



**UCDAVIS**



Aleksander Zujev  
Journal Club talk 2-23-2006

# Thermodynamics of an incommensurate quantum crystal

P. W. Anderson, W. F. Brinkman and David A. Huse  
Department of Physics, Princeton University, Princeton, NJ

# Outline

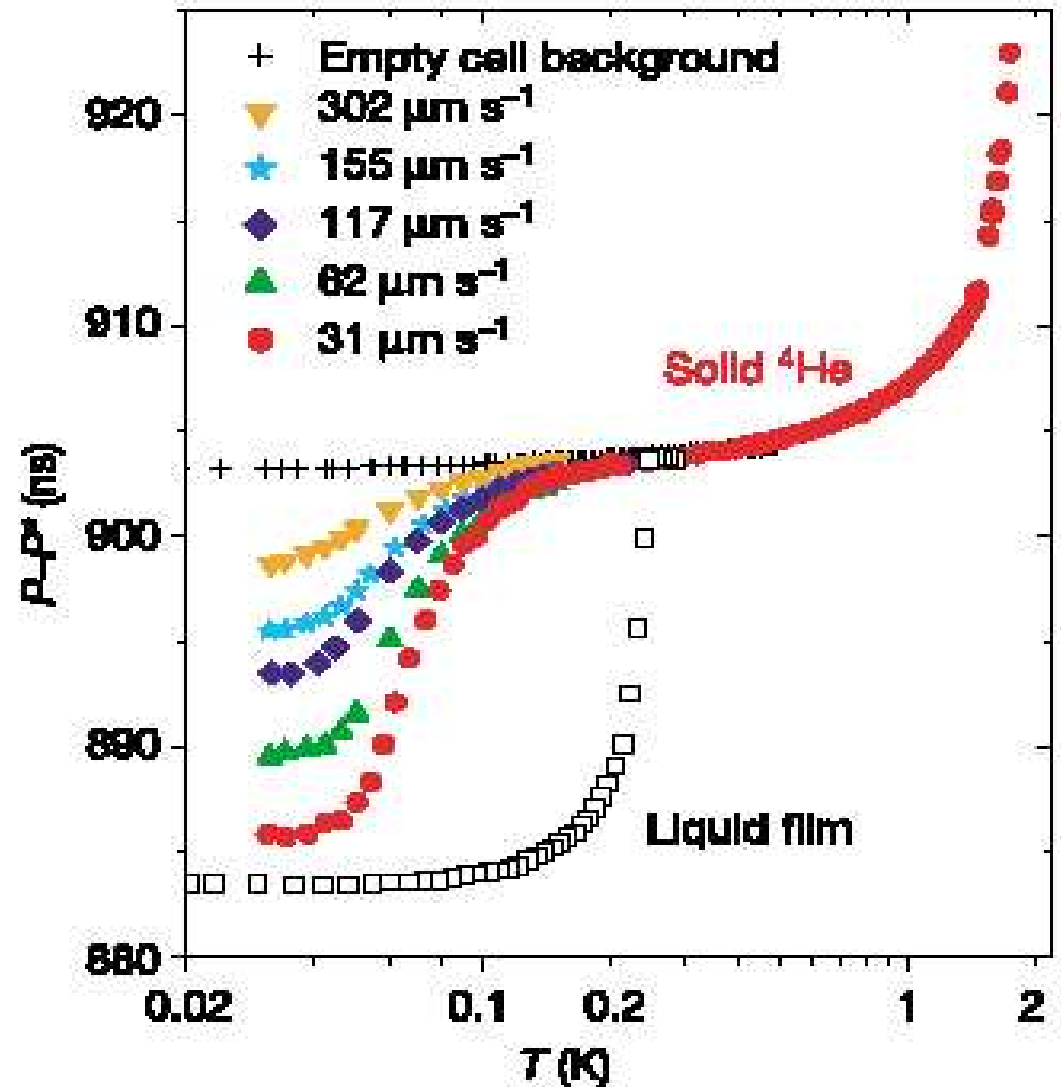
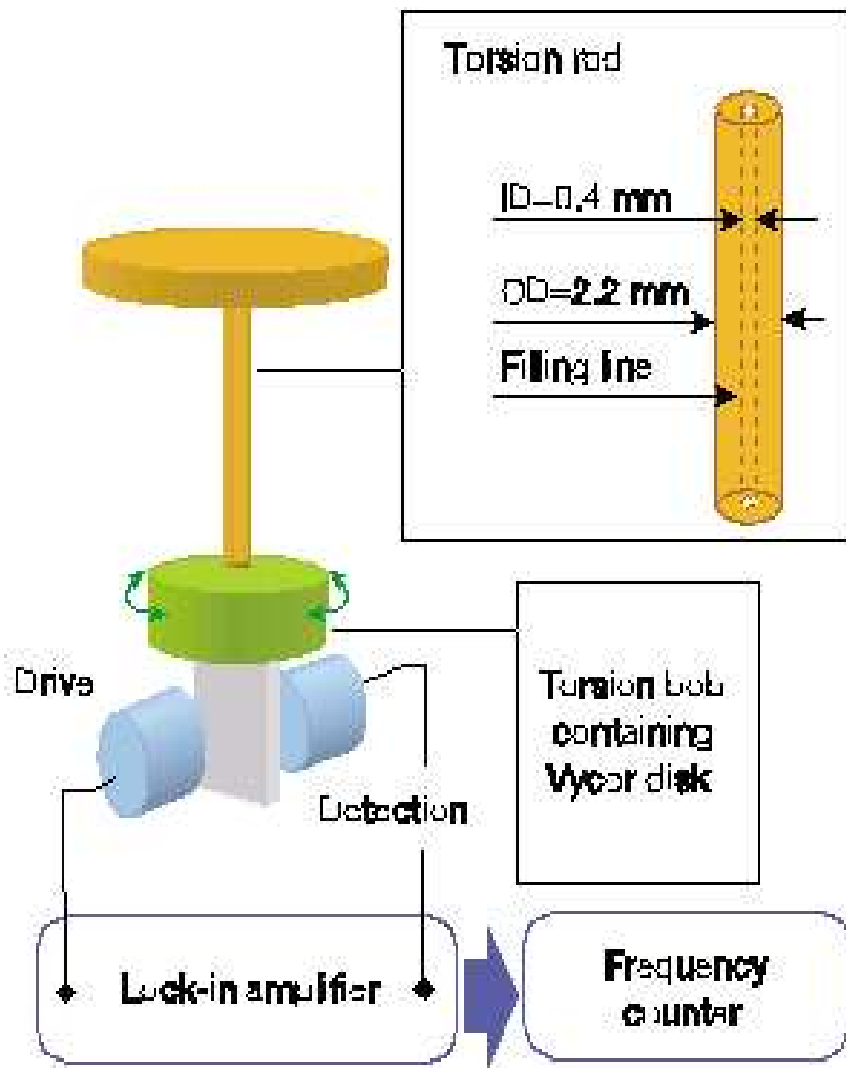
- Supersolid
- Incommensurate crystal
- A simple theory of the thermodynamics of an incommensurate quantum solid.

# Background: Quest for Supersolid

Supersolid: a state of matter - both solid and superfluid.

E. Kim, M. H. W. Chan, Nature 427, 225 (2004):

Recent experiments shows low  $T$  reduction in moment of inertia of crystals of  $^4\text{He}$ .



# Incommensurate crystal

- Ideal crystal: all lattice sites are occupied



- Vacancies: some of the sites are empty



- Interstitials: Some atoms occupy wrong places:



- Incommensurate crystal: crystal with vacancies and interstitials  $\Rightarrow$  **non-integer number of atoms per unit cell.**

- The ground state of the solid: incommensurate crystal, with quantum zero-point vacancies and interstitials.

- Supersolid: believed due to quantum behavior of vacancies and interstitials.

- Proposed phenomenological thermodynamic description of a low-  $T$  incommensurate quantum solid.
- Ground state of a quantum solid need not be commensurate.
- One description of the **Quantum Solid**: a density wave formed in quantum fluid. The periodicity of DW need not match precisely to the particle density, so that the ground state may be incommensurate, with unequal densities of vacancies and interstitials.
- Proposed theory: low  $T$  net change in vacancy density at fixed particle density:  $T^4$  power law.
- The x-ray data: consistent with this  $T$  dependence.
- Also, this model: produces  $T^7$  correction to the specific heat,
- Such a scenario: applicable to any highly quantum solid, not only to bosons.  ${}^3\text{He}$ .
- Perhaps  $H$  also.

# Theory

Hcp lattice, volume  $V$ , lattice constant  $a$ : the number of lattice sites  $N_s = V\sqrt{2}/a^3$ .

Crystal is incommensurate: number  $N$  of atoms  $N \neq N_s$ .

Recent (experimental) data: possibly differ by  $\sim 1\%$ .

Crystal incommensurate: needed a theory where **lattice constant** and **density** can change independently.

- The Approach: fixed particle density, but lattice constant varies, and so does incommensurability.
- Incommensurability

$$\epsilon = \frac{N_s - N}{N_s} = \epsilon_0 + \delta$$

( $\epsilon_0$  - incommensurability at  $T = 0$ .)

- Free energy:

$$F = -E_0 + \frac{E_2}{2}\delta^2 - (D_0 + D_1\delta + \dots)T^4 + \dots$$

(Looks like Landau theory with  $\delta$  being an order parameter(?))

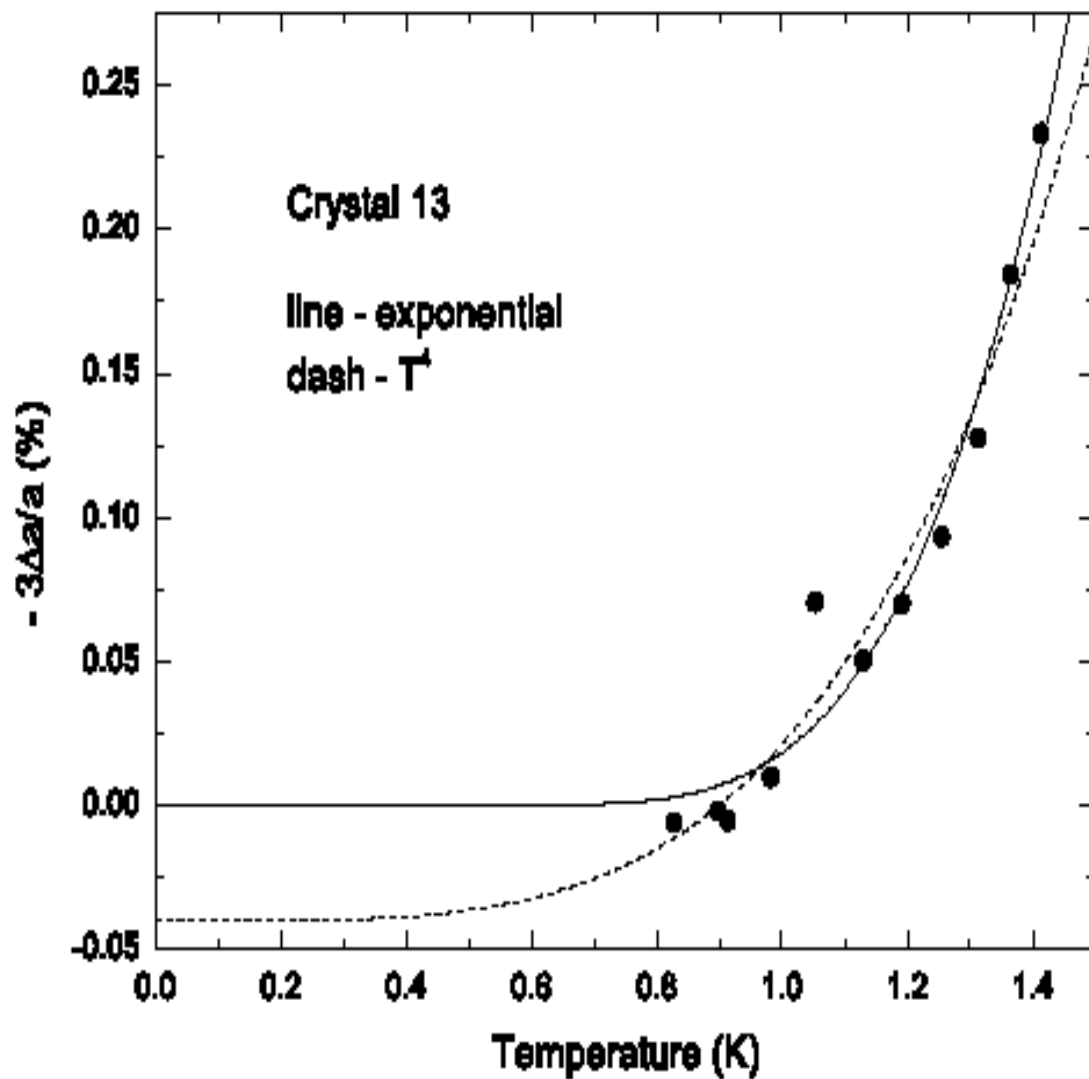
$-E_0$  is the ground state energy,  $E_2$  gives the harmonic increase of the crystal's energy when, staying at  $T = 0$ , the incommensurability is changed away from its ground state value by changing the number of lattice sites and thus the lattice constant.

The value of the incommensurability that minimizes this free energy at a given low temperature, obtaining to lowest order the temperature dependence

$$\delta \approx \frac{D_1}{E_2}T^4$$

instead of classical  $\delta \sim \exp(-\Delta/k_B T)$ .

## Comparison with experiment and the classical theory



On figure: X-ray data on density of vacancies in solid  ${}^4\text{He}$ , together with lines according to two theories, classical and  $T^4$ . Both theories fit, at the moment.



- A known anomaly.

The specific heat of solid  ${}^4\text{He}$  at  $T \sim 1$  K fits nearly exactly

$$C = AT^3 + BT^7$$

Debye formula for phonon heat capacity

$$C_V = 9Nk_B \frac{T^3}{\theta_D^3} \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx \simeq \frac{12\pi^4}{5} Nk_B \frac{T^3}{\theta_D^3} \quad (T \ll \theta_D)$$

The observed  $T^7$  correction is orders of magnitude larger than by Debye formula.

- - Can be explained with proposed theory.

Reminding: our  $F$

$$F = -E_0 + \frac{E_2}{2}\delta^2 - (D_0 + D_1\delta + \dots)T^4 + \dots$$

Minimizing  $F$  wrt  $\delta$ :

$$F = -E_0 - D_0T^4 - D_1^2T^8/2E_2 + \dots$$

$$\Rightarrow C_V = -T \frac{\partial^2 F}{\partial T^2} = 12D_0T^3 + 56D_1^2T^7/2E_2$$

$\Rightarrow$  positive  $T^7$  correction to the phonon specific heat.

Consistent with the experimental  $C$  measurement.

## Application to fermions

- In the argument we did not use the boson nature of  ${}^4\text{He}$ .  $\Rightarrow$  can be used for fermions, like  ${}^3\text{He}$ .
- In fact, the discrepancies found in  ${}^4\text{He}$  between the temperature dependent x-ray vacancy data and the  $C$  data within a classical vacancy model are also there in solid  ${}^3\text{He}$ .

## References

- [1] E. Kim, M. H. W. Chan, *Nature* 427, 225 (2004).
- [2] E. Kim, M. H. W. Chan, *Science* 305, 1941 (2004).
- [3] A. F. Andreev, I. M. Lifshitz, *JETP* 29, 1107 (1969).
- [4] B. A. Fraass, P. R. Granfors, R. O. Simmons, *Phys. Rev. B* 39, 124 (1989).
- [5] C. A. Burns, J. M. Goodkind, *J. Low Temp. Phys.* 95, 695 (1994).
- [6] W. R. Gardner, J. K. Hoer, N. E. Phillips, *Phys. Rev. A* 7, 1029 (1973).
- [7] S. M. Heald, D. R. Baer, R. O. Simmons, *Phys. Rev. B* 30, 2531 (1984).
- [8] D. S. Greywall, *Phys. Rev. B* 15, 2604 (1977).
- [9] P. W. Anderson, cond-mat/0504731.
- [10] B. Chaudhuri, F. Pederiva, G. V. Chester, *Phys. Rev. B* 60, 3271 (1999).
- [11] D. M. Ceperley, B. Bernu, *Phys. Rev. Lett.* 93, 155303 (2004).
- [12] D. E. Galli, M. Rossi, L. Reatto, cond-mat/0503443.
- [13] R. O. Simmons, private communication (2005).
- [14] In the qualitatively similar oscillator data for superfluid  $^4\text{He}$  films near their Kosterlitz-Thouless transitions, the actual transition temperature is well below the dissipation feature. See D. J. Bishop and J. D. Reppy, *Phys. Rev. Lett.* 40, 1727 (1978).
- [15] We thank Moses Chan, Ralph Simmons and Dennis Greywall for helpful discussions. This work was supported in part (D.A.H.) by the NSF through MRSEC grant DMR-0213706.