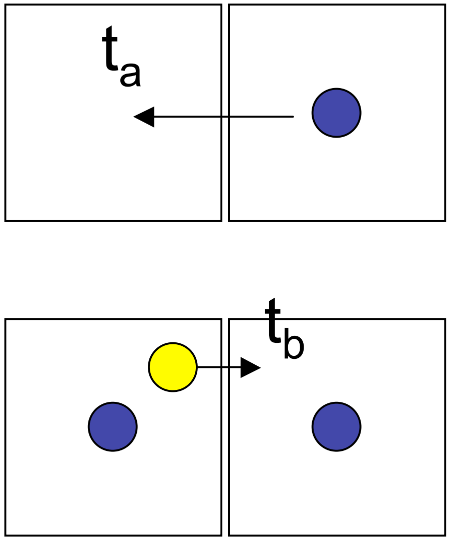
- Successful for other lattice boson models for $d \geq 2$ at $T=0$

- Gives exact instability criteria for Andreev-Lifshitz Model

- Key results for $T=0$ strengthened by quantum fluctuations

T = 0 Phase Diagram



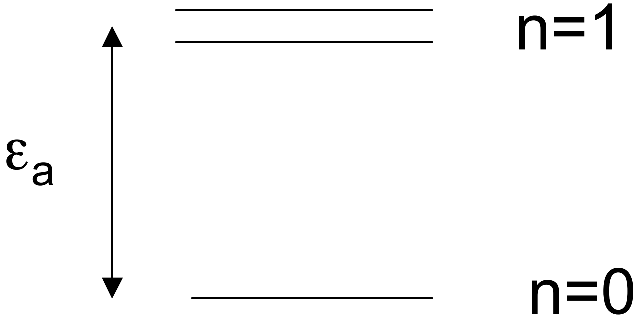


Andreev-Lifhshitz

$\varepsilon_b = 4\,\varepsilon_a$ $\Delta = 0.2\,\varepsilon_a$

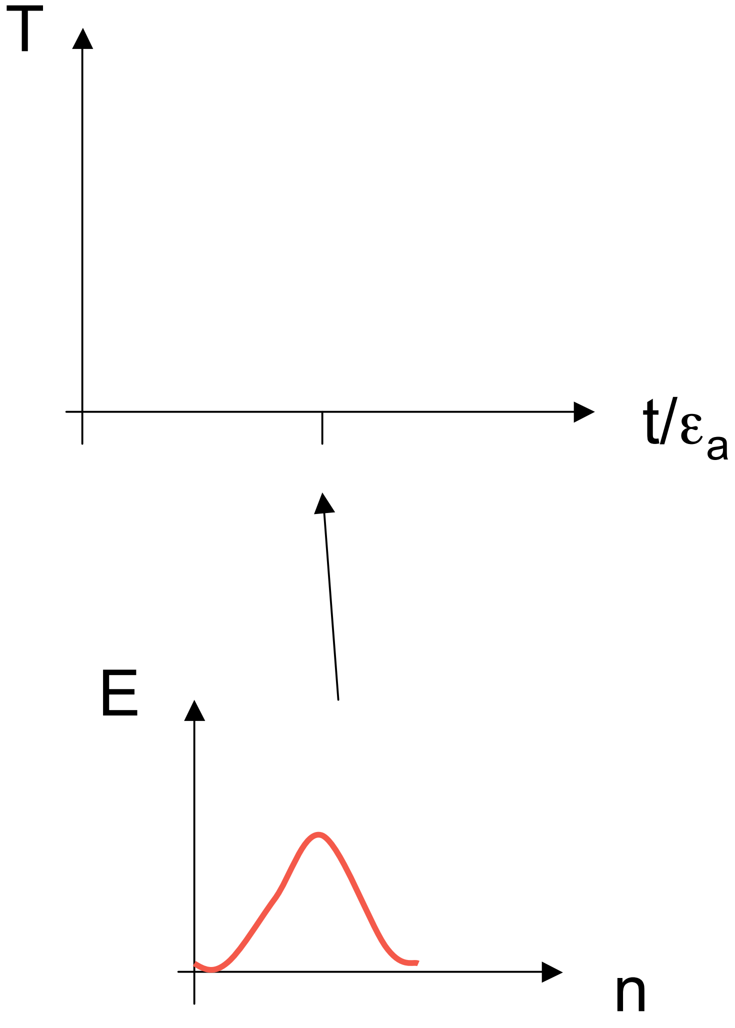
Finite T

Illustrate with ε_b = infinity, $t_a = 0$, $\Delta = \varepsilon_a$

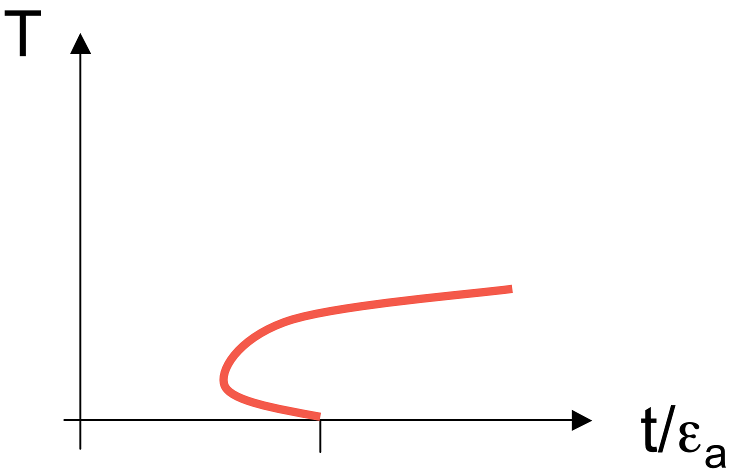


Two coupled order parameters:
n = <n>, defect concentration
b = <b>, condensate amplitude

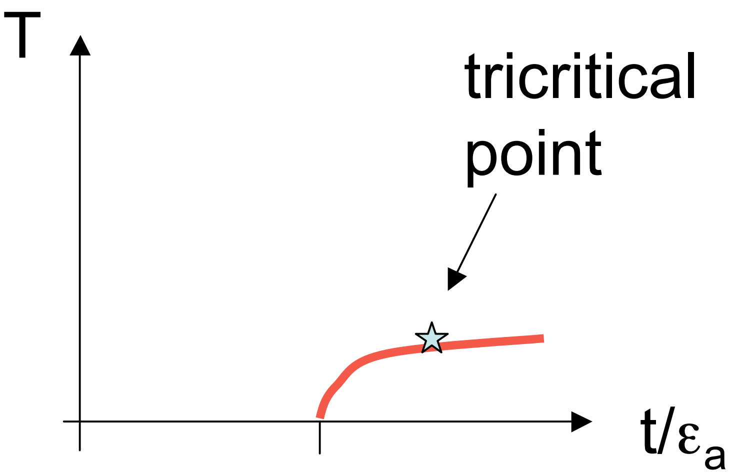
Finite T Phase Diagram (schematic)



Finite T Phase Diagram (schematic)



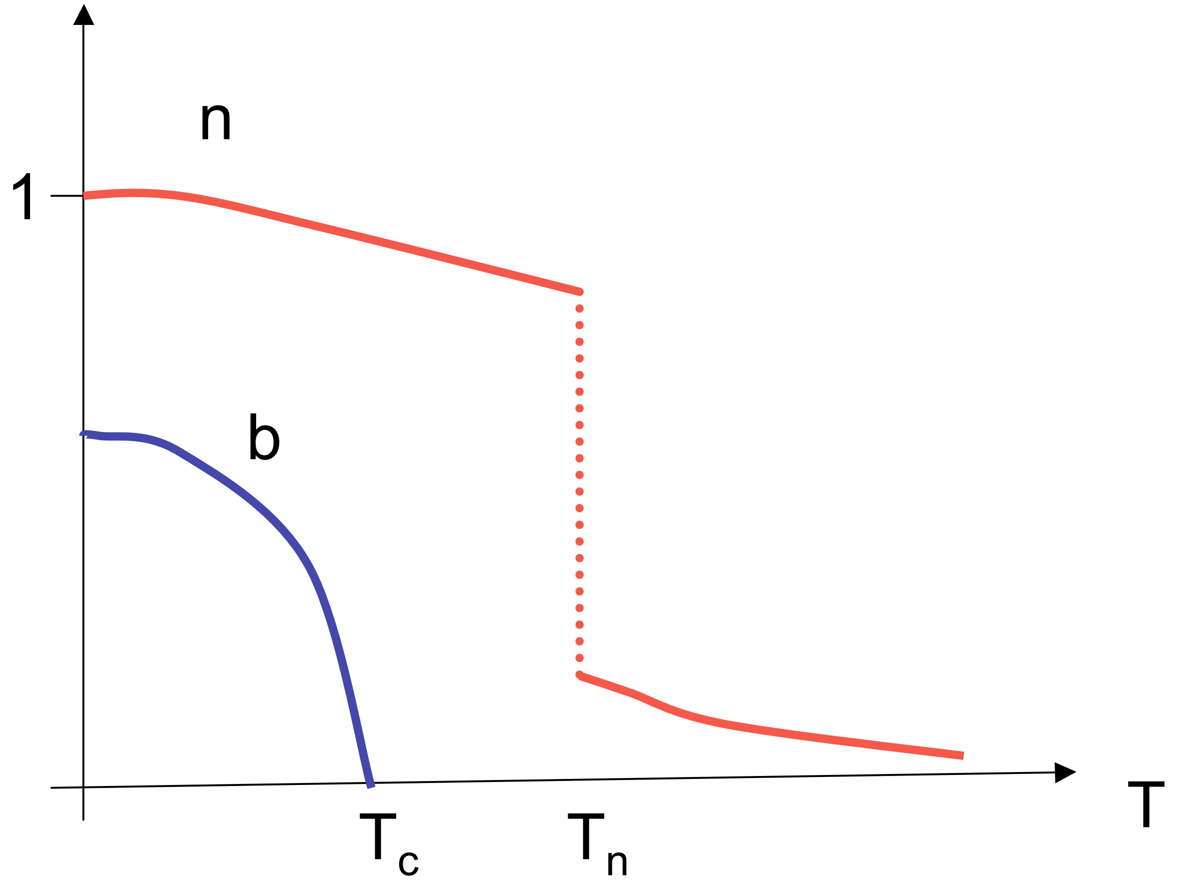
or



These are transition curves for n.
NCRI is related to transition in b

NCRI transition

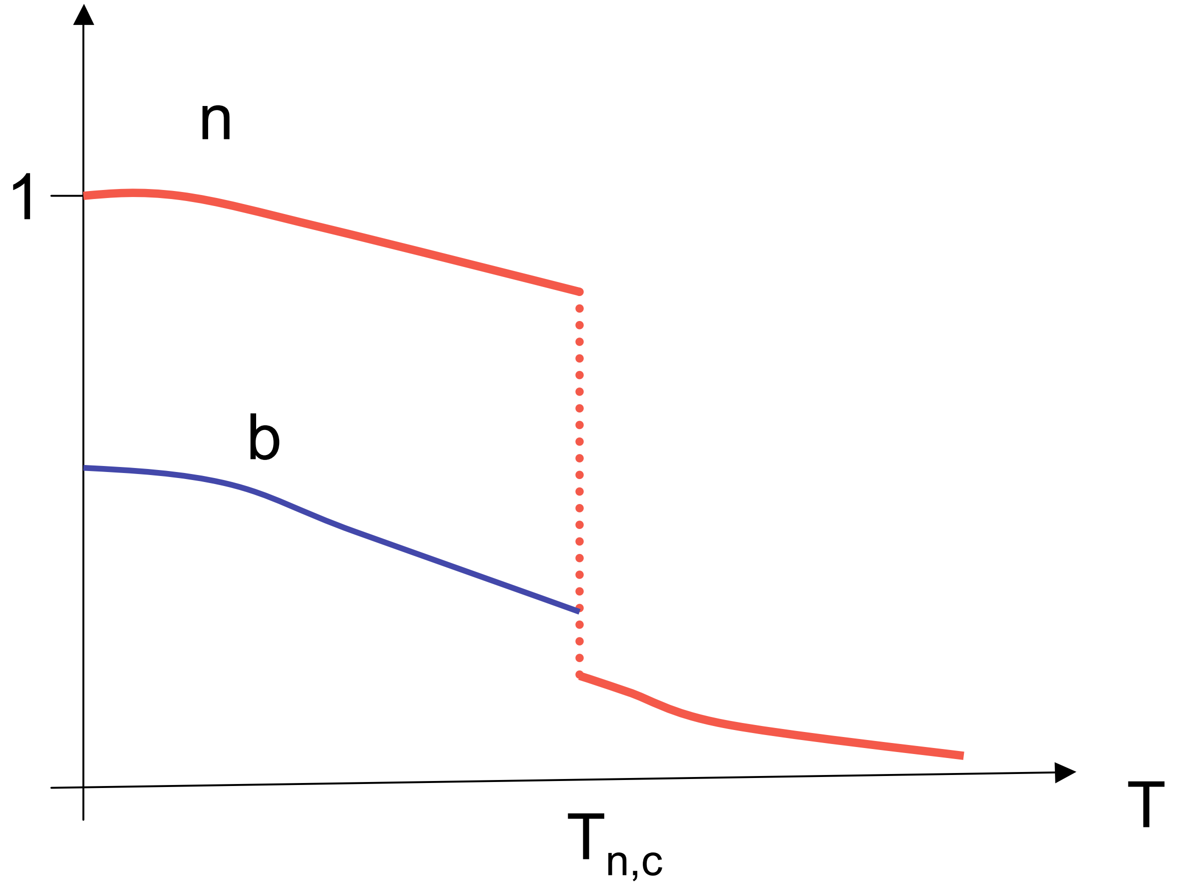
Possibility I



NCRI transition occurs below defect density transition
transition second order

NCRI transition

Possibility II



NCRI transition occurs with defect density transition
transition first order

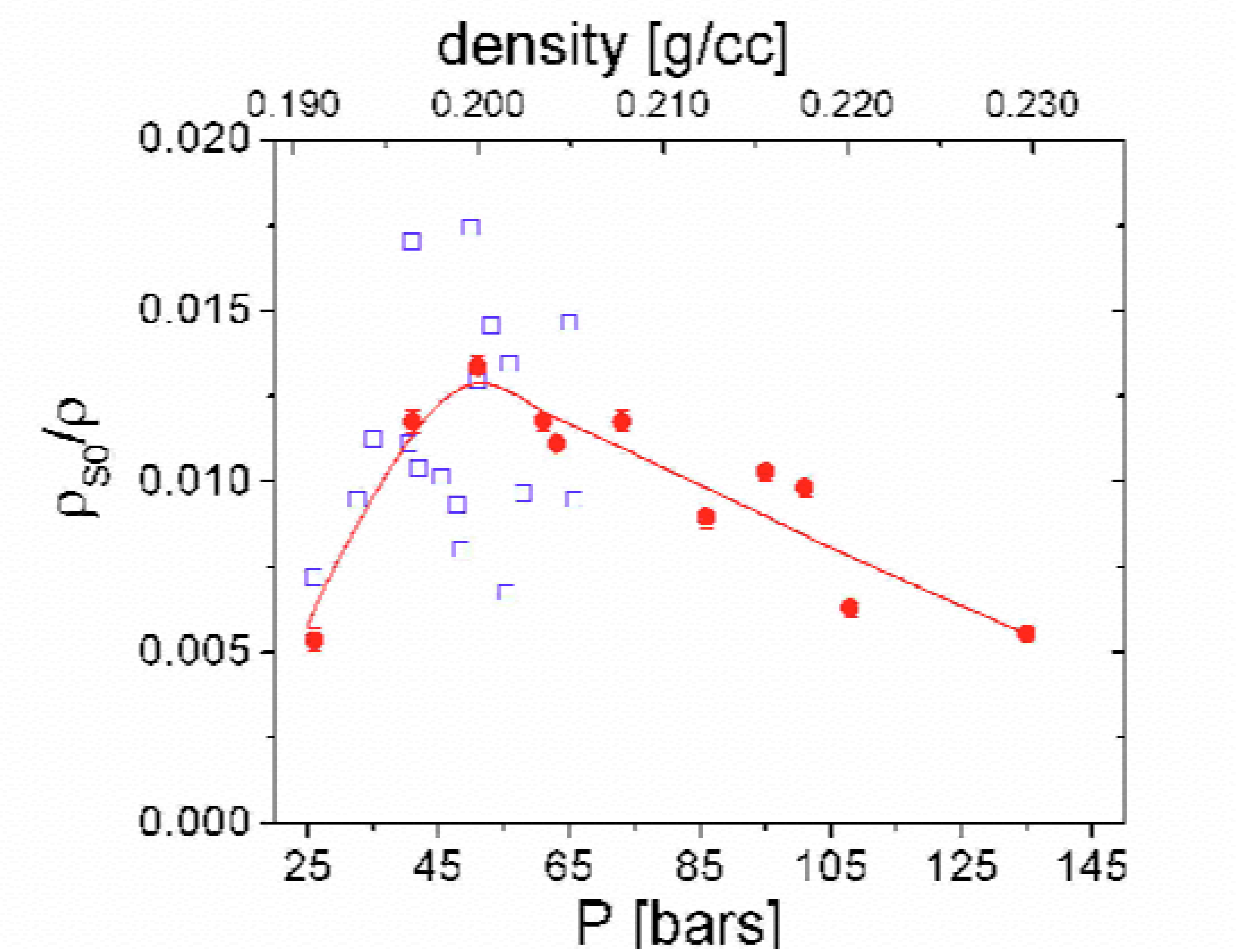
Casual Comparison to Experiments

T=0 Superfluid Density

- Kim and Chan reported max $\rho_s/\rho \sim 1\%$
  Our MFT gives 3 - 9%
  Value should be reduced by quantum (phase) fluctuations
  Fluctuations stabilize supersolid vs. defect free state

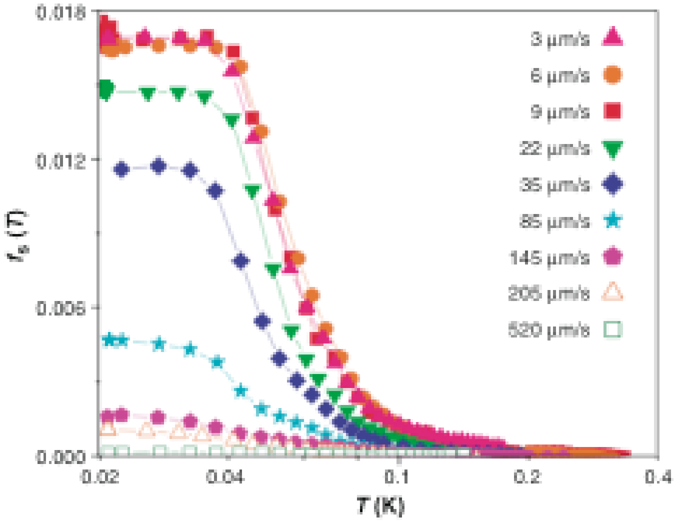
- More recent data shows ρ_s increasing then decreasing with pressure/density
  - Within our model, ρ_s favored by small Δ, ε_a, large $t_{a,b}$
  - $_,$ $t_{a,b}$ may be non-monotonic with ρ

Penn State data



Finite T ρ_s

Finite T



- data suggests transition smeared by disorder
- specific heat shows no critical behavior

Two possibilities for pure system:
-second order transition *not* in X-Y universality class
- first order transition

Transition is first order at T=0 in our model
May also be first order at finite T

He 3 Impurities

Expt, with increasing He3 concentration (ppm):
-T_c increases
- low T ρ_s decreases
- NCRI not observable beyond 0.1% He3 concentration

Qualitative agreement:
- He 3 favors defects due to its smaller mass
  => T_c increases
- Impurities localize vacancies
  => reduce ρ_s and eventually destroys Bose condensation
  (dirty bosons)

Conclusions

- Vacancies can condense in solid He4 in spite of negative evidence from normal state
- Normal solid defect free, supersolid defect rich
  - -- first order transition
  - -- commensurate - incommensurate
  - -- change in local density profile
- No intrinsic contradiction between Kim and Chan’s observation and existing normal solid data