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International Centre for Theoretical Physics

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Workshop on Supersolid 2008

18 - 22 August 2008

The structure and dynamics of hcp He-4 below 1 K

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Structure and dynamics of hcp ^4He below 1 K

Elizabeth Blackburn
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ICTP Trieste – Supersolid 2008

Structure and dynamics of hcp ^{4}He below 1 K

Structure

Joost van Duijn (Madrid)

Oleg Kirichek

Chris Frost

Richard Down

ISIS

Dynamics

John Copley

Yiming Qiu

Ross Erwin

NIST National Institute of Standards and Technology

Both

John Goodkind

Sunil Sinha

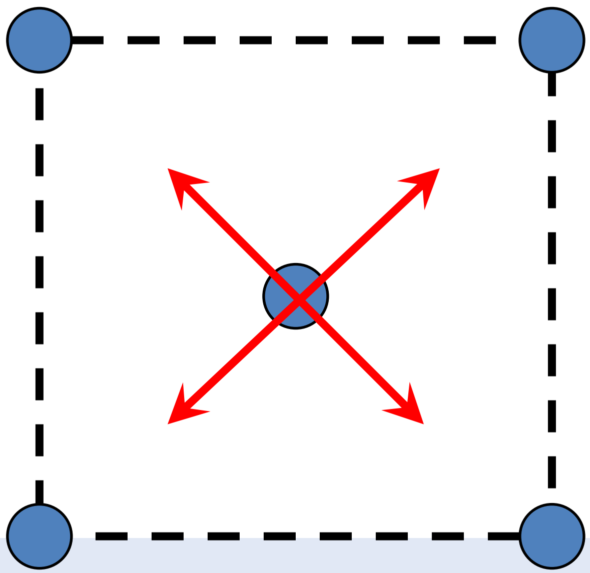
UCSD

Collin Broholm

JOHNS HOPKINS UNIVERSITY

A quantum crystal

- Helium only solidifies under pressure
  - light atom; no overall charge
  - tightly bound electronic shells → small vdW forces
  - large zero-point fluctuations



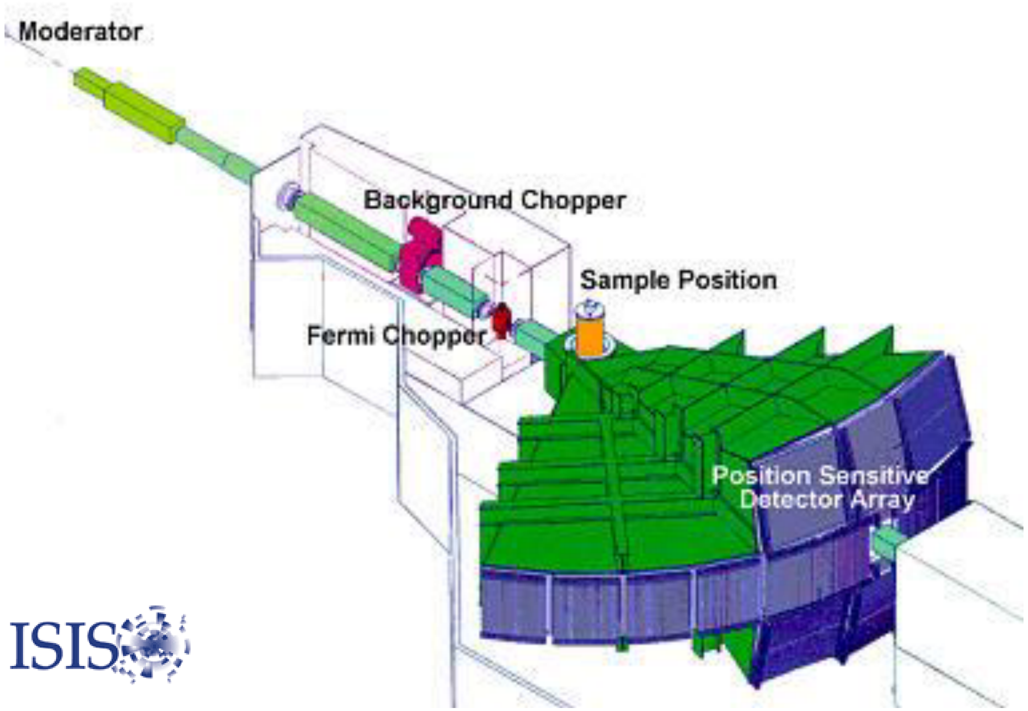
Oscillations much greater than Lindemann criterion

Other potential quantum crystals –
ferroelectrics close to lattice transformations

Ref: Werthamer, Am. J. Phys **37**, 763 (1969).

Are there any structural changes?

MAPS time-of-flight spectrometer



Characteristics

Incident white beam of neutrons

Use time-of-flight detection to extract *d*-spacings.

No need to move sample once grown

Sample growth

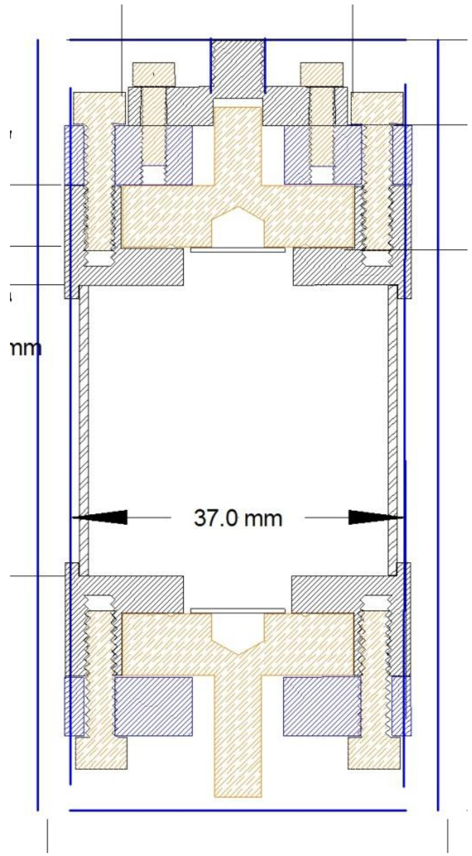
Sample chamber

Stainless steel walls.

Fill line at top; cold spot at bottom.

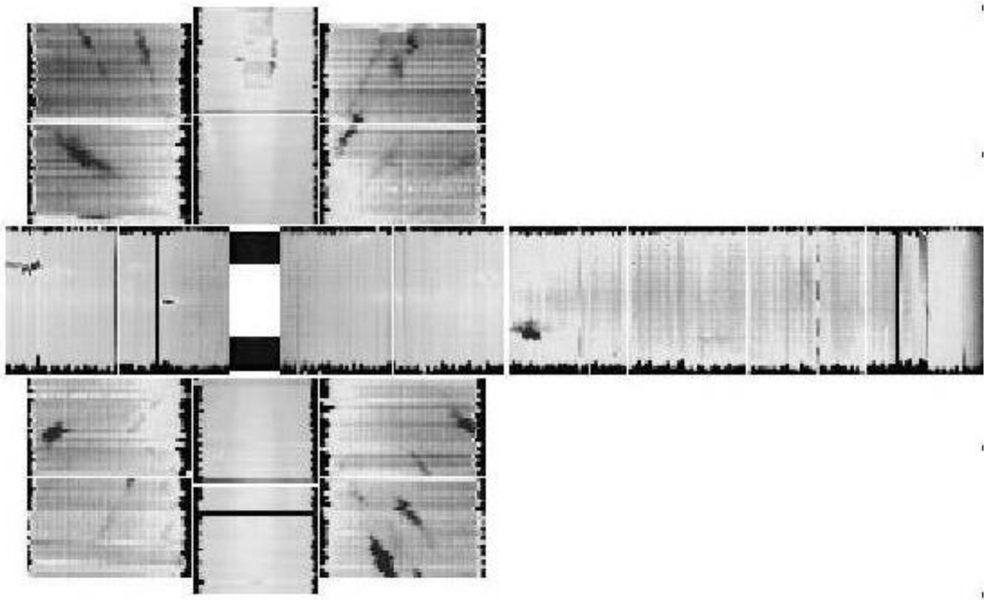
Quartz transducers covering vertical path.

Sample grown *in situ* starting with a pressure of 45 bar at ~ 2 K using the blocked capillary technique.



Finding Bragg peaks

MAPS detector banks



Characteristics

Incident white beam of neutrons

Use time-of-flight detection to extract *d*-spacings.

No need to move sample once grown.

Finding Bragg peaks

Limited choice!

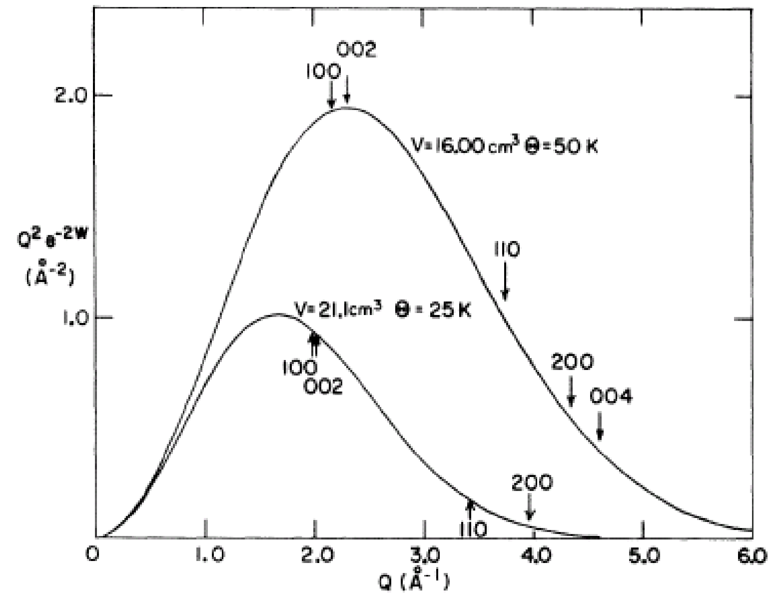


FIG. 2. Function Q^2e^{-2W} for hcp He^4 at molar volumes of 16.00 and 21.1 cm^3.

Peaks seen:

We identified:

100

002

110

101

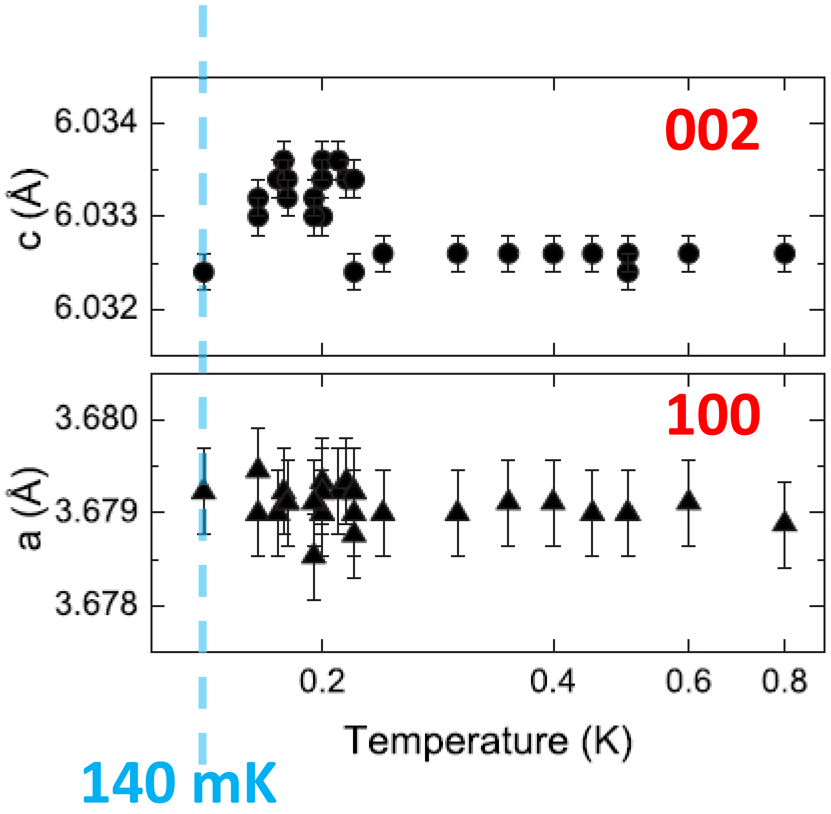
102

200

004

Ref: Reese et al., Phys. Rev. A **3**, 1688 (1971).

Lattice parameters



Peaks seen:

We identified:

100

002

110

101

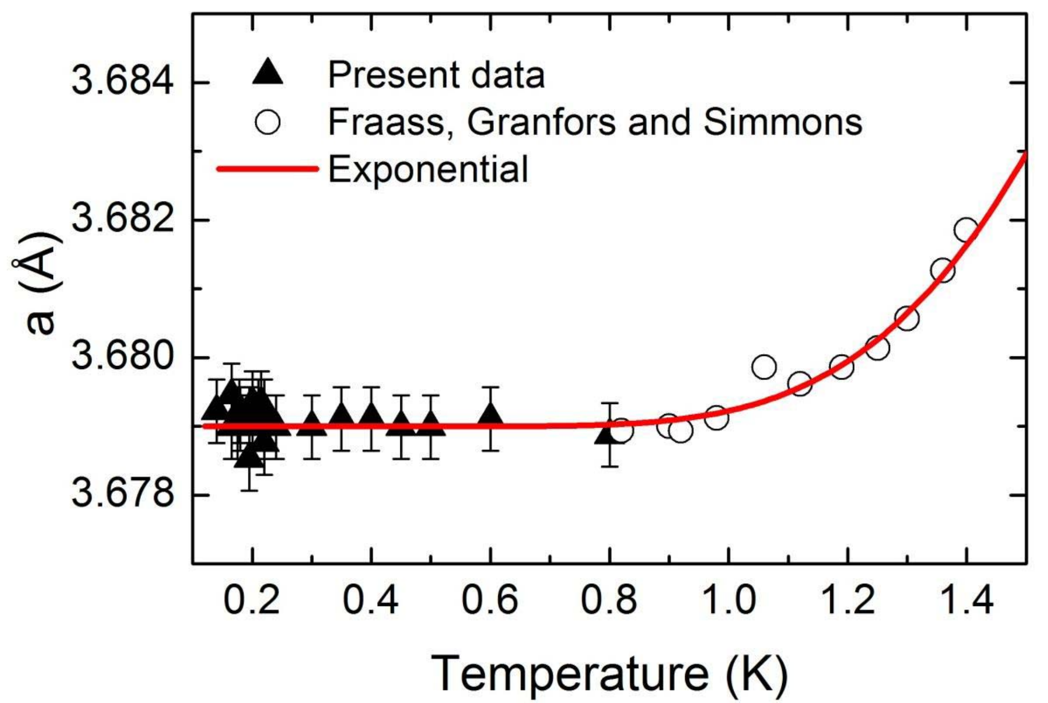
102

200

004

Ref: Blackburn et al., Phys. Rev. B **76**, 024523 (2007).

Vacancy population



The lattice parameter is expected to shift with to the number of vacancies.

Exponential dependence as expected for thermal activation.

Activation energy 8.6 K

Caveat: mass density assumed to remain constant as function of temperature.

Ref: Fraass, Granfors and Simmons, Phys. Rev. B **39**, 124 (1989).

Mean square atomic displacement

For a Bragg reflection at τ,
the structure factor is:

$$F(\tau) = b_{He} \sum_i \exp(i\tau \cdot \mathrm{d}_i) \exp(-W_{\mathrm{d}_i}(\tau)).$$

He scattering length — Bragg condition — Debye-Waller factor

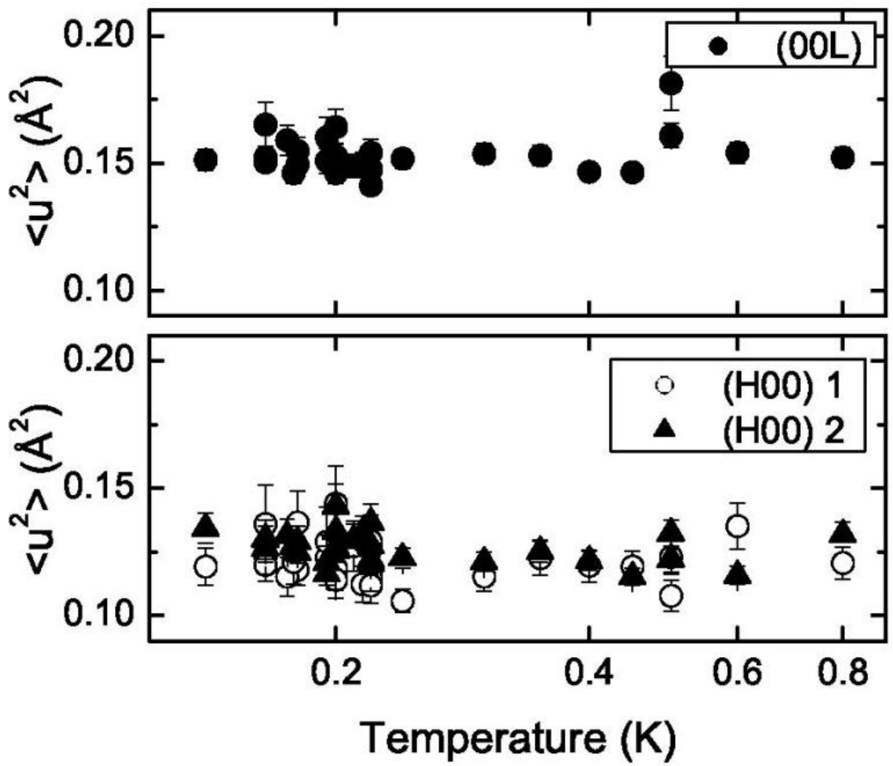
$$W_{\mathrm{d}_i}(\tau) = \langle (\tau \cdot \mathrm{u})^2 \rangle$$

u is the displacement from the average periodic lattice

Peaks used:

100
002
110
101
200
004

Mean square atomic displacement



The mean square displacement is anisotropic, as expected for an hcp crystal.

It does not change with temperature; we are looking at zero-point motion.

Ref: Blackburn et al., Phys. Rev. B **76**, 024523 (2007).

Mean square atomic displacement

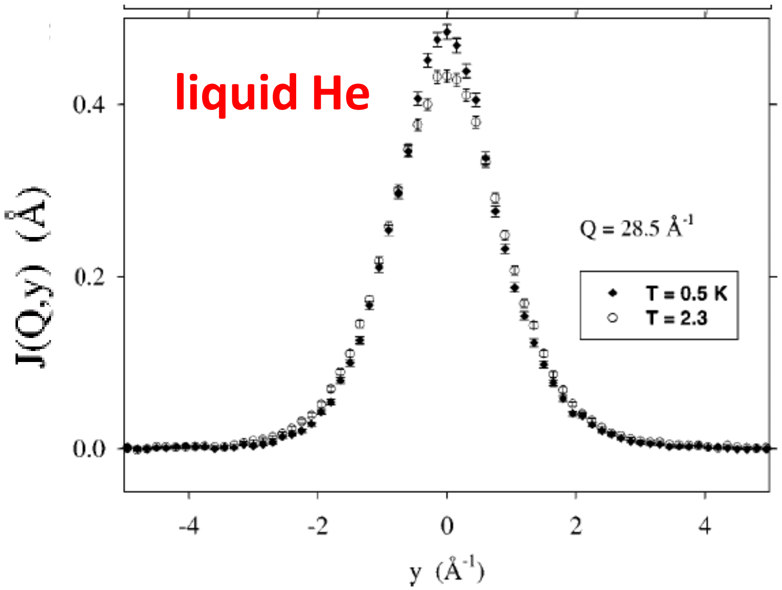
TABLE II. Published values for $\langle u^2 \rangle$ in solid ^{4}He obtained by x-ray and neutron diffraction. In all cases, the harmonic approximation is assumed and for the mixed peak data, no distinction between in-plane and out-of-plane displacements was made.

Molar volume (cm^3)	Temperature (K)	$\langle u^2 \rangle$ ($Å^2$)	Peak type	Reference
11.01	15	0.0593(1)	mixed	Venkataraman and Simmons, PRB **68** (2003) – x-ray
12.06	5.8	0.0466(3)	mixed	Stassis, Khatamian and Kline, SSC **25** (1978) – neutron
12.12	14.8	0.0563(14)	mixed	Arms, thesis (1999) – x-ray
12.13	14.8	0.0513(10)	mixed	Arms, thesis (1999) – x-ray
15.72	5.8	0.0861(9)	mixed	Stassis, Khatamian and Kline, SSC **25** (1978) – neutron
20.9	0.7	0.1537(7)	(00*L*)	Burns and Isaacs, PRB **55** (1997) – x-ray
21.3	<1	0.150(1)	(00*L*)	This work (neutron)
21.3	<1	0.122(1)	(*H*00)	This work (neutron)

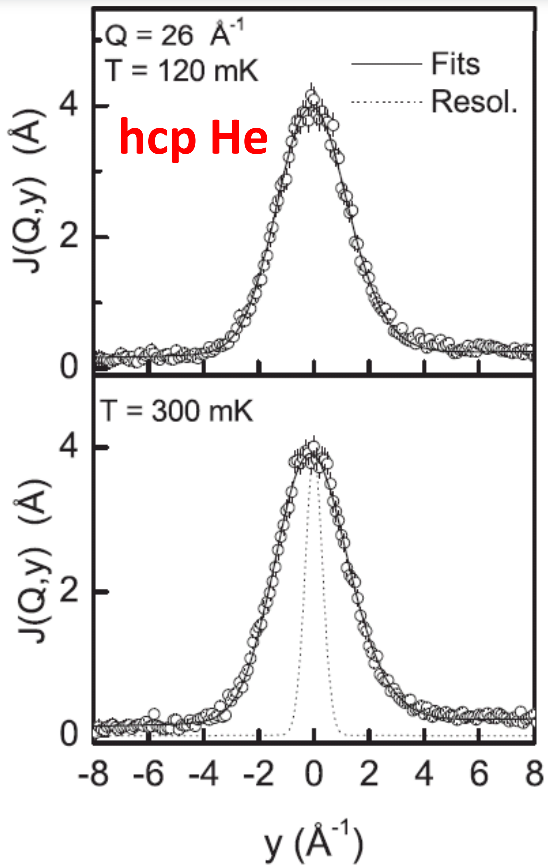
Summary: structure

- No observed temperature dependence
- Mean square displacement consistent with previous values
- Further evidence for thermally activated vacancies

Momentum distribution – signs of ρ_s



from Glyde et al., PRB **62**, 14337 (2000).



from Diallo et al., Phys. Rev. Lett. **98**, 205301 (2007).

Momentum distribution – signs of ρ_s

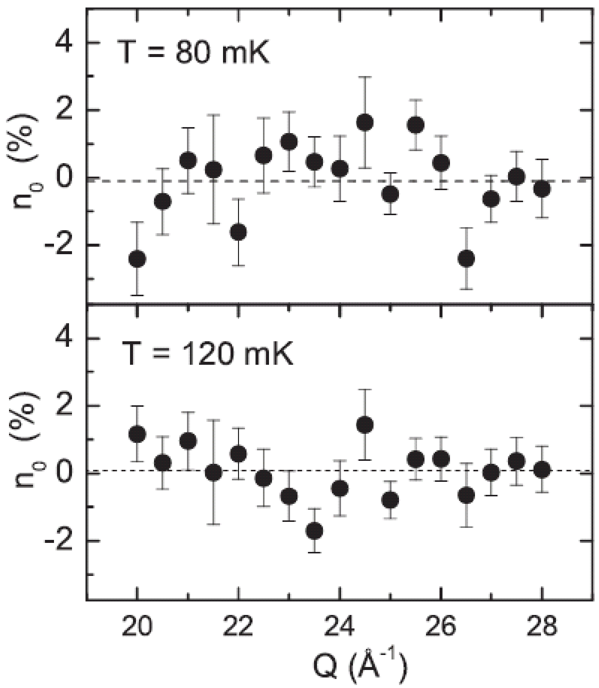
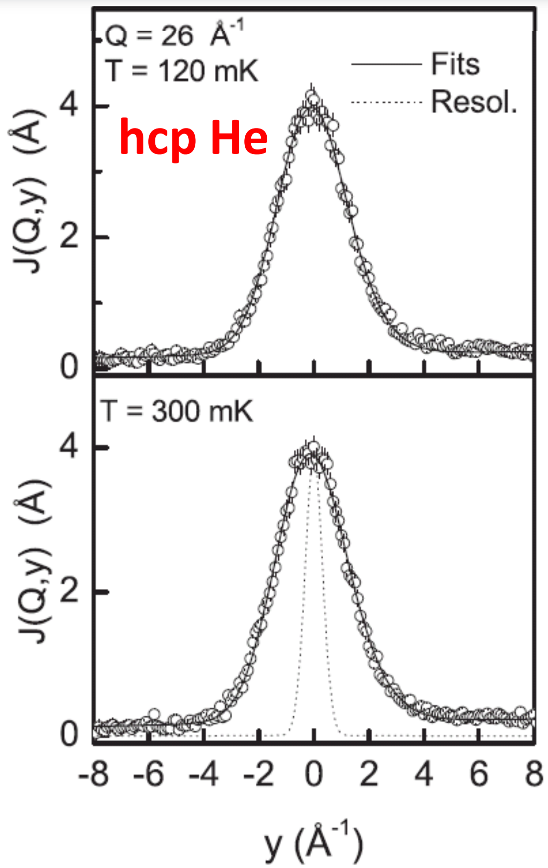


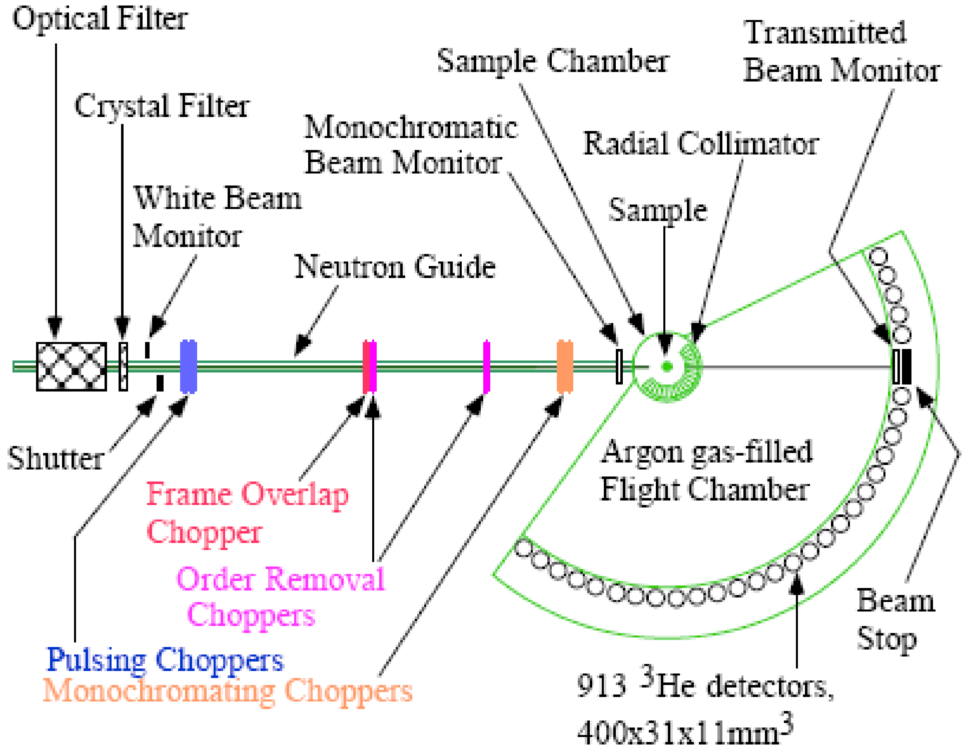
FIG. 3. Condensate fractions obtained by fitting the CA at T = 80 and 120 mK with the width of $n(\mathbf{k})(\bar{\alpha}_2)$ held fixed at its values shown in Fig. 2. We find $n_0 = (-0.10 \pm 1.20)\%$ at T = 80 mK and $n_0 = (0.08 \pm 0.78)\%$.



Refs: Adams et al., Phys. Rev. Lett. **98**, 085301 (2007), Diallo et al., Phys. Rev. Lett. **98**, 205301 (2008).

What about the excitation spectrum?

DCS time-of-flight spectrometer



Characteristics

Monochromatic beam.

Use time-of-flight detection to extract energy transfer information.

Sample needs limited rotation to get full coverage.

NIST National Institute of Standards and Technology

Sample growth

Sample chamber

Stainless steel walls.

Fill line at top; cold spot at bottom.

Quartz transducers covering vertical path, and X-cut transducers horizontally at top.

Sample grown *in situ* along the melting curve, at ≈ 1.2 K.

Sample growth

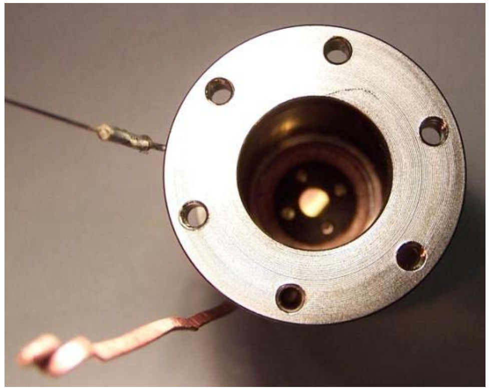
Sample chamber

Stainless steel walls.

Fill line at top; cold spot at bottom.

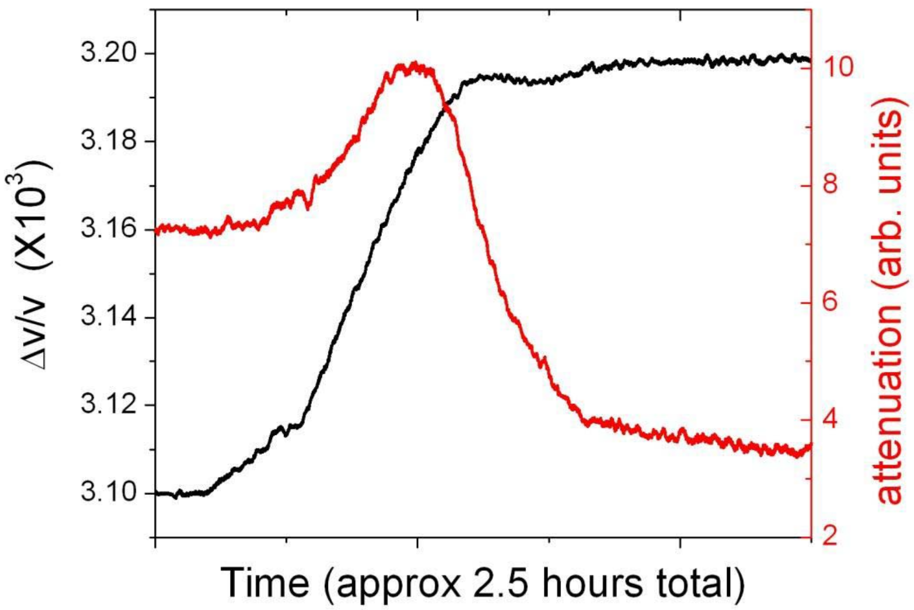
Quartz transducers covering vertical path, and X-cut transducers horizontally at top.

Sample grown *in situ* along the melting curve, at ≈ 1.2 K.

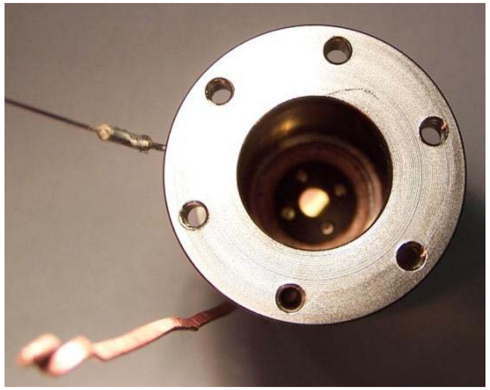


Sample growth

Acoustic measurements



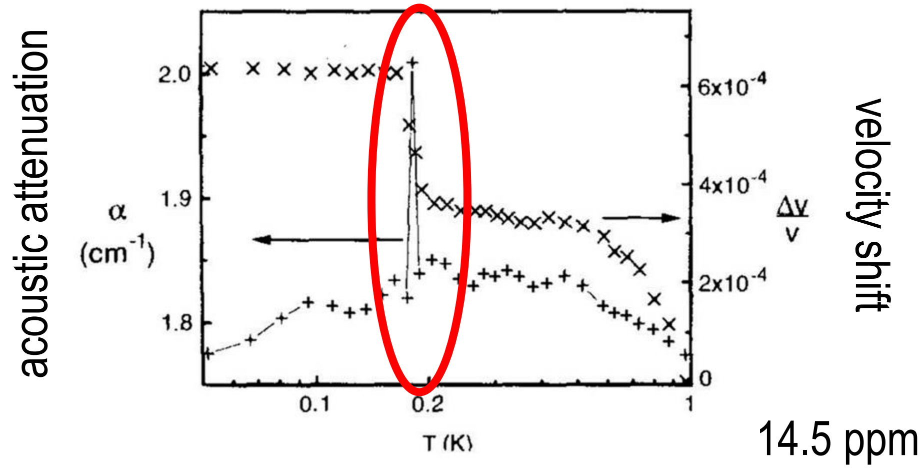
<- Temperature



Definitely got below 200 mK; thermometry seemed correct.
Closest thermometer was on mixing chamber.

Ultrasound measurements

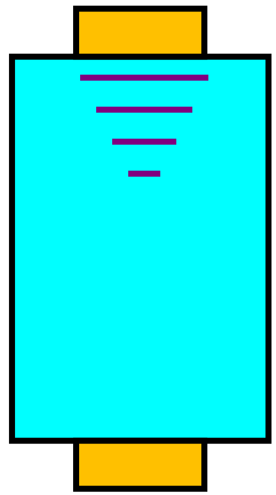
Sharpest attenuation peak seen:



14.5 ppm ^{3}He

Measured at f = 9.3, 28 and 46.8 MHz – freq. dependence unclear

^{3}He required – too much destroys effect



Ref: Ho, Bindloss and Goodkind, J. Low. Temp Phys. **109**, 409 (1997).

Ultrasound measurements

Non phonon thermal excitation seen.

The excitation has a speed of 226 ms^{-1}.

Indication that for T > 200 mK these excitations are gapped.

This gap disappears below 200 mK.

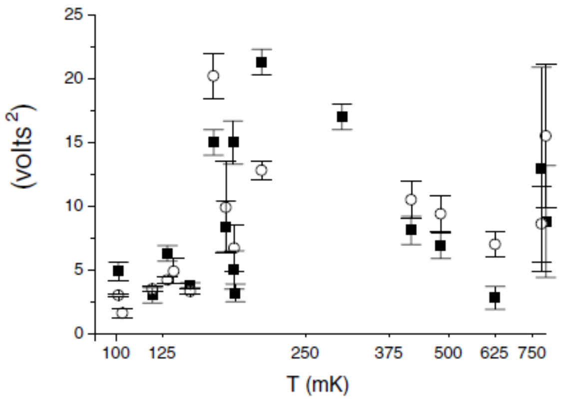
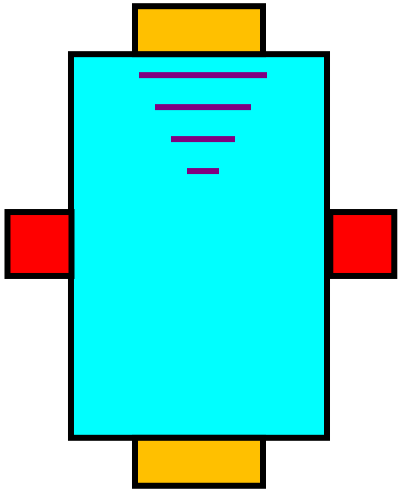


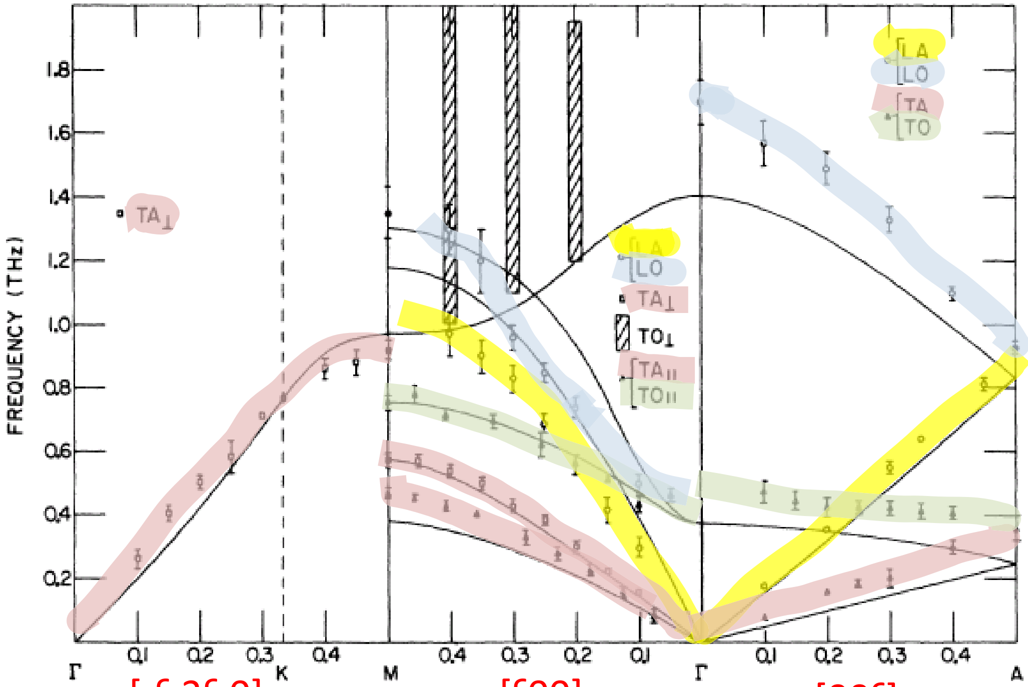
FIG. 5. Values of ϕ from fits of an exponential function to the shifts of α and v vs V_{hp}^2. ■ from attenuation; ○ from velocity.



Ref: Goodkind, Phys. Rev. Lett. **89**, 095301 (2002).

What has previously been measured?

Summary of measured spectra



zone centre [-ξ,2ξ,0] [ξ00] zone centre [00ξ]

References

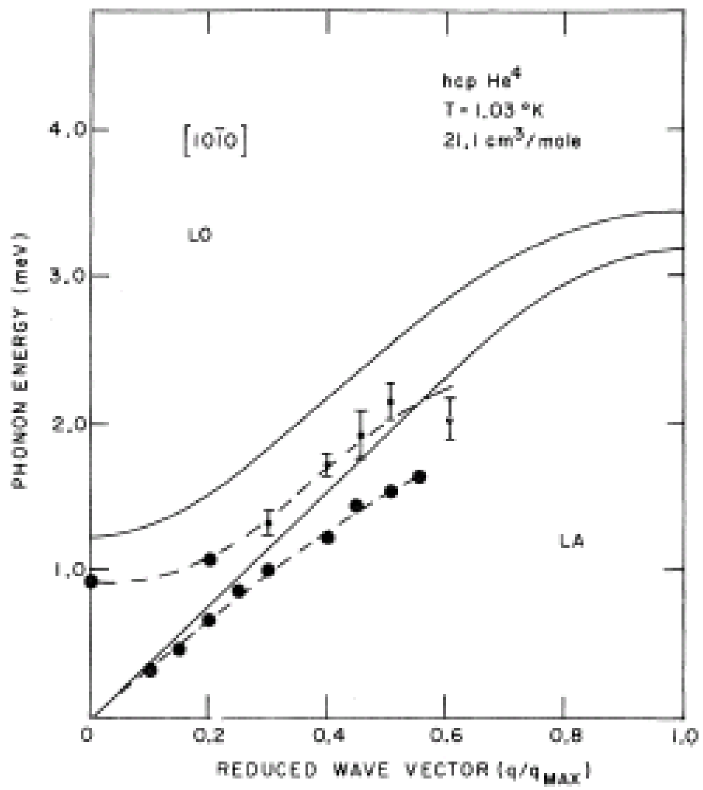
Molar volume 16cm^3

Reese et al., PRA **3**, 1688 (1971).

Molar volume 21.1cm^3

Minkiewicz et al., PR **174**, 267 (1968).

Phonon spectrum in the basal plane



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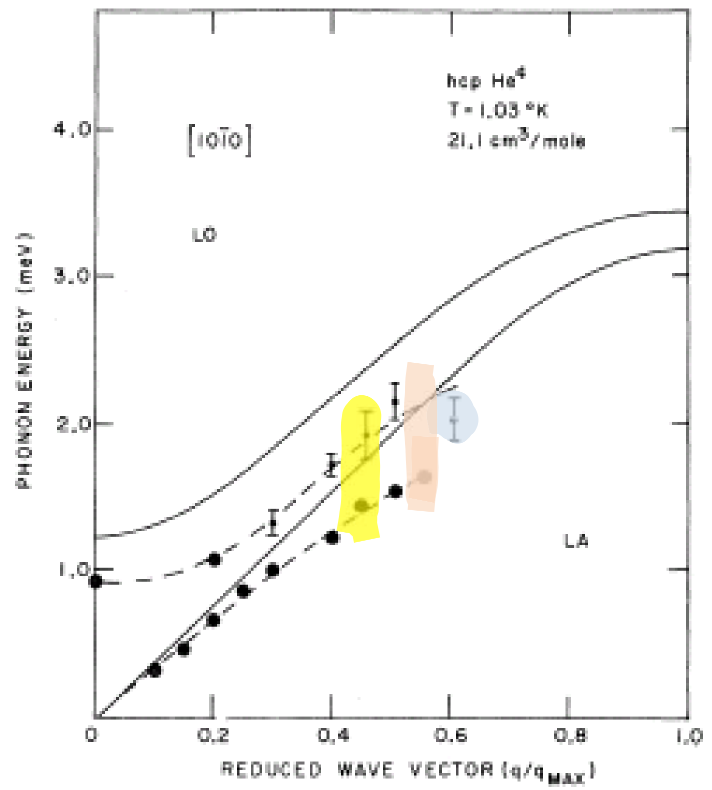
Phonon spectrum in the basal plane



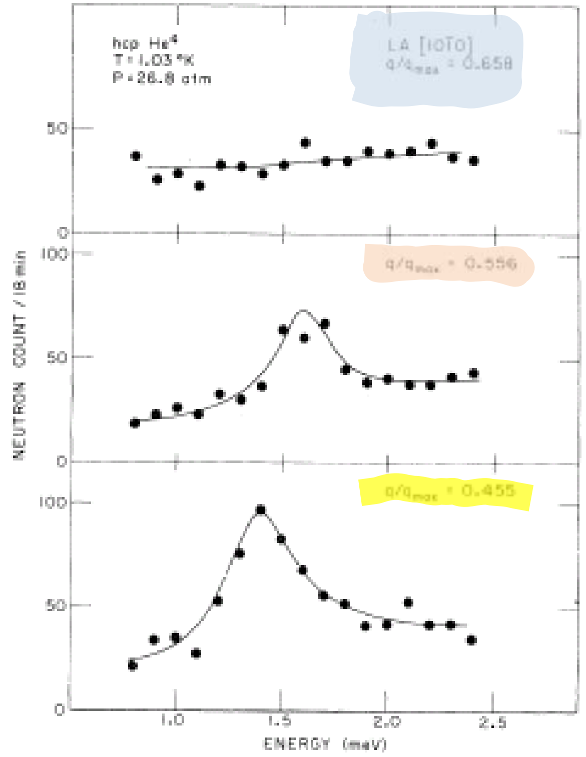
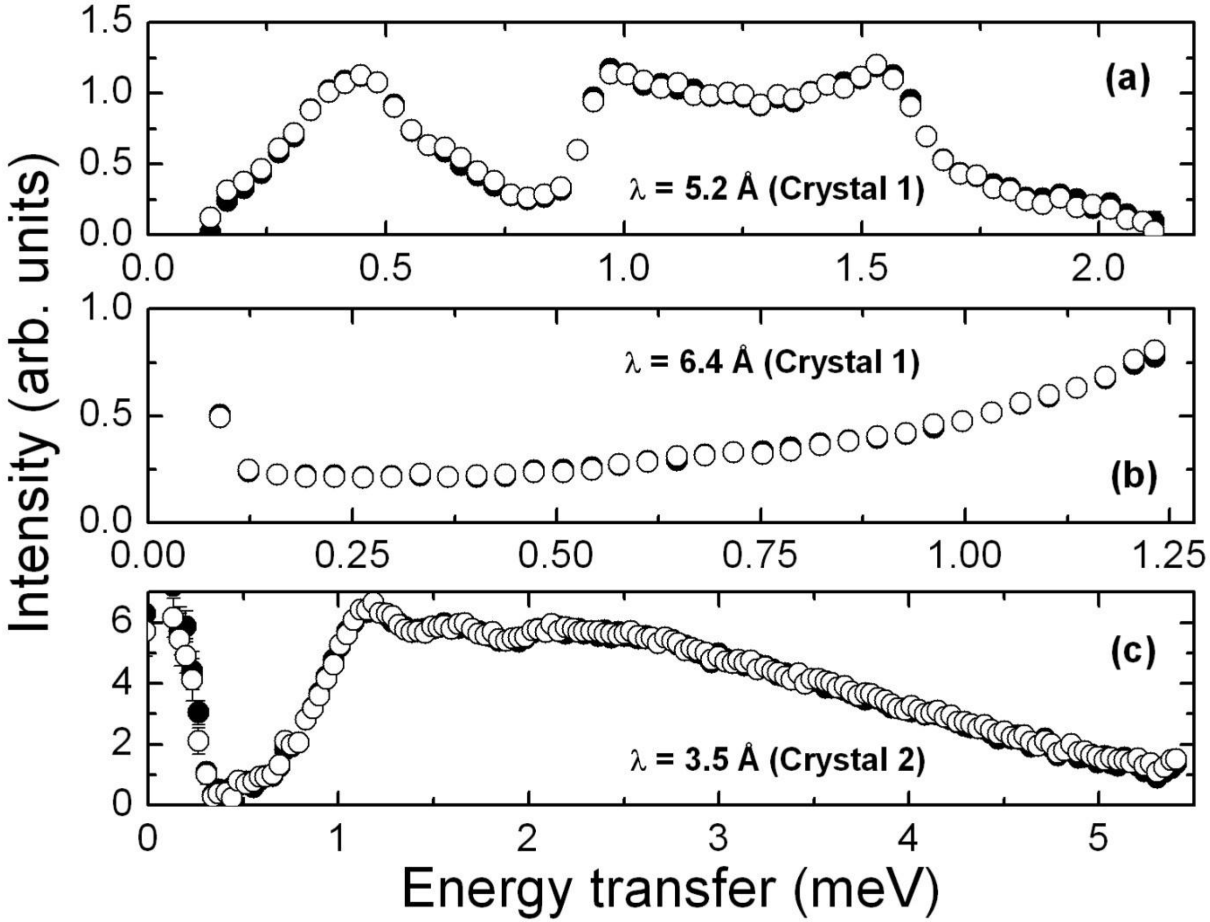


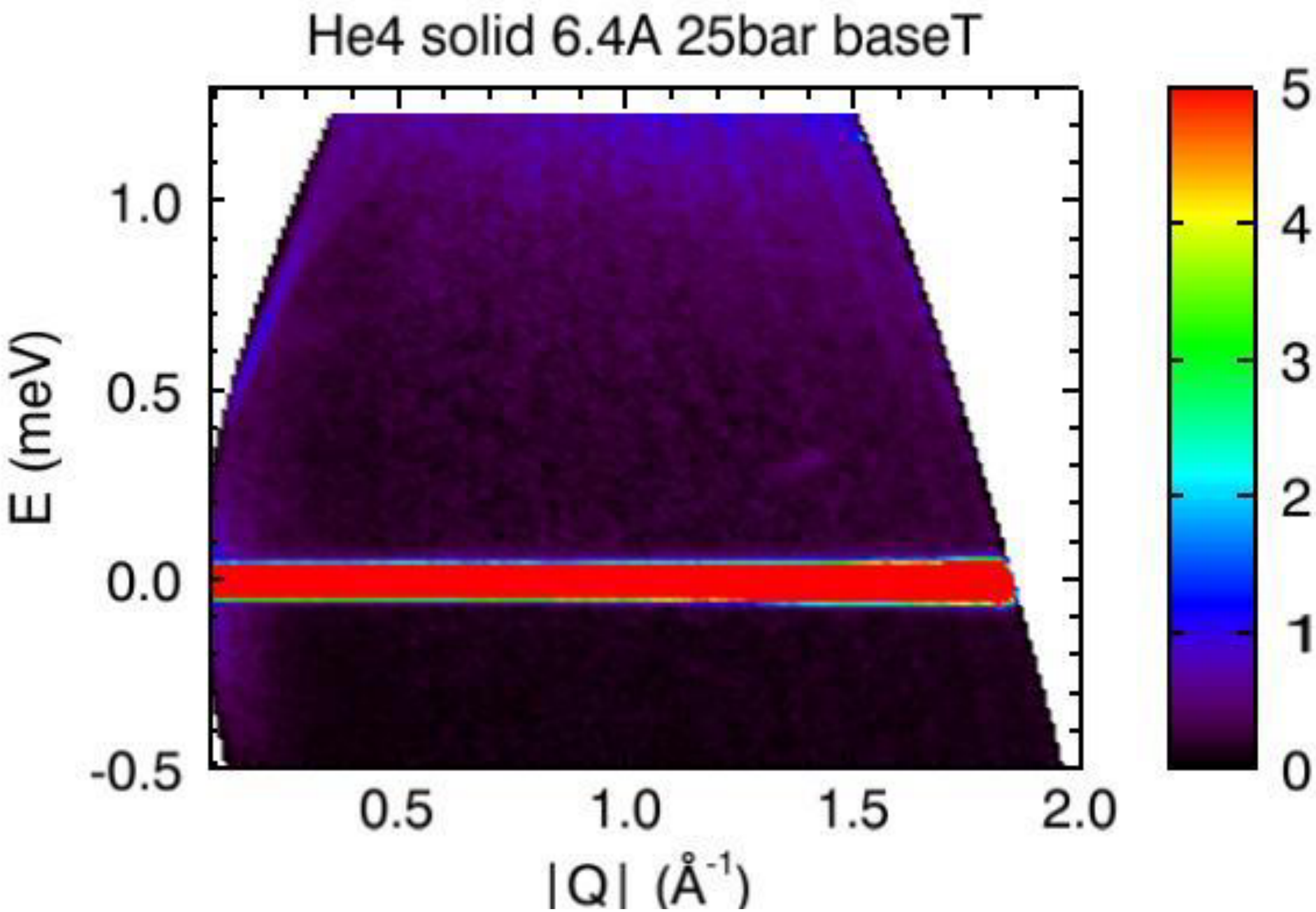
FIG. 8. Examples of the phonon group profiles for the [10$\bar{1}$0] LA branch of the phonon spectrum of hcp He^4.

Temperature dependence

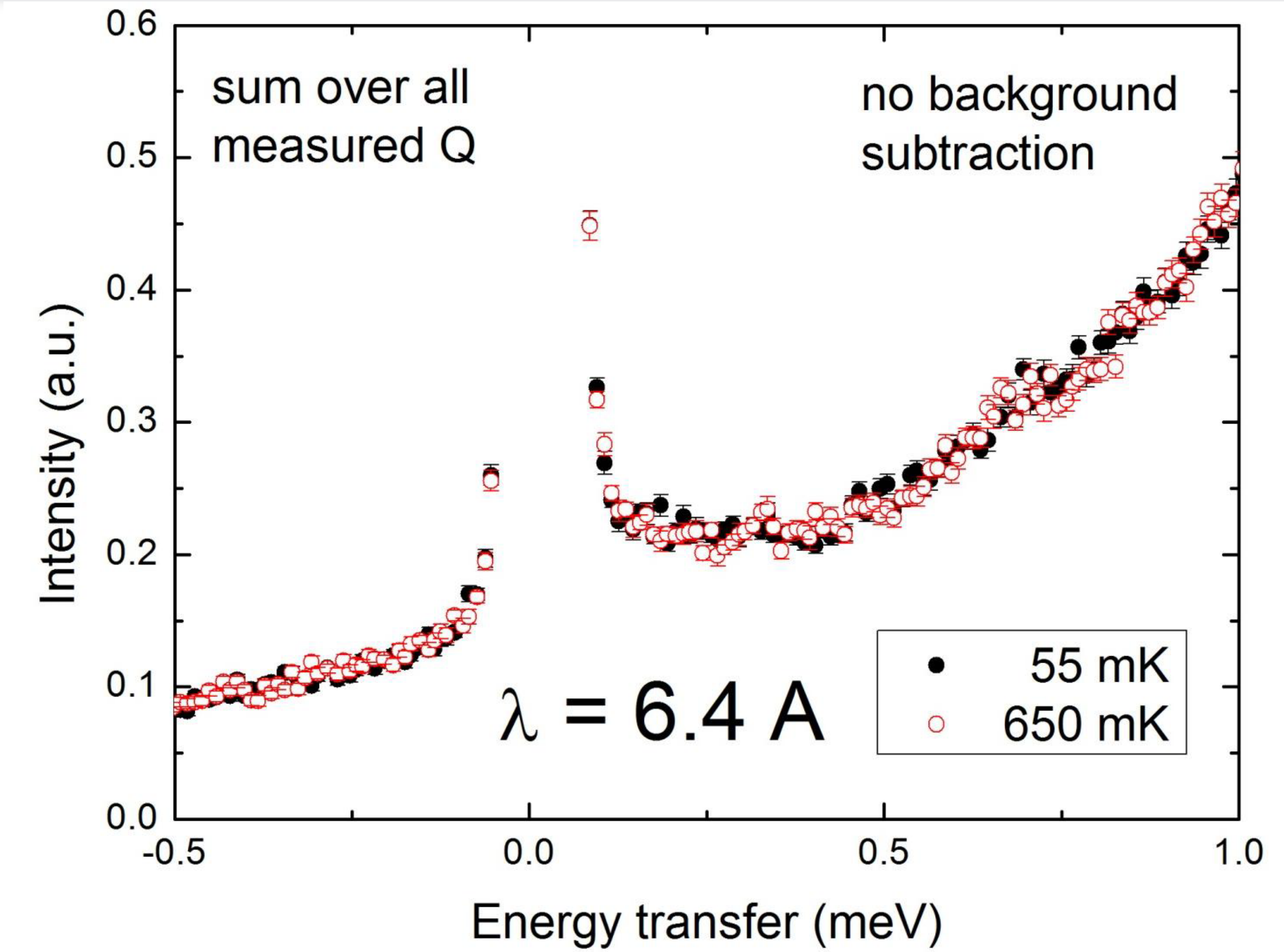


Closed circles = base temperature (55 mK); Open circles = high temperature

Temperature dependence

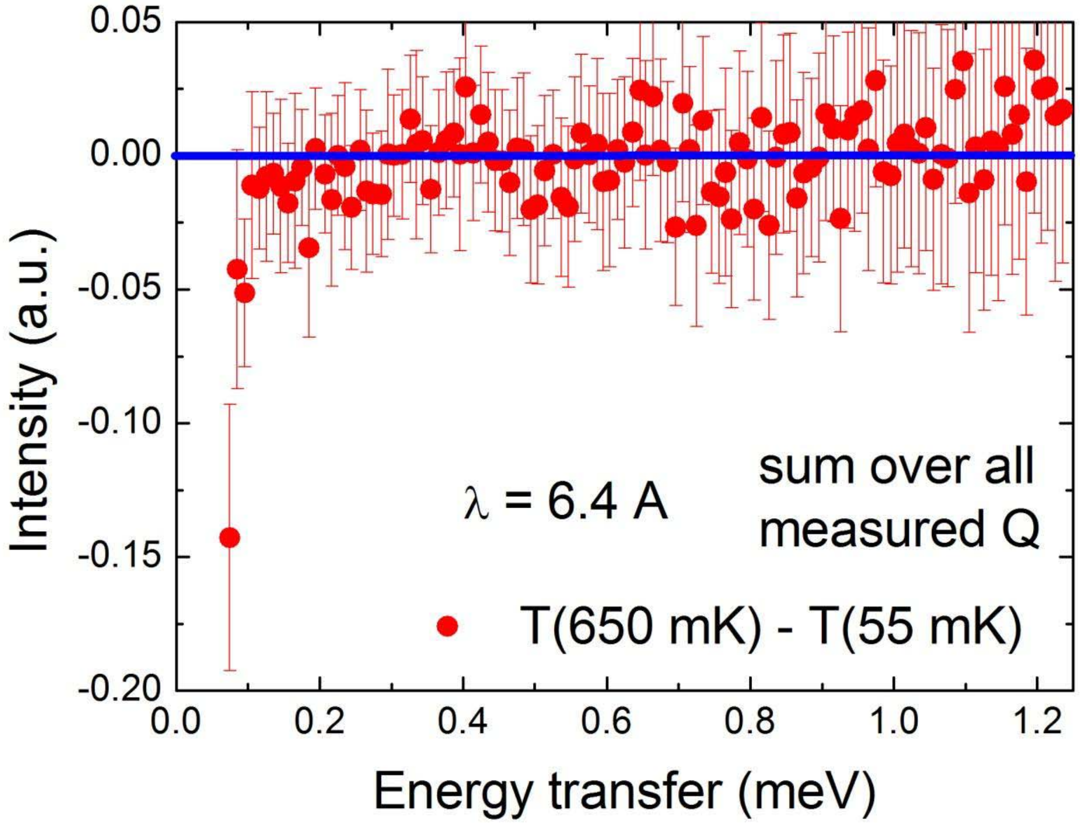


Temperature dependence



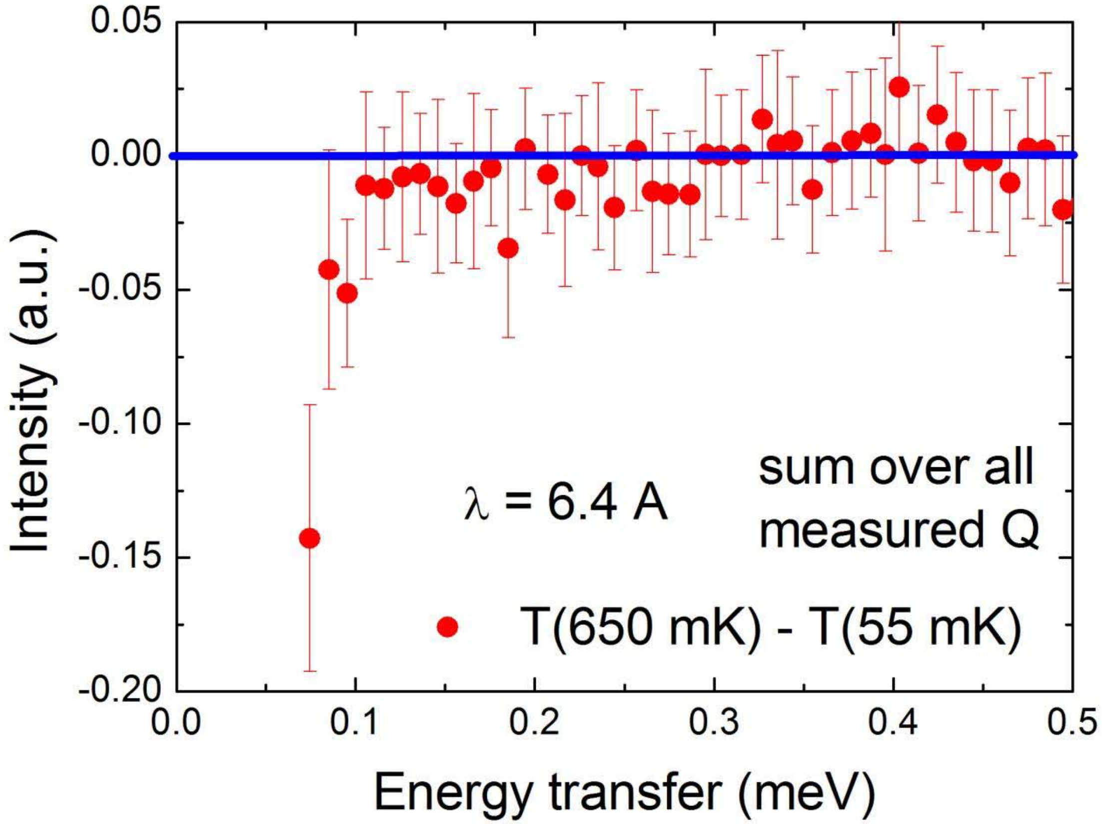
Closed circles = base temperature (55 mK); Open circles = high temperature

Temperature dependence



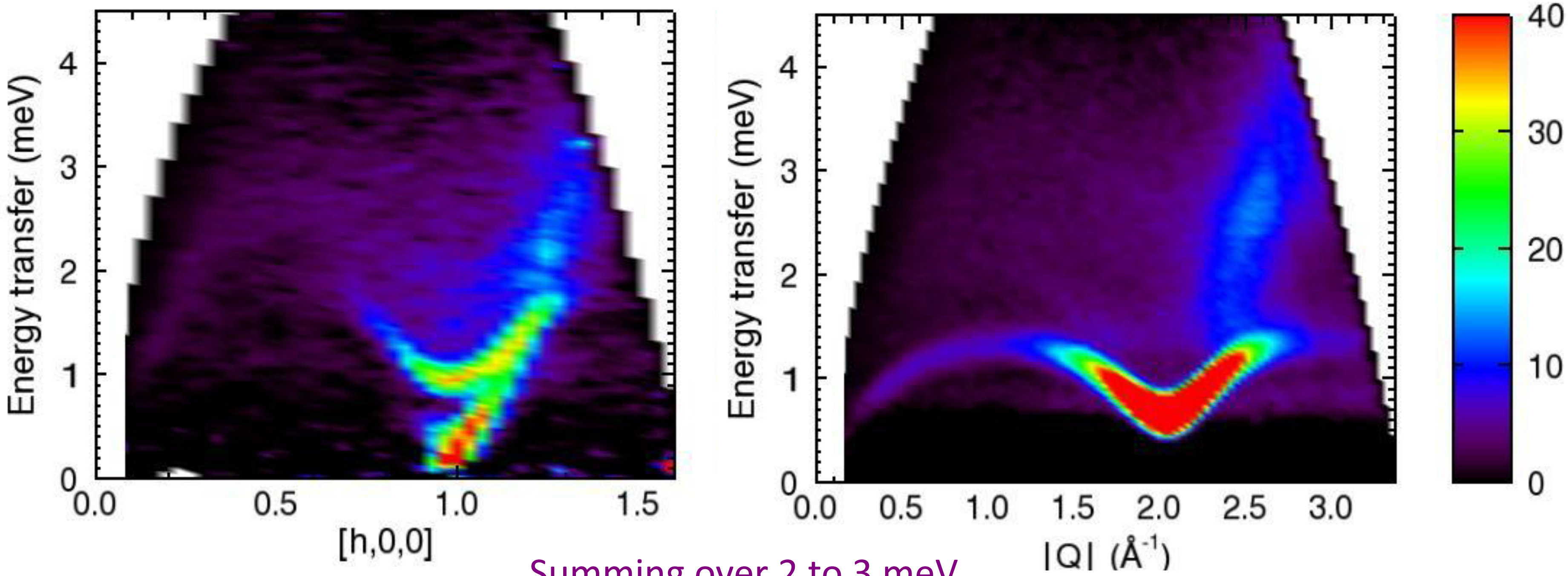
Closed circles = base temperature (55 mK); Open circles = high temperature

Temperature dependence

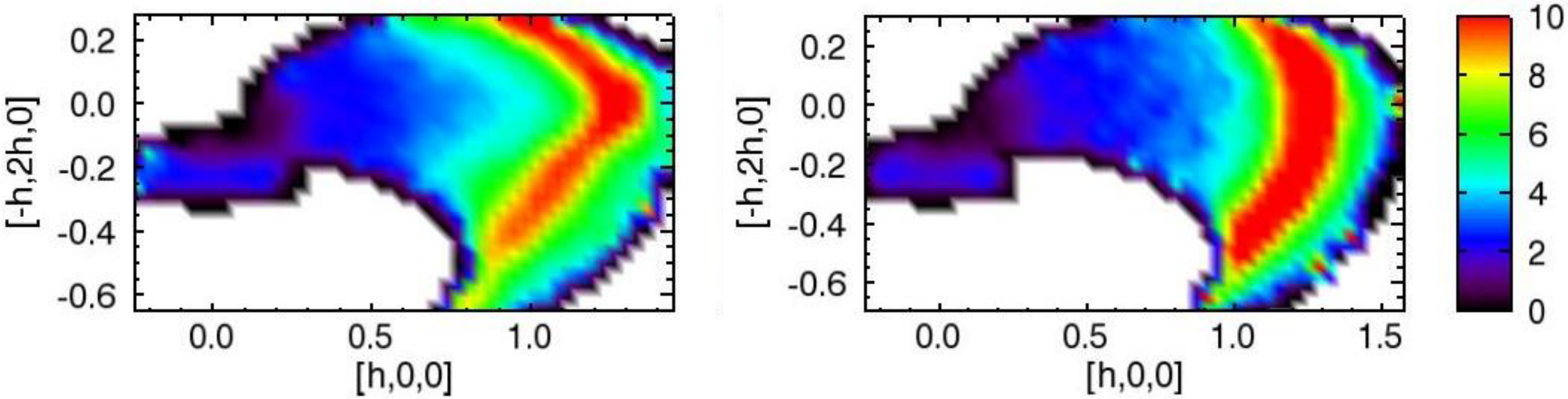


Closed circles = base temperature (55 mK); Open circles = high temperature

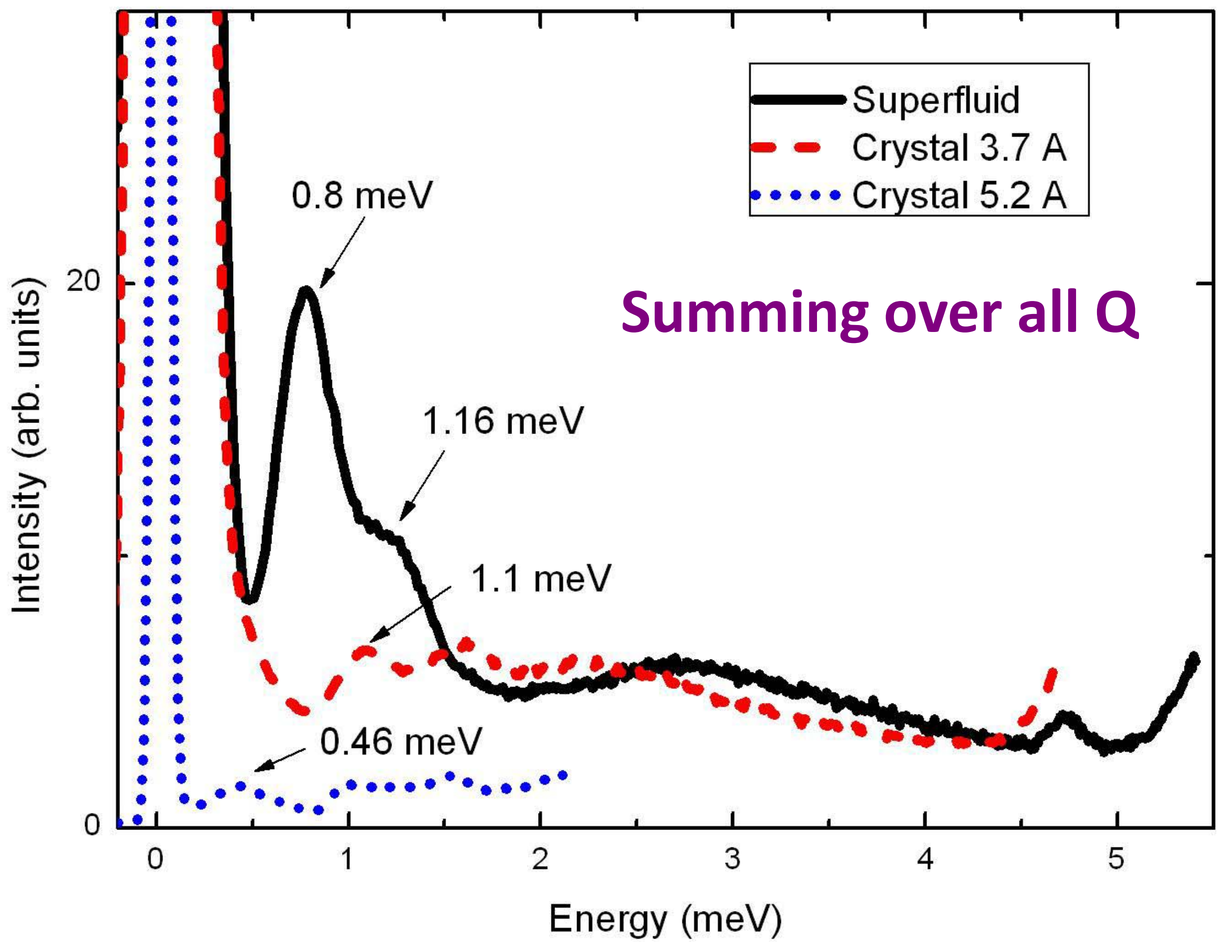
Comparison with the superfluid



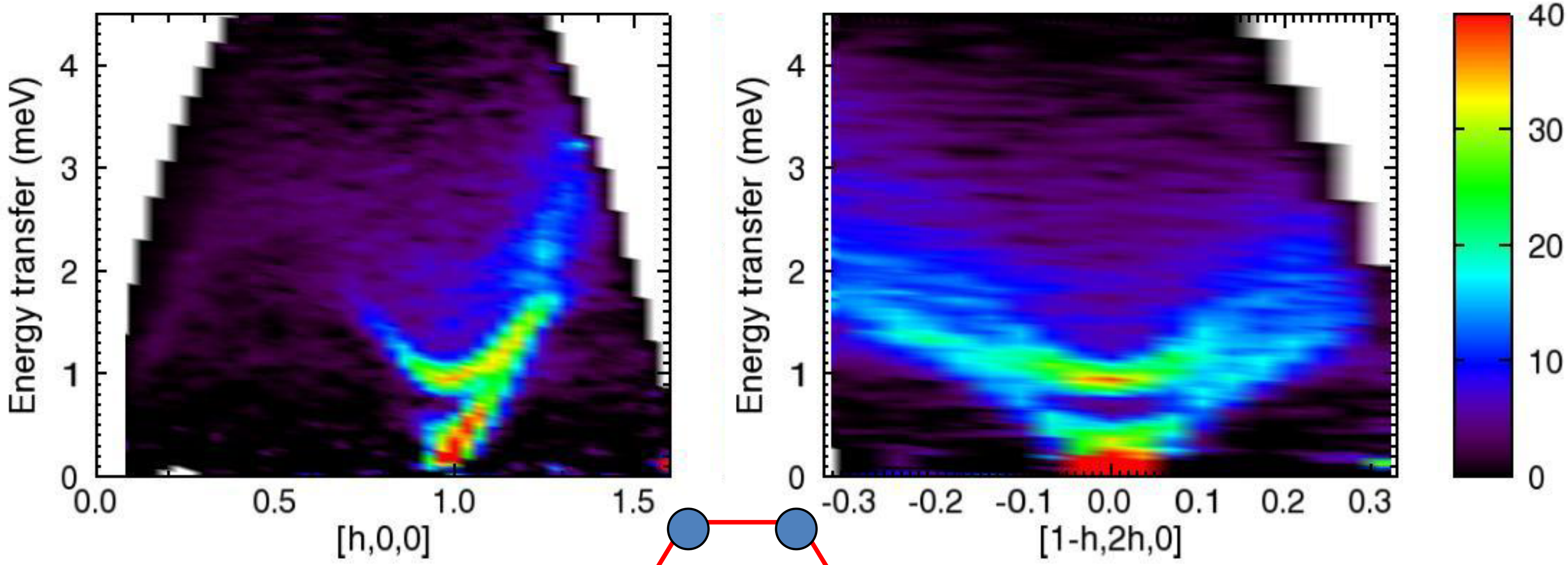
Summing over 2 to 3 meV

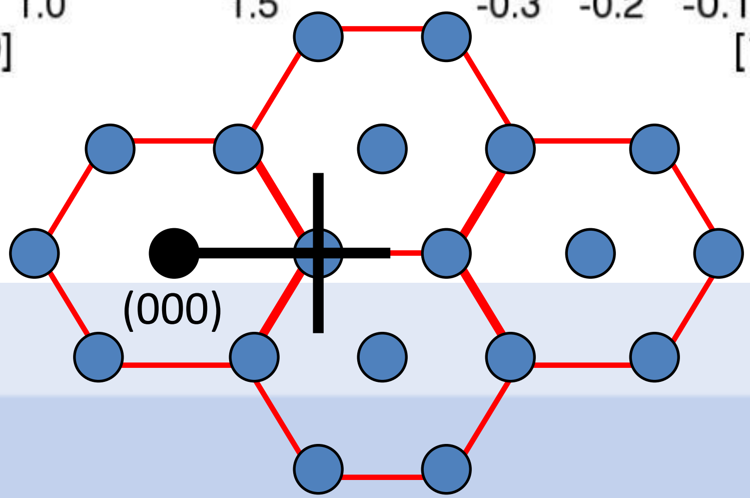


Any superfluid in the sample?

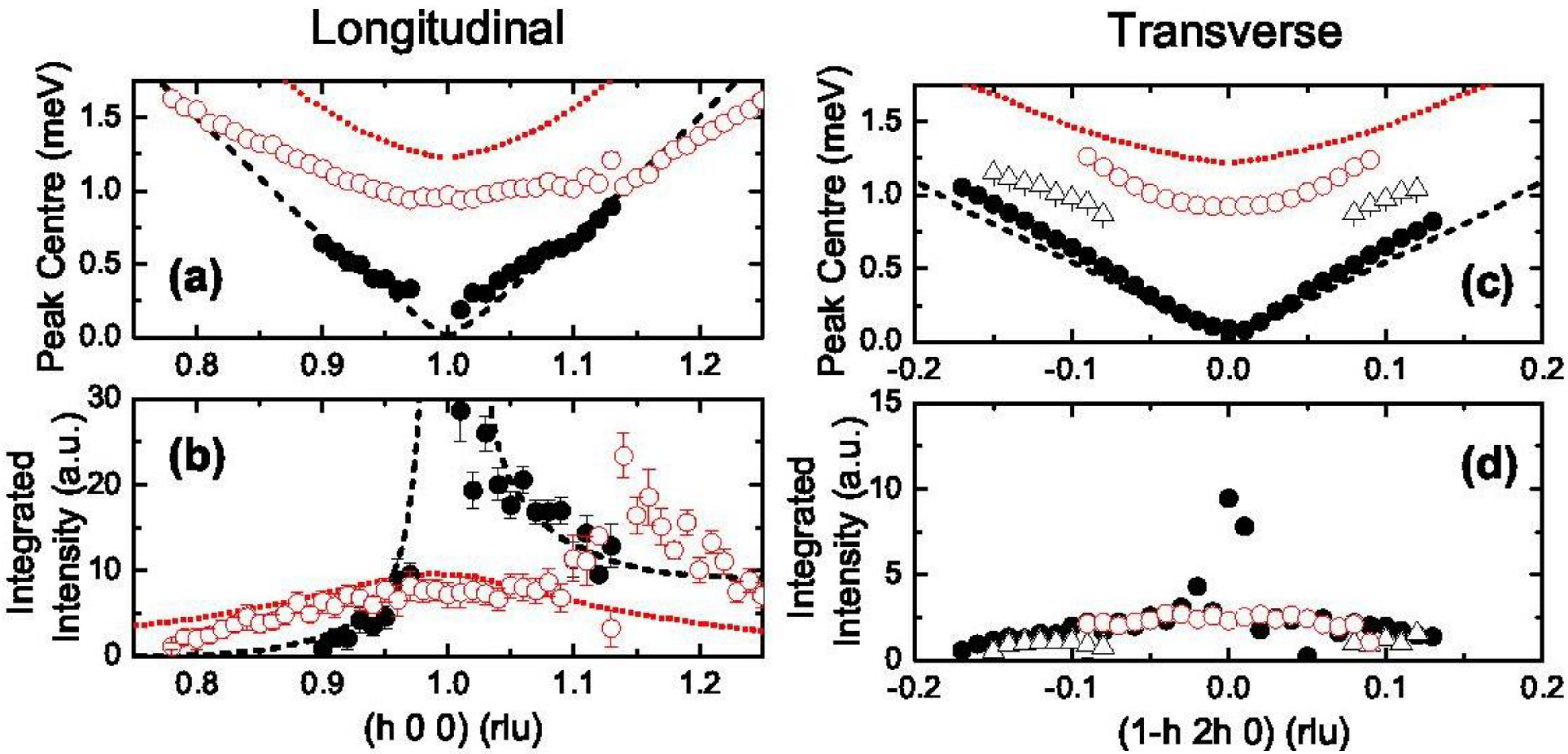


Excitation spectra in the basal plane





Sharp, resolution-limited modes



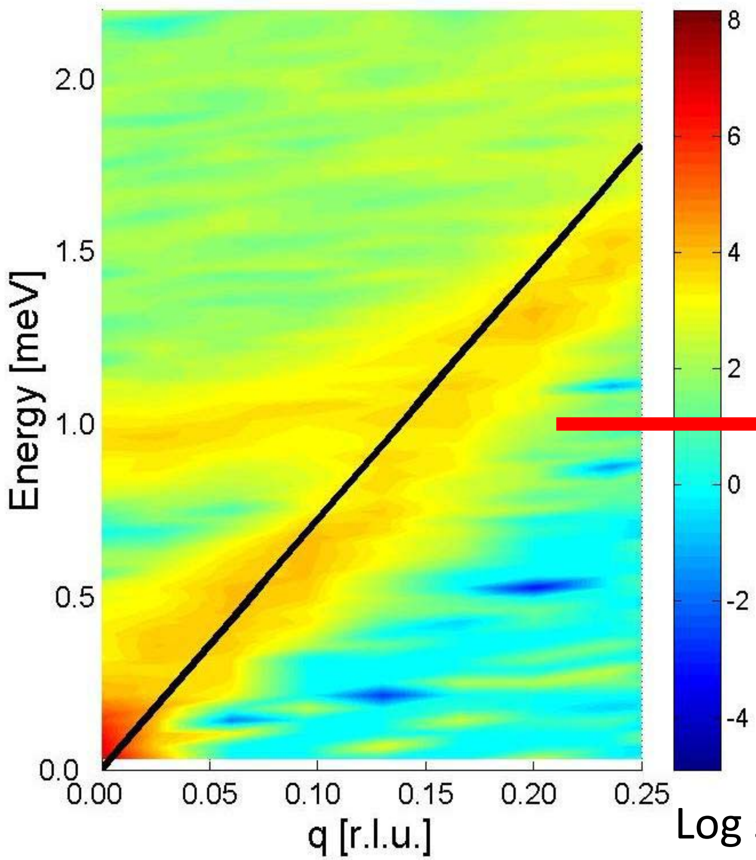
Lines are from calculations using a self-consistent phonon theory

Ref: Gillis, Koehler and Werthamer, Phys. Rev. **175**, 1110 (1968).

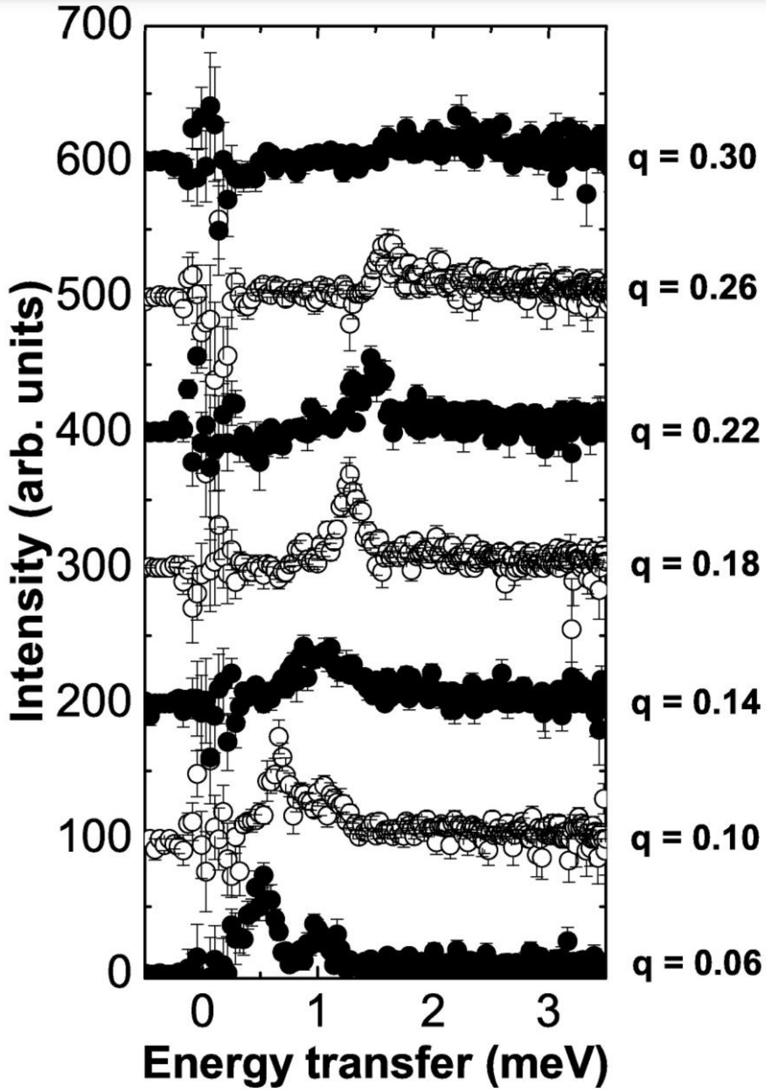
Material	Mode	Effective mass m_{He}	Energy gap meV	$Q_{minimum}$ $Å^{-1}$
Crystal 1	Longitudinal	0.107(3)	0.951(4)	1.964(6)
Crystal 2	Longitudinal	0.114(5)	1.002(3)	1.970(6)
Crystal 1	Transverse	0.144(2)	0.916(2)	1.970(1)
Superfluid	Roton	0.094(2)	0.680(1)	2.054(1)

Table I: Characteristics of the vacancy mode in the solid and the roton mode in the superfluid at 24 bar.

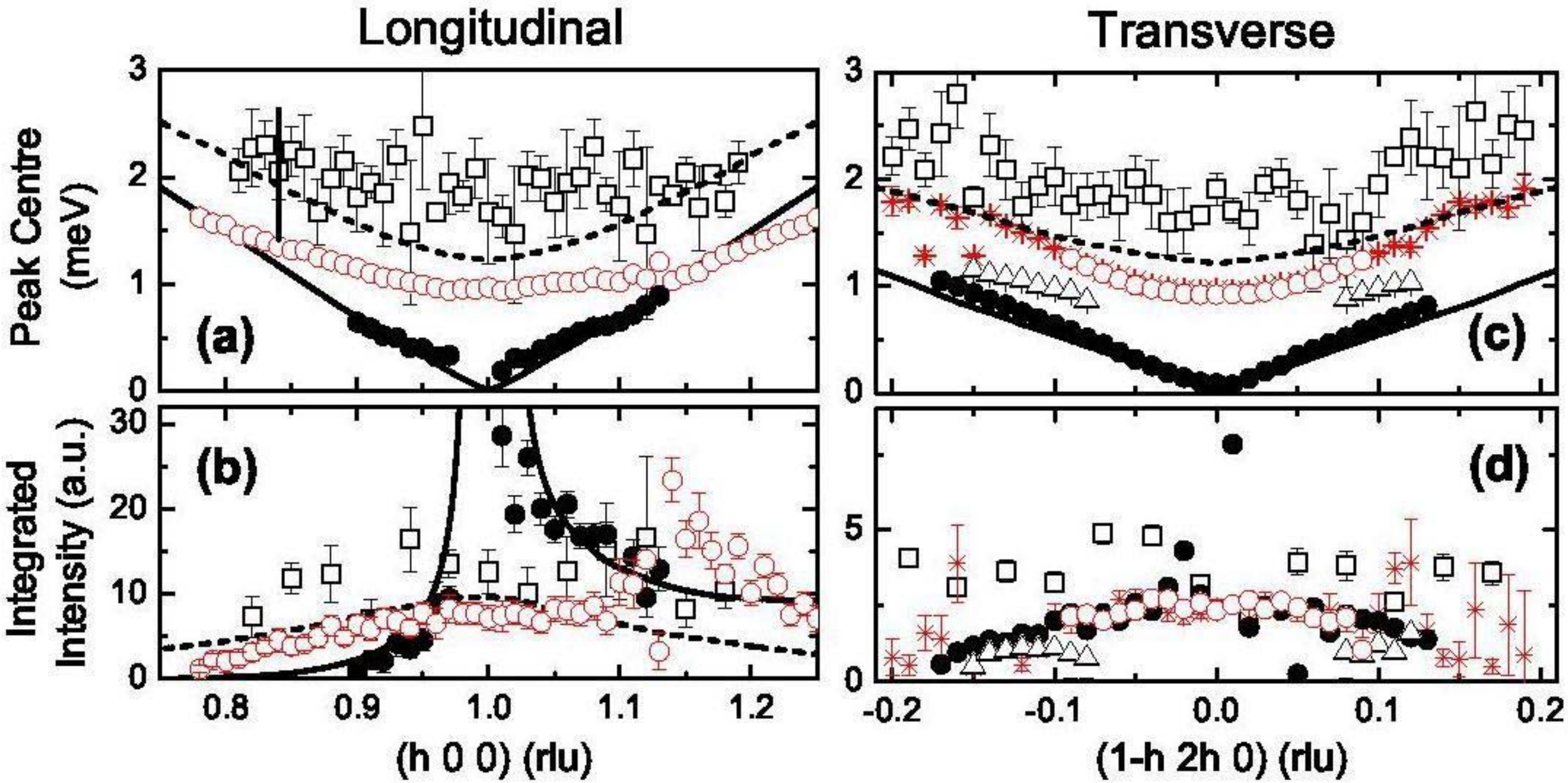
Intersection region



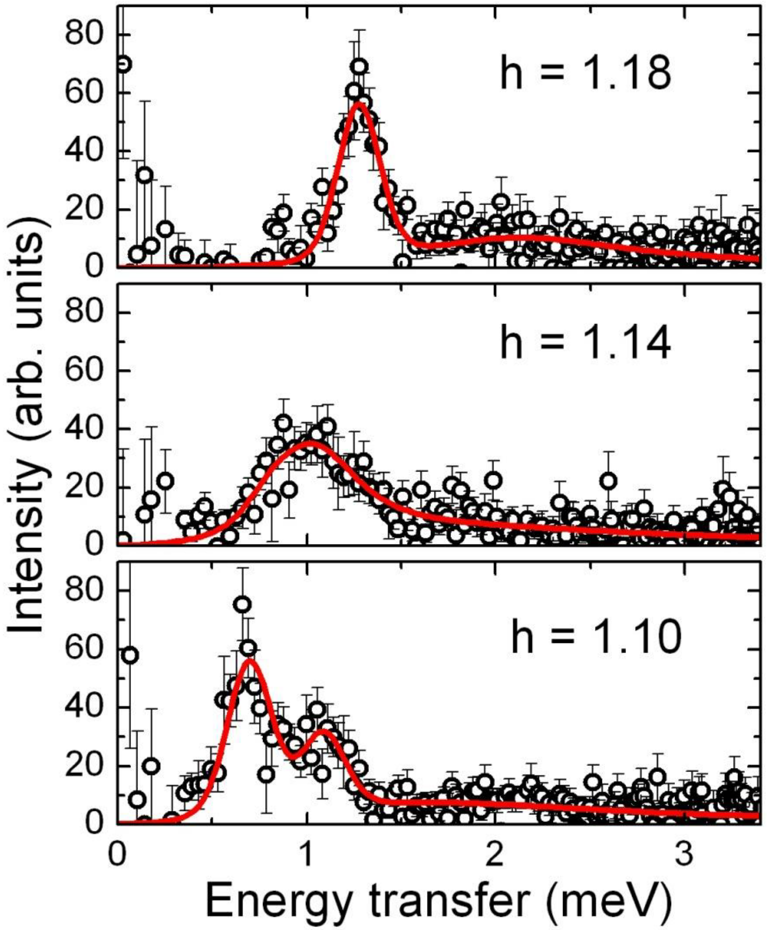
Log scale intensity



Above the sharp mode



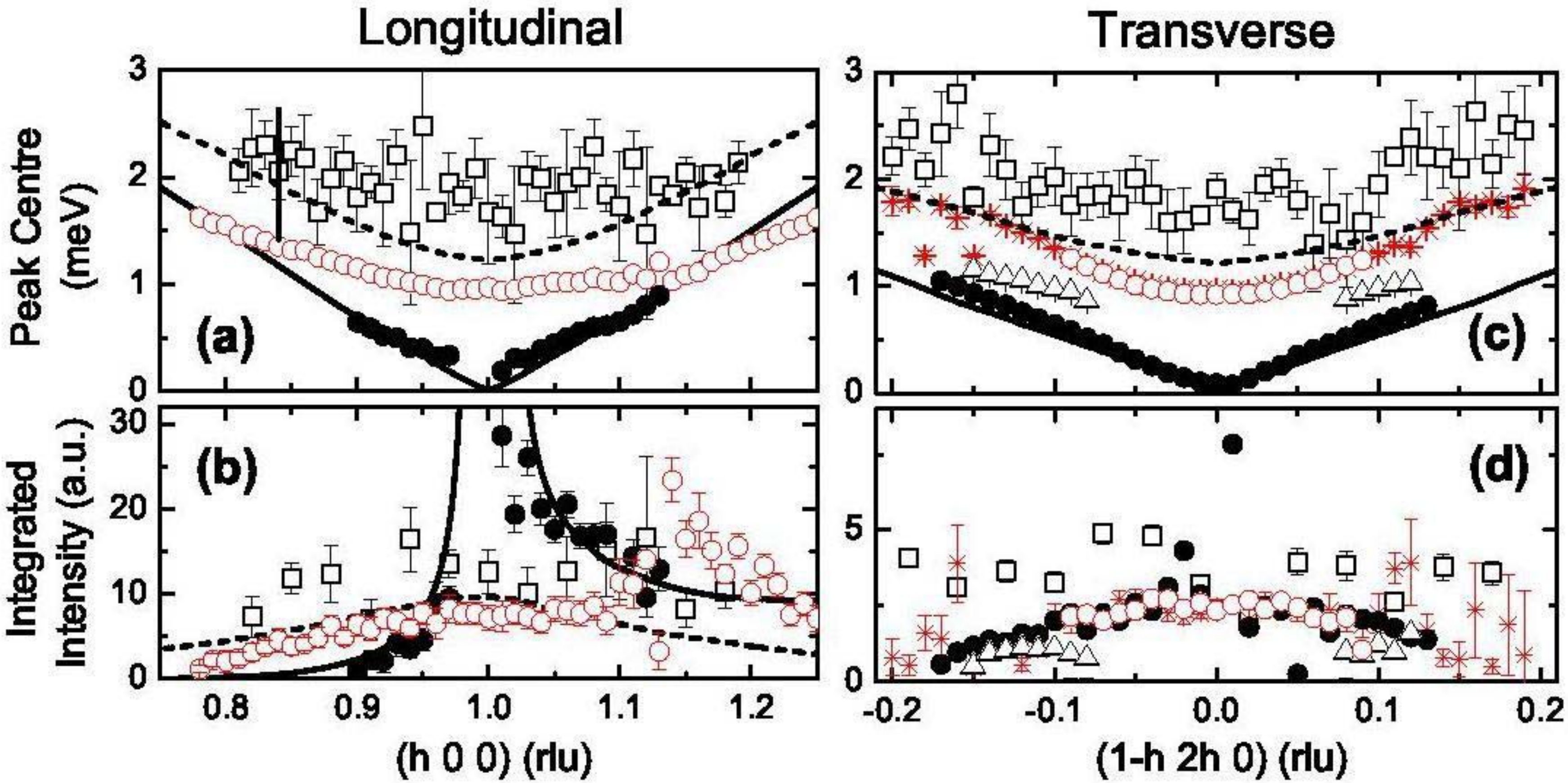
So where is the optic phonon?



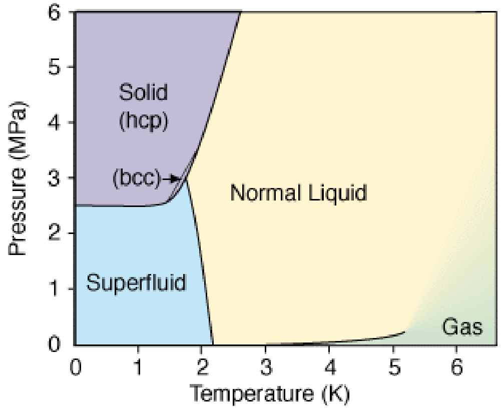
Fitting using damped harmonic oscillators for all of poles, with positions and relative intensities of the acoustic and optic modes fixed using the GKW calculations.

Convoluted with instrumental resolution.

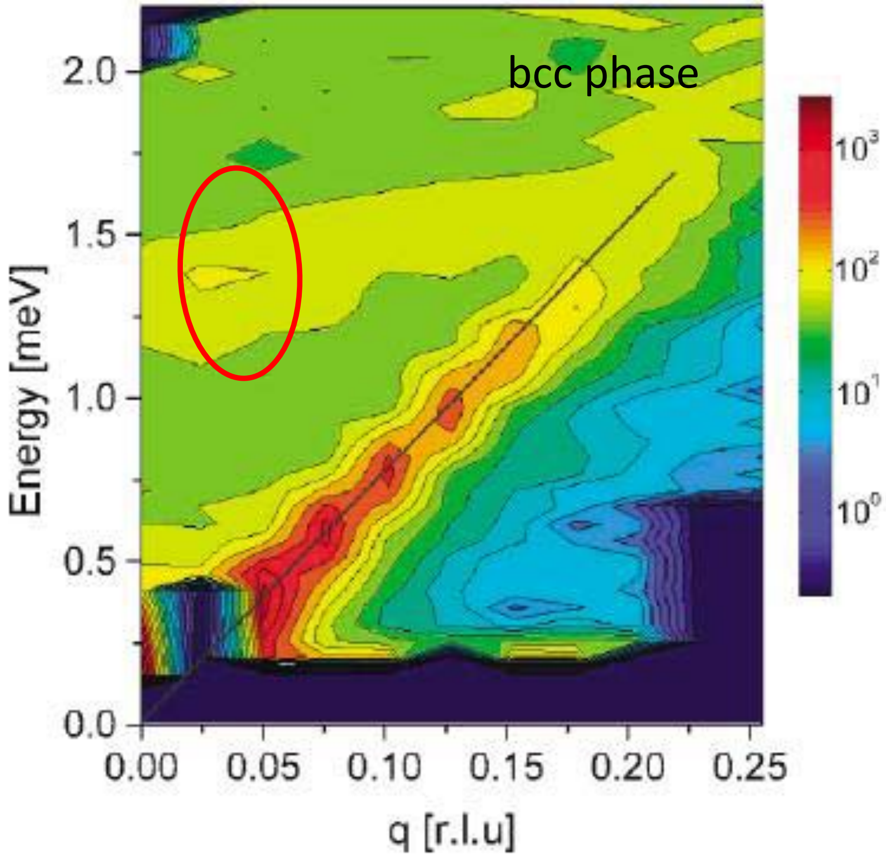
Above the sharp mode



Comparison with bcc phase

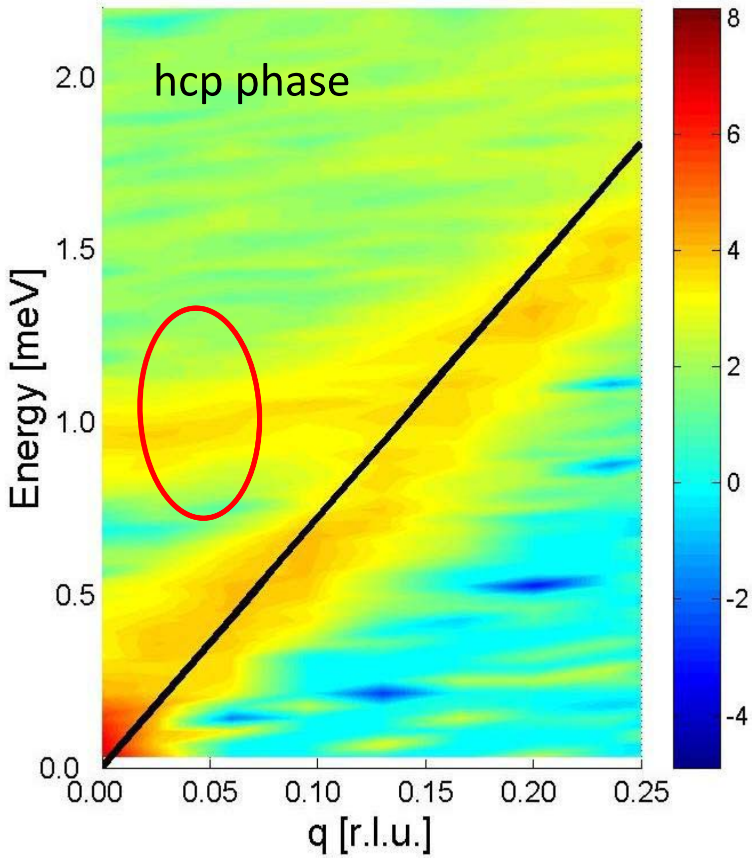


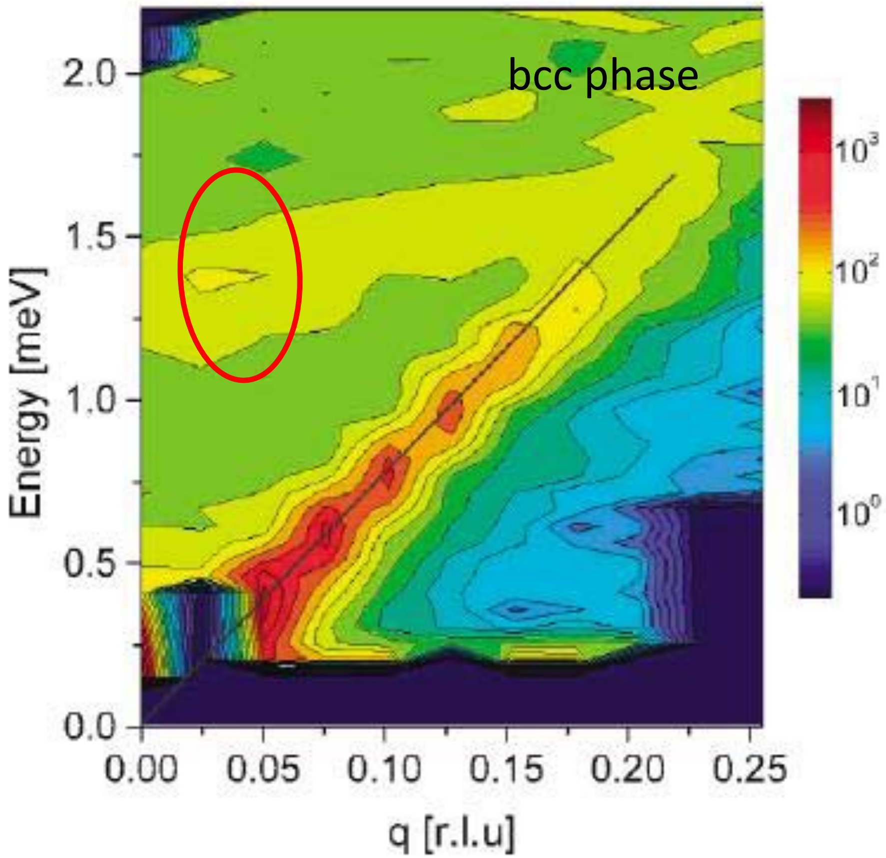
The bcc phase has one atom per unit cell therefore there is no optic phonon



from: Markovich et al.,
Phys. Rev. Lett. **88,** 195301 (2002).

Comparison with bcc phase





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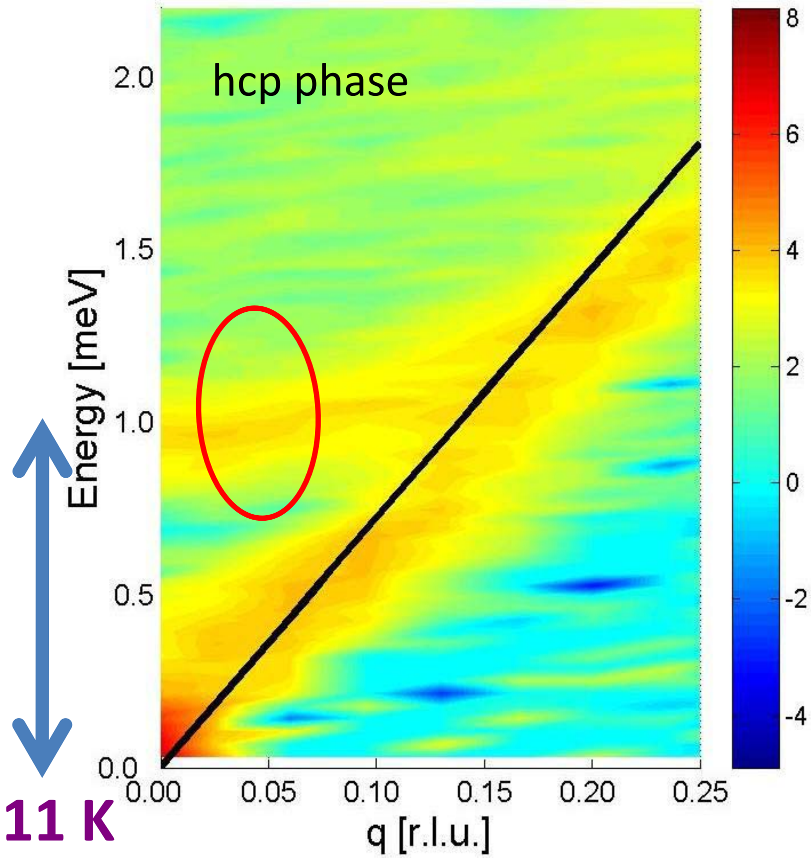
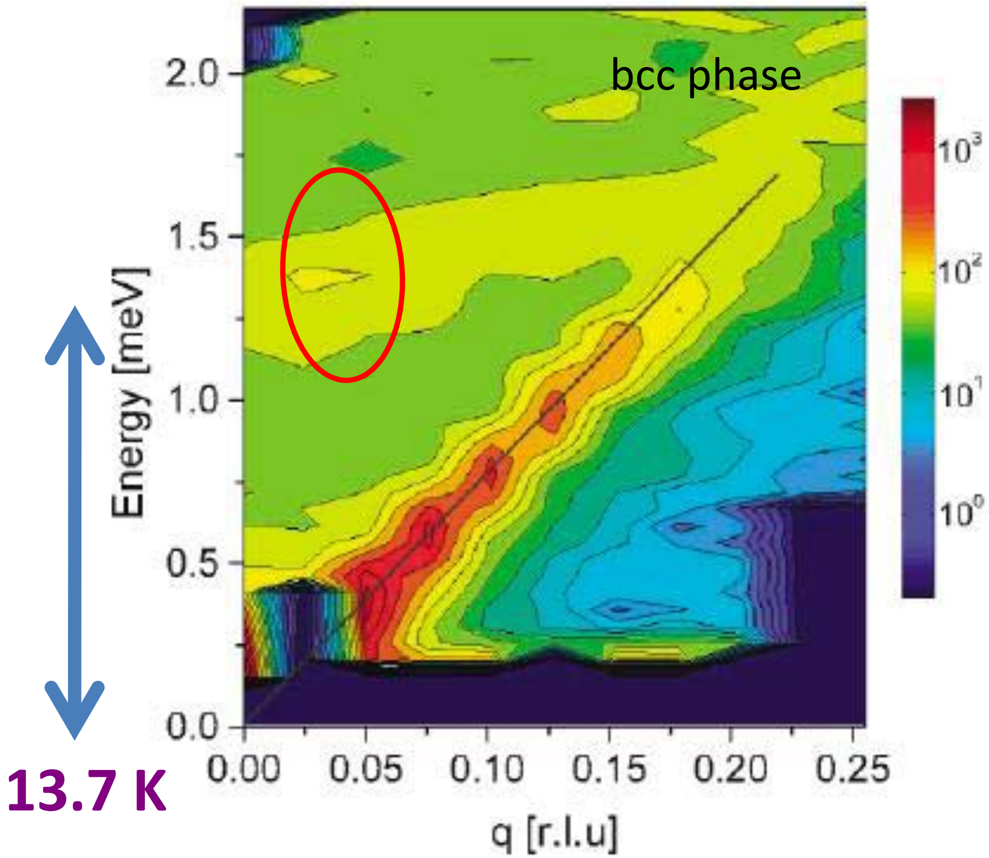
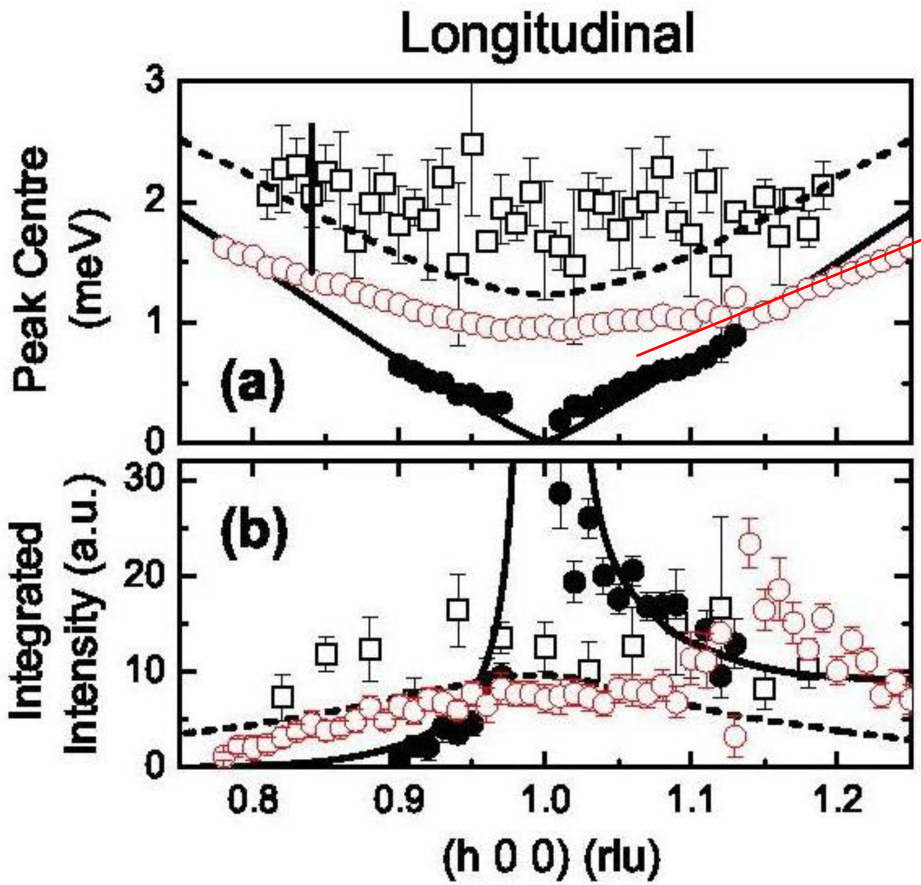
Comparison with bcc phase





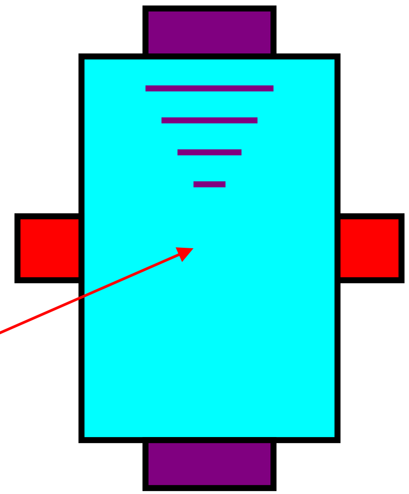
from: Markovich et al.,
Phys. Rev. Lett. **88,** 195301 (2002).

Relation to bolometer expt?



375   8 m/s

226 m/s



For second sound on a gas of excitations with a linear dispersion

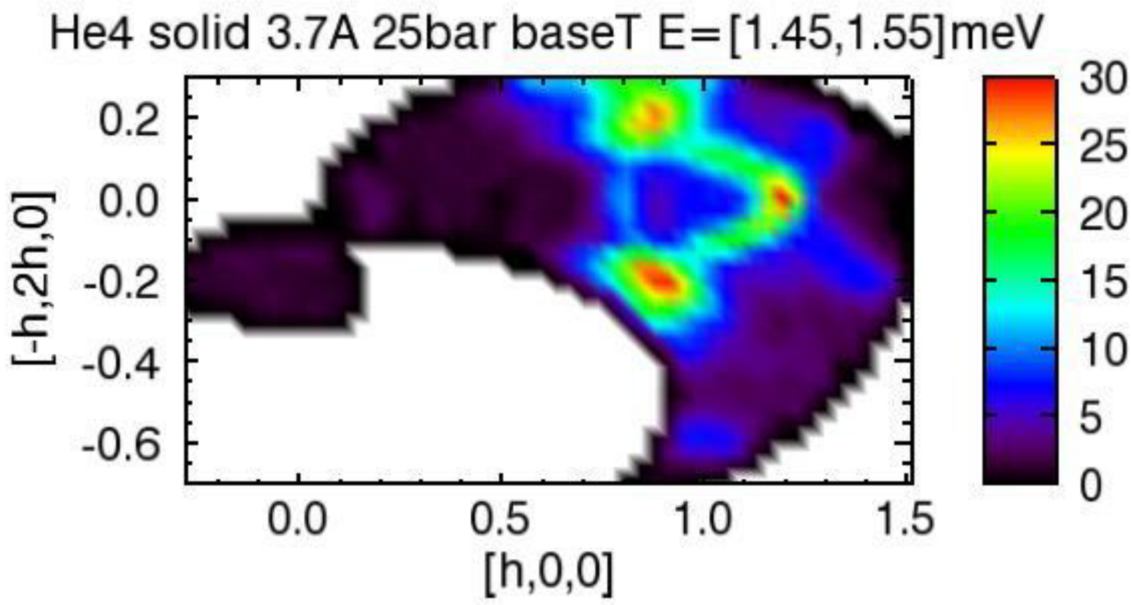
$c_2 = c_1/\surd 3$

so for the linear dispersion here

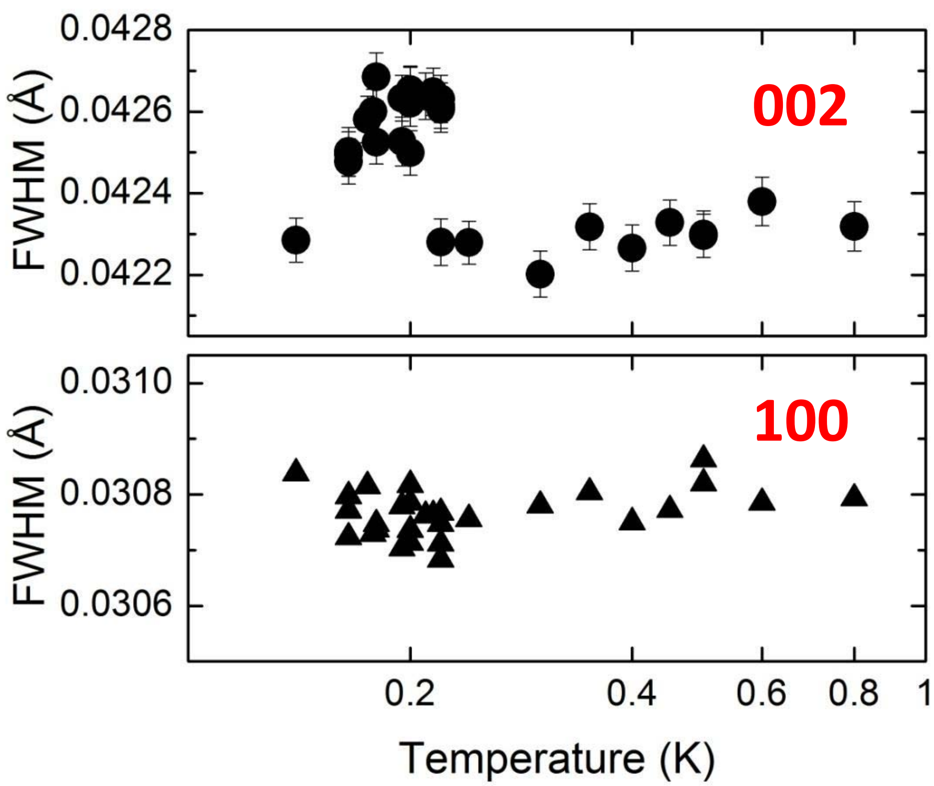
$c_2 = 217 \pm 5$ m/s

Summary

- Observation of a possible delocalized vacancy excitation
- No temperature dependence observed



Bragg peak width



Peaks seen:

We identified:

100

002

110

101

102

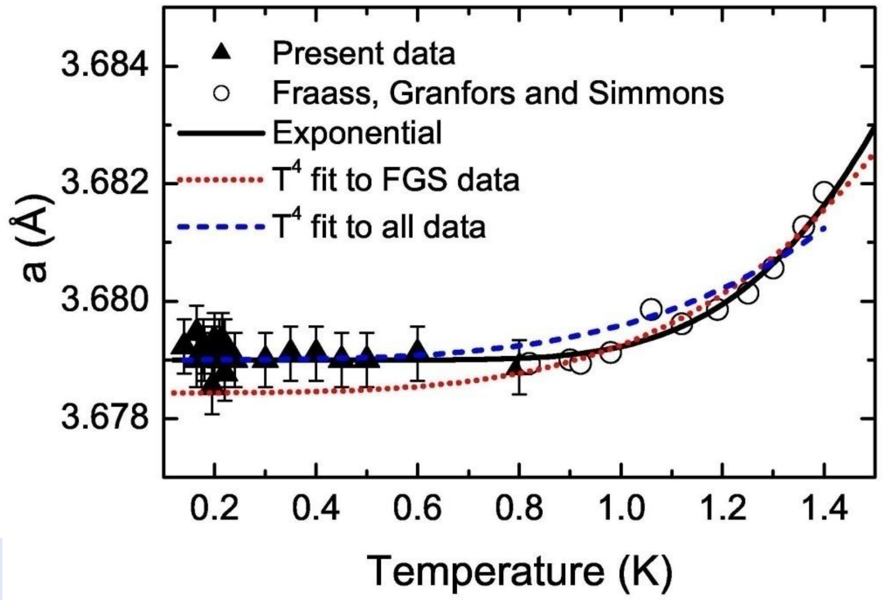
200

004

Vacancies in helium crystals

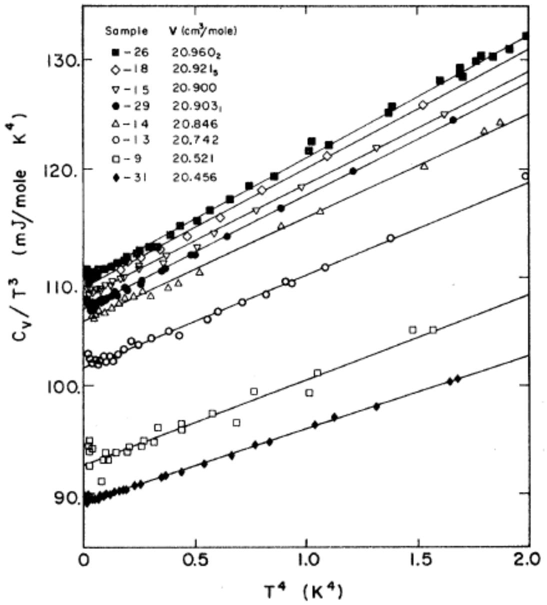
There is a lot of evidence for the presence of thermally activated vacancies above 1 K.

Anderson, Brinkman and Huse proposed a model of (delocalized) zero-point vacancies forming a condensate at low temperatures.



Ref: Blackburn et al., Phys. Rev. B **76**, 024523 (2007).

The heat capacity of solid helium shows a roughly T^7 dependence, as yet unexplained.

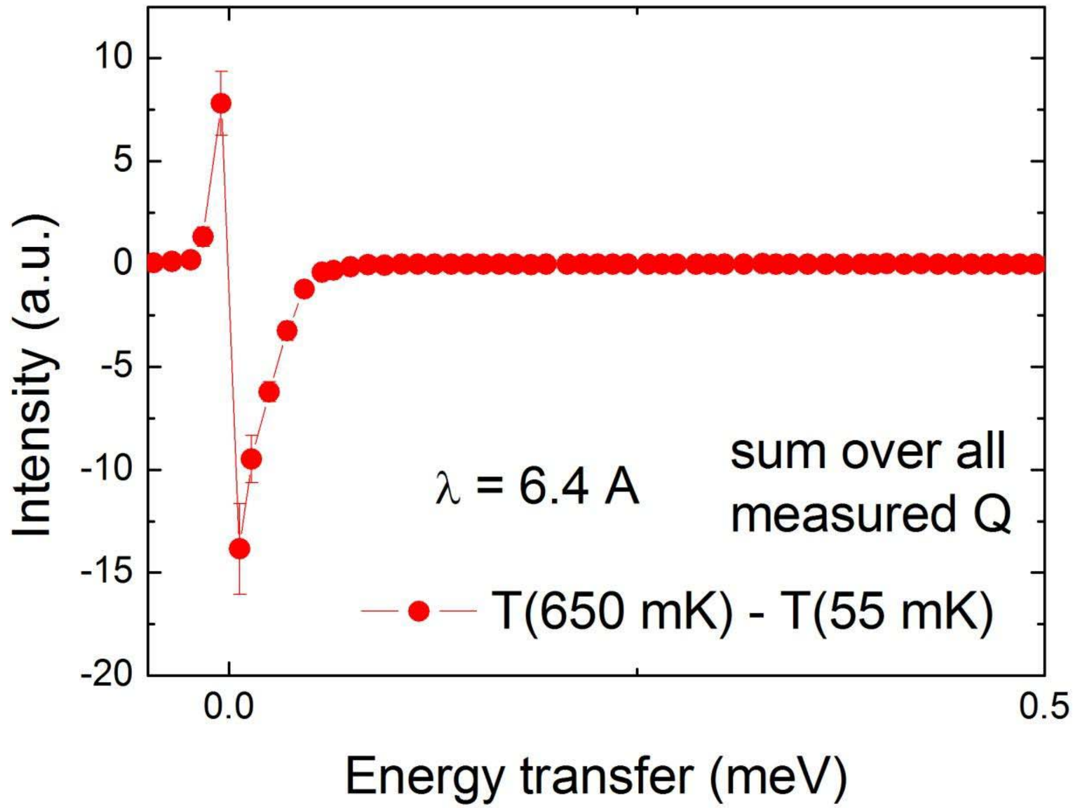


from: Gardner, Hoffer and Phillips, Phys. Rev. A **7,** 1029 (1973).

ABH used this to calculate a vacancy concentration with a T^4 dependence.

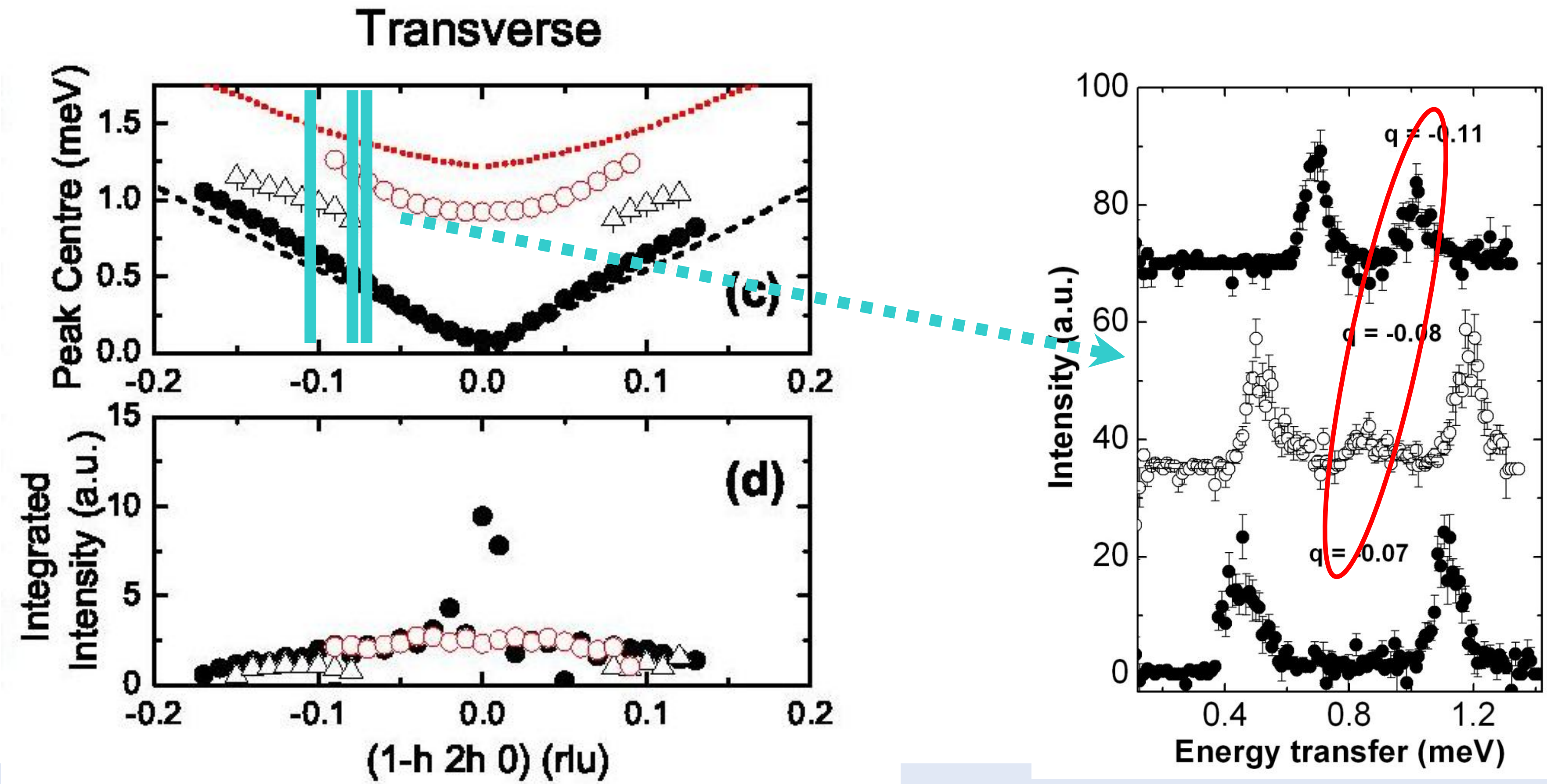
Ref: Anderson, Brinkman and Huse, Science **310**, 1164 (2005).

Temperature dependence - extra



Closed circles = base temperature (55 mK); Open circles = high temperature

A new mode?


Transverse
Peak Centre (meV)
1.5
1.0
0.5
0.0
(c)
-0.2
-0.1
0.0
0.1
0.2
Integrated Intensity (a.u.)
15
10
5
0
(d)
(1-h 2h 0) (rlu)
100
80
60
40
20
0
Intensity (a.u.)
q = -0.11
q = -0.08
q = -0.07
0.4
0.8
1.2
Energy transfer (meV)