Theories of Superfluid Fraction f_s for Solid ^{4}He

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How to Calculate Superfluid Fraction f_s

- Not in Andreev and Lifshitz, nor in Chester.
- Leggett (1970) gives a prescription based on a variational estimate (intrinsically an upper bound).
- Pollock and Ceperley (1987) give an exact relationship for f_s, based upon fluctuations (both thermal and quantum) in the "winding number". Builds on Gordon Baym (Boulder?) lecture notes.
- I don't know of another microscopic way to get f_s.

Outline (pre-KITP Supersolids miniconference)

- Two distinct mechanisms for supersolid:
  (a) by Andreev&Lifshitz (and Chester), who consider vacancy condensation and flow with density changes ("mass transport by means of the motion of the zero-point defectons while the lattice sites remain essentially fixed"); and
  (b) by Leggett, who considers commensurate particle condensation and flow with no density (or lattice) changes ("**phase flow**").
- Two classes of experiment:
  (a) one set (pressure driven), involving density changes, disfavors vacancy flow, and
  (b) another set (rotation driven), involving no density changes, favors "phase flow".

Outline (pre-KITP Supersolids miniconference)

- Leggett approach (1970) is probably appropriate only for BEC into a single commensurate and periodic state. Gives upper limit for **superfluid fraction f_s** at T=0, using a one-body phase. A sum-of-gaussians estimate of density profile (circa 1976) give f_s=0.02 (good). Fcc and hcp lattices are almost equivalent. However, latest hcp Monte Carlo density profile from Galli and Reatto gives f_s=0.20.
- What's new in many-body physics? Higher order correlations in phase function should lower f_s from 0.20. Current density is more complex than for single atom.
- Phase flow implies quantum vortex lines and rings. Ion ring experiments?

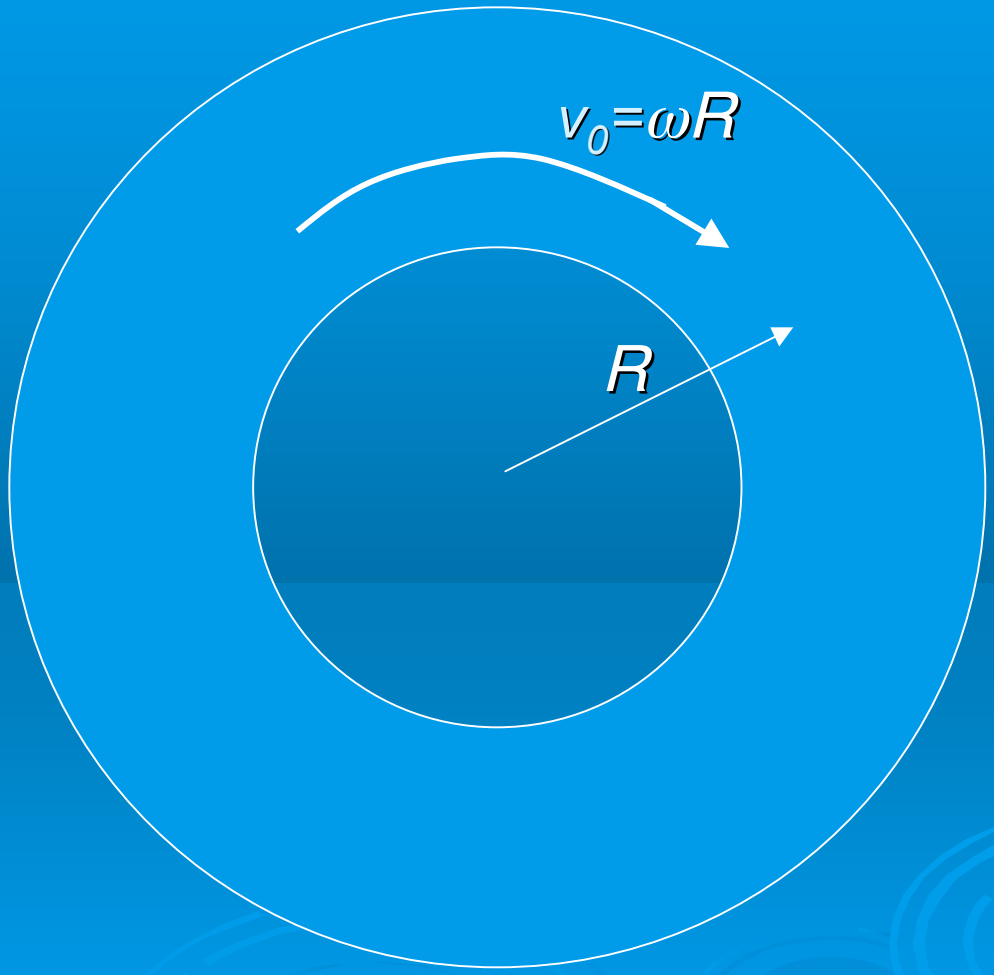
Addendum (KITP Supersolids miniconference)

- How do we include the effect of vacancies in making a good estimate of the superfluid fraction f_s?
- What could the wavefunction possibly look like?
- Does ^{3}He play an essential role in affecting the wavefunction?

What is "Phase Flow"?

- Simple for one-body system, where $\Psi = \rho^{1/2}\exp(i\phi)$. Particle flux is $j=\rho v_s$, where $v_s=(\hbar/m)\nabla\phi$, and $d\rho/dt+\mathrm{div}\ j=0$ (continuity). j gives "phase flow".
- Consider electron for hydrogen atom in 2p state with l=1. (Neglect proton.) Have non-zero j (to get net angular momentum), but no net momentum, and $d\rho/dt=0$, div j=0. Hence the density is constant, but there is local particle flow. This is phase flow at constant density.
- Particle flux $j=\rho v_s$ also pretty literally applies to the center-of-mass motion of all atoms, even of atoms like lead or uranium, which we think of as classical. However, for translational motion of an atom, the density changes. Nevertheless, this is still phase flow.
- Any motion of a massive object can be described (perhaps in more complex form than $j=\rho v_s$, because of many-body effects) as phase flow. For a ring system with 10 sites and 9 atoms, coherent motion of 9 atoms can be described as phase flow, but is easier to think of as vacancy flow. This may be what Andreev and Lifshitz had in mind.

Leggett Phys. Rev. Lett. **25**, 1543 (1970)
Superflow for a Solid in an Annulus



$L=2\pi R$

A.J.Leggett (1970) - Overview

- Expanded on Kohn's discussion of conductors vs. insulators, replacing applied electric field by rotation.
- (a) Notes that in rotating frame the Hamiltonian is time-invariant (good for solving Schrodinger equation) but the boundary condition on the wavefunction becomes more complex. Notes that if ground state energy E_0 is sensitive to the new b.c., then there will be a Non-Classical Rotational Inertia (NCRI). Note: torsion oscillator experiment measures NCRI and NCRIF, but only if we have supersolid does NCRIF=f_s. For localized states, the energy is insensitive to rotation, so no superfluidity. Also, states that can decay give no superfluidity.
- (b) Assuming bosons to have common (one-body) phase function ϕ that depends only on coordinate in direction of rotational motion, developed theory for upper bound on superfluid density ρ_s.
- Local superfluid velocity $v_s=(\hbar/m)\nabla\phi$ (can vary on atomic scale); spatial-average superfluid velocity $v_0=(\hbar/m)\Delta\phi/\Delta x$.

Solid ^{4}He Wavefunctions - I

- Generically, two types of wavefunctions have been considered for solid ^{4}He.
- Both build on Jastrow form, used in liquid ^{4}He: for three particles,
  $\Phi_J(r_1,r_2,r_3) = \exp(u(r_{12}))*\exp(u(r_{23}))*\exp(u(r_{13}))$.
  Already symmetrized (Bose statistics).
- The u (r_{12})'s keep the particles from getting too close to one another.

Solid ^{4}He Wavefunctions - II

- Localised form (Nosanow). For r_1 a particle site and s_1 a lattice site, etc, take $\Phi(r_1,r_2,r_3) = \Phi_J(r_1,r_2,r_3)*f(r_1-s_1)*f(r_2-s_2)*f(r_3-s_3)$; perhaps even symmetrize the last three terms (important for exchange). $f(r_1-s_1)$ localizes r_1 around s_1.

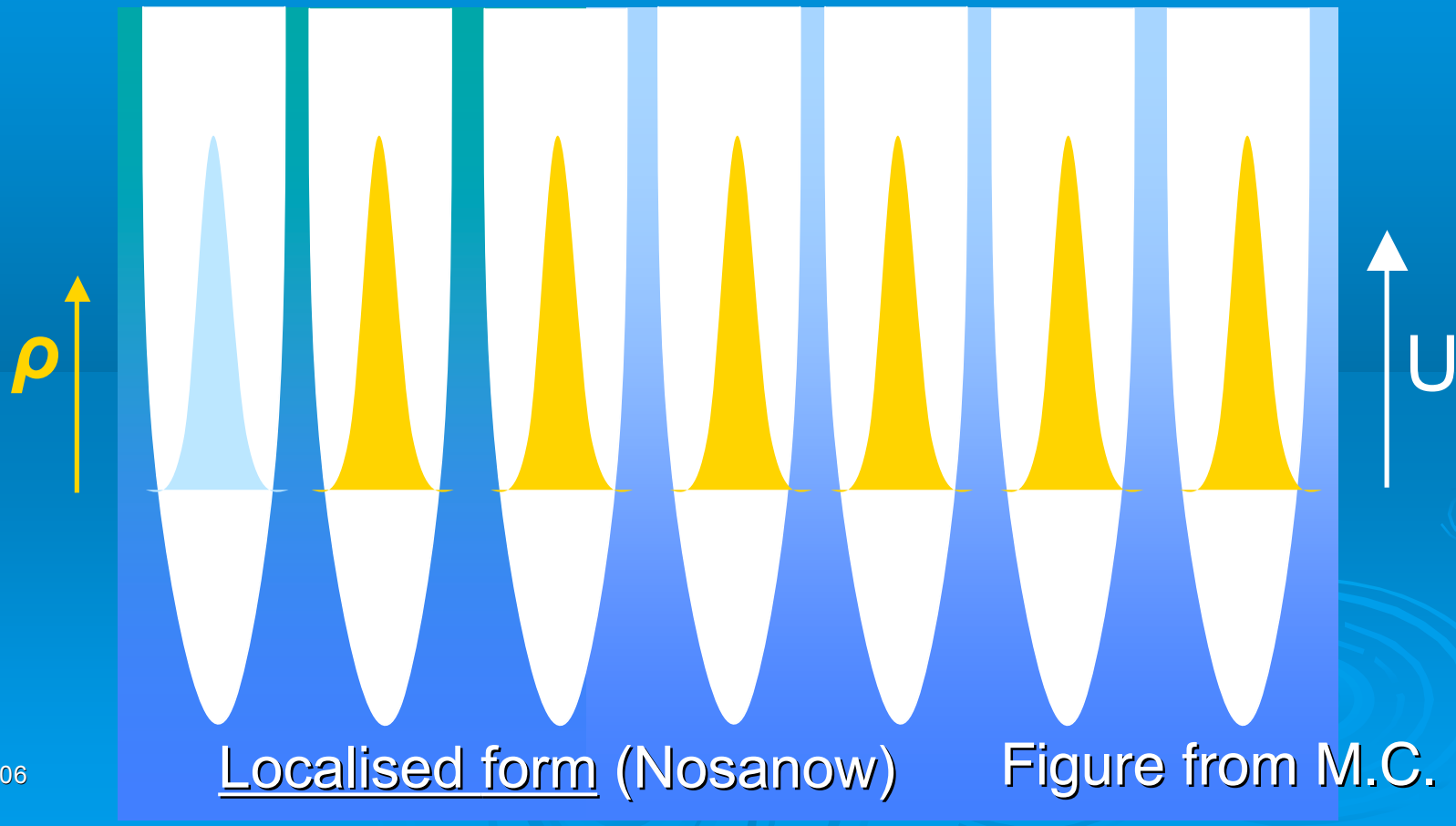
  Like a Mott insulator. NOT SUPERFLUID

- Delocalized form (Lowy-Woo). $\Phi(r_1,r_2,r_3) = \Phi_J(r_1,r_2,r_3)*g(r_1)*g(r_2)*g(r_3)$; automatically symmetrized. $g(r_1)$ is periodic (covers all lattice sites).

  Like a partially localized fluid. POSSIBLY SUPERFLUID.

  (But gives high ground state energy for Yukawa interaction.)

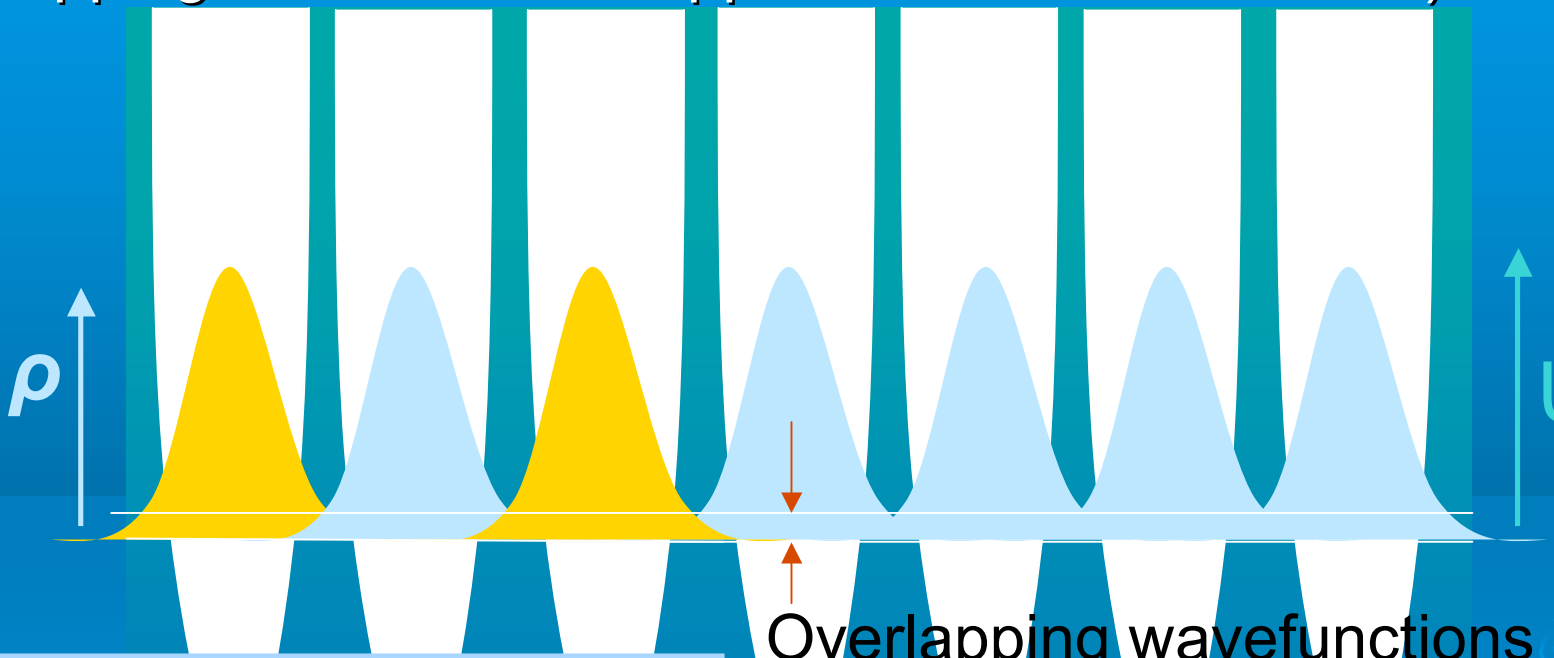
- According to Leggett, if the atomic wavefunctions are disconnected relative to the entire sample (even though they may overlap), then no superflow and no NCRI.



Localised form (Nosanow)

Figure from M.C.

- If the atomic wavefunctions are connected relative to the entire sample (so they must overlap), then have ODLRO and expect superflow and NCRI. (Picture below, borrowed from M.C., isn't quite appropriate for this point because it makes the overlapping wavefunctions appear to be disconnected.)



Remember: $\gamma_L = \frac{\sqrt{< u^2 >}}{d_a} = 0.26$

Delocalized form (Lowy-Woo).

A.J.Leggett (1970) - (a)

- In lab frame $\Psi(x+L,t)=\Psi(x,t)$ is boundary condition. If walls move at v_0, then (neglecting particle-particle interactions)

  $$H_0(x,t)= -[\hbar^2/2m](d^2/dx^2) + V(x-v_0t)$$

- In $H_0\Psi=i\hbar d\Psi/dt$, potential $V(x-v_0t)$ varies with time - not good.

- In moving frame ($x'=x-v_0t$, $t'=t$), potential is time-independent.

  $$H_0(x,t)= H_0(x')= -[\hbar^2/2m]d'^2/dx'^2 +V(x')$$

- Define $\Psi(x,t)= exp(ikx)\,\Psi'(x',t)$. Then
  $\Psi'(x'+L,t)=exp(-ikL)\,\Psi'(x',t)$ is new boundary condition.

- With $k=mv_0/\hbar$, $H_0\Psi=i\hbar d\Psi/dt$ becomes
  $(H_0+[(\hbar k)^2/2m])\Psi'=i\hbar d\Psi'/dt$,
  where $H_0(x')$ is independent of time, and Ψ' is subject to new boundary condition, with $\Delta\phi= -kL= -mv_0L/\hbar= -mv_0(2\pi R)/\hbar$.

A.J.Leggett (1970) - (b)

- Assume that $\Psi=\Psi_0 \exp(i\phi)$, and that $\phi=\Sigma\phi_1(x_i)$; a one-body phase. Density doesn't change, so potential energy doesn't change. From Ψ_0 can get the atomic number density $\rho(r)$.
- Then flow pattern v_s minimizes energy and defines ρ_s (!!!!)
  $E = \int d^3r\, \rho(r)\, v_s^2/2 \equiv (1/2)\rho_s v_0^2 \Omega$, ($\Omega$ is volume)
  subject to imposed $\Delta\phi = -kL = -mv_0L/\hbar = -mv_0(2\pi R)/\hbar$. Both $\rho(r)$ and v_s vary on the atomic level, with v_0 (average value of v_s) known and $\rho(r)$ known. $v_s = v_0 + v'_s$. Atomic scale backflow v'_s is unknown.
- Minimum value of E defines Non-Classical Rotational Inertia (NCRI), here ρ_s. Let ρ_0 be the average density.
- Developed variational upper bound for ρ_s/ρ_0, using ϕ depending only on coordinate along direction of average motion.
- Estimated (not calculated) ρ_s/ρ_0 of order 10^{-4} by tunneling analogy.

W. M. Saslow

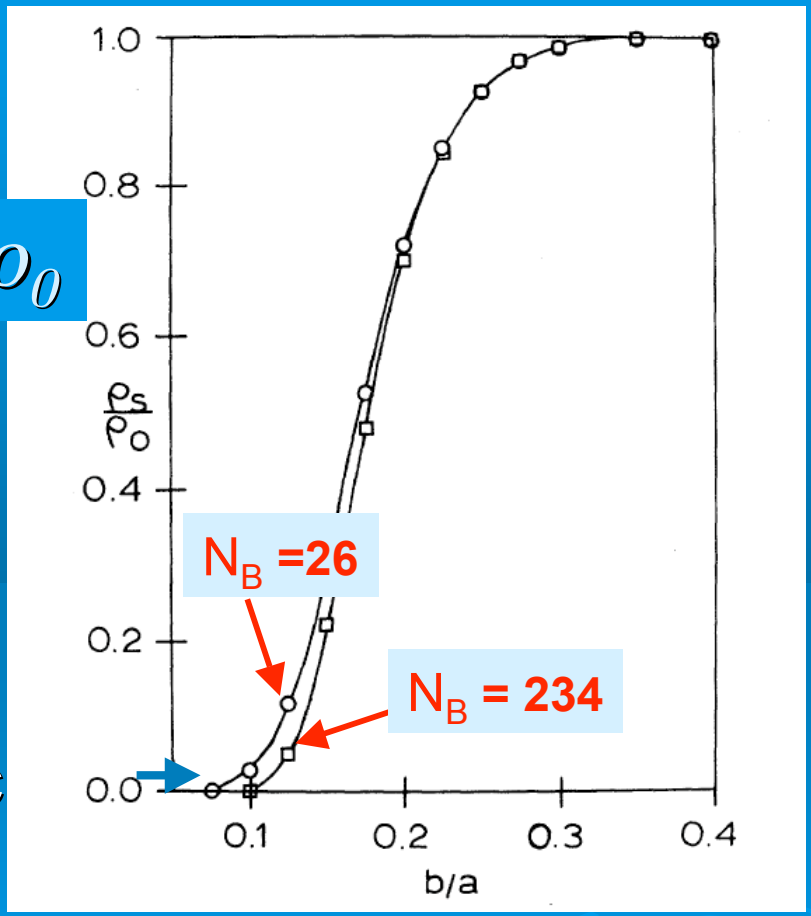
Phys. Rev. Lett. **36**, 1151 (1976)

- Upper bound on ρ_s for ϕ depending on <u>all three</u> coordinates.
- Variationally minimize $E=(\hbar^2/2m)\int \rho(r)(\nabla\phi)^2 d^3r \equiv (1/2)\rho_s v_0^2 \Omega$ with respect to ϕ. Let average density be ρ_0.
- Minimization gives $0 = \nabla \cdot j = \nabla \cdot \rho v_s$. <u>Thus satisfy continuity equation</u>: $d\rho/dt = -\nabla \cdot j = 0$. With $v_s = v_0 + v'_s$, write
  $\nabla \cdot \rho v'_s = -\nabla \cdot \rho v_0$.
  Average velocity v_0 serves as a source term. If $\rho(r)$ is known, can get flow profile $v_s(r)$.
- Take $\rho(r)$ as a sum over gaussians with width b, for fcc lattice constant a. Can solve for $v_s(r)$ and then E and then $f_s = \rho_s/\rho_0$ vs. b/a. Use N_B fourier components.

Superfluid fraction $f_s = \rho_s/\rho_0$ vs *b/a*

(1976 mainframe - Maximum N_B = 234)

Localized: not converged Delocalized: converged



KC = Kim & Chan (2004)

b= width of gaussians
a= fcc lattice constant

Large b/a - classical fluid
Small b/a - quantum solid

For convergence: N_B = no. of plane waves in basis set

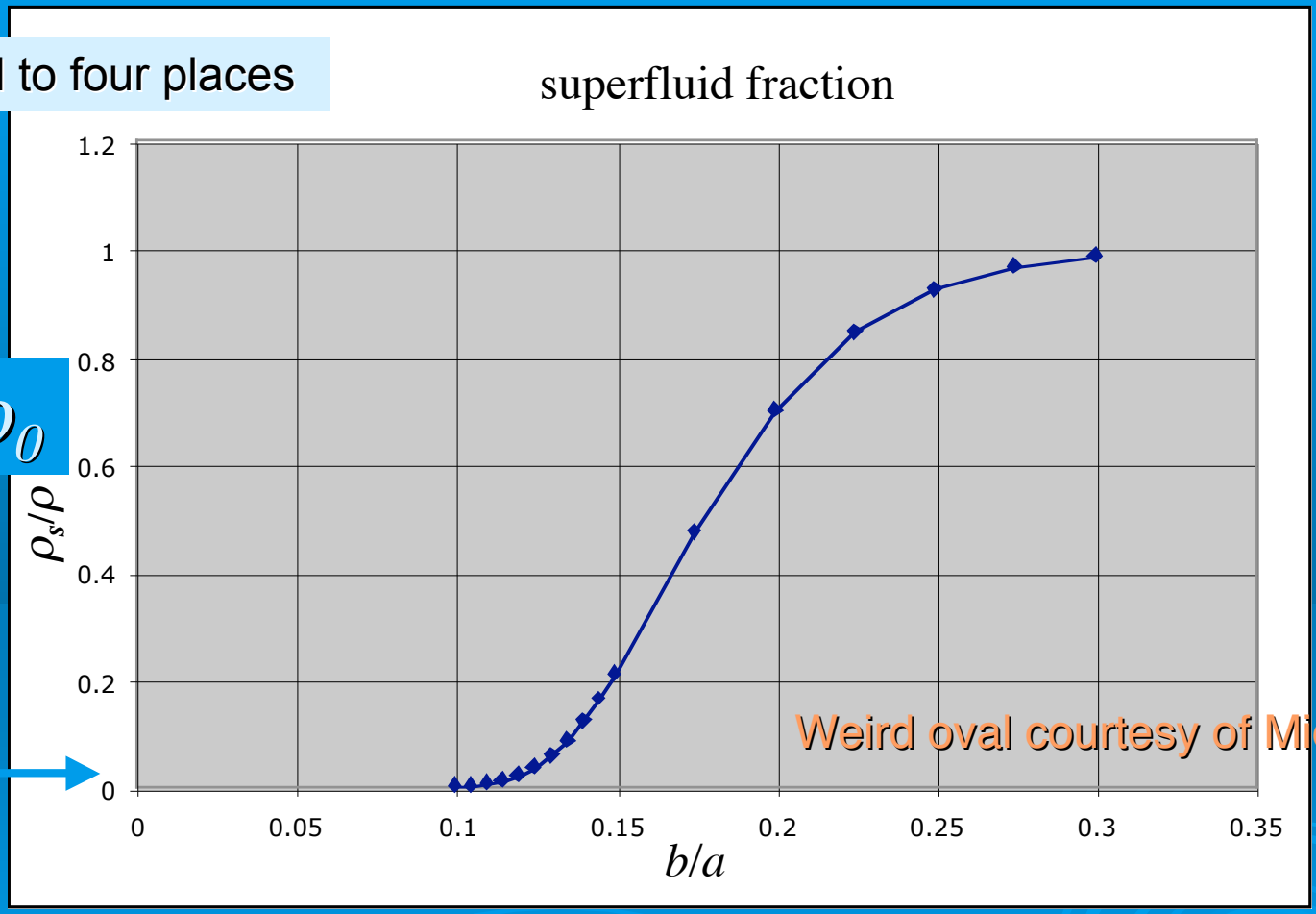
For expected *b/a=0.12*, ρ_s/ρ is of order *5%–20%*. Smaller ρ_s/ρ_0 is below limit of convergence.

Superfluid fraction $f_s = \rho_s/\rho_0$ vs b/a

(2004 - on this Powerbook, Maximum $N_B > 6000$)

W. M. Saslow, Phys. Rev. B 71, 092502 (2005)

Converged to four places



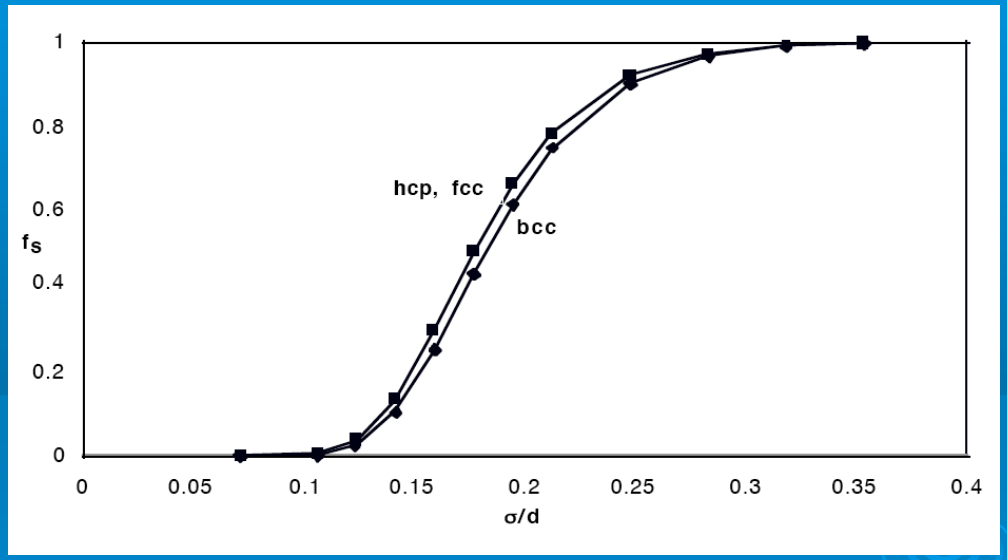
ρ_s/ρ_0

Kim-Chan

Weird oval courtesy of Microsoft

f_s for fcc, hcp, and bcc (sum-of-gaussians density)

- f_s is actually a tensor.
- f_s is expected to be diagonal for cubic lattices. Confirmed for sum-of-gaussians model.
- For sum-of-gaussians model, and $\sigma/d=b/a$=gaussian width/nn distance, f_s for hcp is same as f_s for fcc, to 0.001.
- f_s for bcc is lower, because of more open structure.



The good news: get experimental ρ_s/ρ_0 for b/a~0.115-0.12

The Bad News: Modern Monte Carlo Densities Give Too Much Superfluid Density

- Using density profiles provided by D. Galli and L. Reatto gives $\rho_s/\rho_0=f_s=0.20$. Newer density profiles indicate that solid ^{4}He is much less localized than thought thirty years ago.
- Problem: superfluid fraction f_s now is much higher than experiment. (We used to worry it would be much lower!)
- Not necessarily bad, because 20% is still an upper limit.
- How can we get around this? Extend our view of phase function.

But First: for Monte Carlo density superflow is nearly Isotropic

(Saslow, Galli and Reatto, unpublished)

TABLE I: Superfluid fraction for hcp lattice with $\rho_0 = 0.029$ Å^3.

N is a measure of basis set size

converged

N	$f_s(100)$	$f_s(010)$	$f_s(001)$
1	0.405498723	0.380100695	0.569434049
2	0.288404628	0.273327405	0.334029644
3	0.246381157	0.238923885	0.261835390
4	0.230966475	0.226688728	0.234649864
5	0.224924997	0.221915928	0.222438944
6	0.222396304	0.219891477	0.216574767
7	0.221292170	0.218987446	0.213748538
8	0.220798253	0.218572811	0.212366358

More Complex Phase Function

- Phase functions $\phi(x_1,x_2,\ldots)$ used to date are one-body functions; a bit like mean-field theory.

$$\phi = \sum_i^N \phi_1(x_i)$$

- Hence one-body phase seems to work exactly for superfluids, with uniform density profiles.

- Must try a more complex function to represent the phase of a supersolid. (Saslow, Galli, Reatto, unpublished)

$$\phi = \sum_i^N \phi_1(x_i) + \frac{1}{2(N-1)} \sum_{i \neq j}^N \phi_2(x_i, x_j) + \ldots$$

Two-Body Phase Function

- Ψ_0 is ground-state wavefunction. Define one-body, two-body, and three-body densities. $\rho(r) \equiv \rho_1(r)$.

$$\rho_1(1) \equiv \rho_1(x_1) \equiv N \int |\Psi_0|^2 dx_2 \dots dx_N,$$

$$\rho_2(1,2) \equiv \rho_2(x_1, x_2) \equiv N(N-1) \int |\Psi_0|^2 dx_3 \dots dx_N,$$

$$\rho_3(1,2,3) \equiv \rho_3(x_1, x_2, x_3) \equiv N(N-1)(N-2) \int |\Psi_0|^2 dx_4 \dots dx_N$$

- Energy minimization yields two "continuity" conditions.

$$0 = \frac{1}{\hbar} \frac{\delta \Delta E}{\delta \phi_1} = \vec{\nabla}_1 \cdot [\rho_1(x_1) \vec{v}_s(1) + \frac{1}{N} \int dx_2 \rho_2(x_1, x_2) \vec{v}_s(1,2)]$$

$$0 = \frac{1}{\hbar} \frac{\delta \Delta E}{\delta \phi_2} = \vec{\nabla}_1 \cdot [\rho_2(x_1, x_2) \vec{v}_s(1) + \frac{1}{N} \int dx_3 \rho_3(x_1, x_2, x_3) \vec{v}_s(1,3)]$$

- [illegible] use new term to lower their NCRI, as observed experimentally (at T=0 superfluids have f_s=1).

More Complex Form for One-Body Current Density j

$$j(x_1) = [\rho_1(x_1)\vec{v}_s(1) + \frac{1}{N}\int dx_2 \rho_2(x_1, x_2)\vec{v}_s(1,2)]$$

What if there are Vacancies?

- Imagine a ring of three sites with two particles and one vacancy. Try a ground state wavefunction
  $\Psi = \Psi_1 + \Psi_2 + \Psi_3$, where the subscript indicates the vacant site.
- On rotation we expect
  $\Psi \Rightarrow \Psi' = \Psi_1 \exp(i\phi_1) + \Psi_2 \exp(i\phi_2) + \Psi_3 \exp(i\phi_3)$, where ϕ has the same (unknown) form in each case. This form permits density changes, so the potential energy can change.
- Have to work out implications of this structure.

That’s all folks!