MEASUREMENT OF ATOMIC MOMENTUM DISTRIBUTIONS BY HIGH ENERGY NEUTRON SCATTERING J Mayers (ISIS)

Lectures 1 and 2. How n(p) is measured

The Impulse Approximation. Why high energy neutron scattering measures the momentum distribution n(p) of atoms.

The VESUVIO instrument.

Time of flight measurements. Differencing methods to determine neutron energy and momentum transfers Data correction; background, multiple scattering Fitting data to obtain sample composition, atomic kinetic energies and momentum distributions.

Lectures 1 and 2. Why n(p) is measured

What we can we learn from measurements of n(p)

(i) Lecture 3 n(p) in the presence of Bose-Einstein condensation.(ii)Lecture 4 Examples of measurements on protons.

The "Impulse Approximation" states that at sufficiently high incident neutron energy.

- (1) The neutron scatters from single atoms.
- (2) Kinetic energy and momentum are conserved in the collision.

Initial Kinetic Energy

Final Kinetic Energy

$$\kappa_i = p^2 / 2M$$

 $\kappa_f = (\mathbf{p} + \mathbf{q})^2 / 2M$

Momentum transfer

Energy transfer

$$\omega = \frac{\left(\mathbf{p} + \mathbf{q}\right)^2}{2M} - \frac{p^2}{2M}$$

Gives momentum component along **q**

$$y = \mathbf{p}.\hat{\mathbf{q}} = \frac{M}{q} \left(\omega - \frac{q^2}{2M} \right)$$

The Impulse Approximation

$$\frac{d^2\sigma(E_0, E_1, \theta)}{d\Omega dE_1} = \left|b\right|^2 \sqrt{\frac{E_1}{E_0}S(q, \omega)}$$

$$S(\mathbf{q},\omega) = \int n(\mathbf{p})\delta\left(\omega + \frac{p^2}{2M} - \frac{(\mathbf{p}+\mathbf{q})^2}{2M}\right)d\mathbf{p}$$

Kinetic energy and momentum are conserved

Why is scattering from a single atom?



If q >> $1/\Delta r$ interference effects between

different atoms average to zero.

Incoherent approximation is good for q such that; Liquids S(q) ~1 q >~10Å⁻¹ Crystalline solids – q such that Debye Waller factor ~0. Why is the incoherent $S(q,\omega)$ related to n(p)?

$$S(\mathbf{q},\omega) = N \sum_{f} |A_{f}(\mathbf{q})|^{2} \delta(\omega + E_{f} - E)$$

Single particle In a potential

$$A_f(\mathbf{q}) = \int \psi^*(\mathbf{r}) \exp(i\mathbf{q}\cdot\mathbf{r}) \psi_f(\mathbf{r}) d\mathbf{r}$$

E = Initial energy of particle

 ω = energy transfer

- $E_f = Final energy of particle$
- **q** = wave vector transfer

$$A_f = \int \psi^*(\mathbf{r}) \exp(i\mathbf{q}\cdot\mathbf{r}) \psi_f(\mathbf{r}) d\mathbf{r}$$

IA assumes final state of the struck atoms is a plane wave.

$$\psi_f(\mathbf{r}) = C \exp(-i\mathbf{k}_f \bullet \mathbf{r}) \qquad E_f = \frac{\hbar^2 \mathbf{k}_f^2}{2M}$$



 \mathbf{a}

$$A_f = C \int \psi^*(\mathbf{r}) \exp[i(\mathbf{q} - \mathbf{k}_f) \cdot \mathbf{r}] \psi(\mathbf{r}) d\mathbf{r}$$

$$n(\mathbf{p}) = \left| \int \psi(\mathbf{r}) \exp[i\mathbf{p} \cdot \mathbf{r}] d\mathbf{r} \right|^{2} \qquad \text{momentum distribution}$$

$$\left| A_{f} \right|^{2} = \left| C \right|^{2} n(\mathbf{q} - \mathbf{k}_{f})$$

$$\downarrow$$

$$S(\mathbf{q}, \omega) = \sum_{f} n(\mathbf{q} - \mathbf{k}_{f}) \delta(\omega + \frac{k_{f}^{2}}{2m} - E)$$



p in Å⁻¹ throughout - multiply by ħ to get momentum

$$S(\mathbf{q},\omega) = \sum_{\mathbf{p}} n(\mathbf{p}) \delta \left(\omega - \frac{(\mathbf{p} + \mathbf{q})^2}{2M} - E \right)$$

Final state is plane wave

$$S(\mathbf{q},\omega) = \int n(\mathbf{p})\delta\left(\omega - \frac{(\mathbf{p}+\mathbf{q})^2}{2M} + \frac{p^2}{2M}\right)d\mathbf{p}$$

Impulse Approximation

 $q \rightarrow \infty$ gives identical expressions

Difference due to "Initial State Effects" Neglect of potential energy in initial state. Neglect of quantum nature of initial state.

 $A_f = \int \psi^*(\mathbf{r}) \exp(i\mathbf{q}\cdot\mathbf{r}) \psi_f(\mathbf{r}) d\mathbf{r}$

Infinite Square well





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Quantum effects in deep inelastic neutron scattering

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T=0

Initial state effects in deep inelastic neutron scattering

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G. Baciocco Dipartimento di Fisica, Università "La Sapienza," Rome, Italy (Received 8 August 1988)







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All deviations from IA are known as Final State Effects in the literature.

Can be shown that (V. F. Sears *Phys. Rev. B.* **30,** 44 (1984).

$$J(y) = J_{IA}(y) - \frac{M\langle \nabla^2 V \rangle}{36\hbar^2 q} \frac{d^3 J_{IA}(y)}{dy^3} + \frac{M^2 \langle F^2 \rangle}{72\hbar^4 q^2} \frac{d^4 J_{IA}(y)}{dy^4} + \dots$$

Thus FSE give further information on binding potential (but difficult to measure)

Neutron-scattering study of the impulse approximation in ZrH₂

A. C. Evans* and D. N. Timms

Division of Physics, Portsmouth University, Park Building, King Henry I Street, Portsmouth POI 2DZ, United Kingdom

J. Mayers and S. M. Bennington Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, United Kingdom (Received 14 August 1995)



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FSE in Pyrolytic Graphite

A L Fielding,, J Mayers and D N Timms Europhys Lett 44 255 (1998)





FSE in ZrH₂



Measurements of momentum distributions of atoms

Need q >> rms p

For protons rms value of p is 3-5 $Å^{-1}$

q > 50 Å⁻¹, ω > ~20 eV required

Only possible at pulsed sources such as ISIS UK, SNS USA

Short pulses ~1µsec at eV energies allow accurate measurement of energy and momentum transfers at eV energies.

Lecture 2

• How measurements are performed

Time of flight measurements



Time of flight neutron measurements

Fixed
$$v_0$$
 (incident v)
(Direct Geometry) $t = \frac{L_0}{v_0} + \frac{L_1}{v_1} \longrightarrow v_1$

Fixed v₁ (final v) (Inverse Geometry)

$$t = \frac{L_0}{v_0} + \frac{L_1}{v_1} \longrightarrow v_0$$

 $k_{0} = \frac{mv_{0}}{\hbar} \qquad E_{0} = \frac{1}{2}mv_{0}^{2} \qquad \qquad k_{1} = \frac{mv_{1}}{\hbar} \qquad \qquad E_{1} = \frac{1}{2}mv_{1}^{2}$

$$q^2 = k_1^2 + k_2^2 - 2k_1k_2\cos\theta$$

Wave vector transfer

$$\omega = E_0 - E_1$$

Energy transfer

The VESUVIO Inverse Geometry Instrument





Foil cycling method



E M Schoonveld, J. Mayers et al Rev. Sci. Inst. **77** 95103 (2006)



Filter Difference Method





Blue = intrinsic width of lead peak

Black = measurement using Filter difference method

Red = foil cycling method



YAP detectors give

Smaller resolution width

Better resolution peak shape

100 times less counts on filter in and filter out measurements Thus less detector saturation at short times

Similar count rates in the differenced spectra

Larger differences between foil in and foil out measurements therefore more stability over time.

Comparison of chopper and resonance filter spectrometers at eV energies C Stock, R A Cowley, J W Taylor and S. M. Bennington

Phys Rev B **81**, 024303 (2010)





Gamma background









Need detectors on rings

Rotate secondary foils keeping the foil scattering angle constant

Should almost eliminate gamma background effects








 $p^2n(p)$ without a background correction

with a background correction

Multiple Scattering

J. Mayers, A.L. Fielding and R. Senesi, Nucl. Inst. Methods A 481, 454 (2002)



Multiple Scattering



A=0.048. A=0.092, A=0.179, A=0.256.



Correction for Gamma Background and Multiple Scattering

Automated procedure. Requires;

Sample+can transmission

Atomic Masses in sample + container

Correction determined by measured data

30 second input from user

Correction procedure runs in ~10 minutes



Data Analysis

Impulse Approximation implies kinetic energy and momentum are conserved in the collision between a neutron and a single atom.

Initial Kinetic Energy

Final Kinetic Energy

$$\kappa_i = p^2 / 2M$$

 $\kappa_f = \left(\vec{p} + \vec{q}\right)^2 / 2M$

Momentum transfer

Energy transfer

$$\omega = \frac{(\vec{p} + \vec{q})^2}{2M} - \frac{p^2}{2M}$$

$$\mathbf{p}.\hat{\mathbf{q}} = \frac{M}{q} \left(\omega - \frac{q^2}{2M} \right)$$

Y scaling

$$y = \mathbf{p}.\hat{\mathbf{q}} = \frac{M}{q} \left(\omega - \frac{q^2}{2M} \right)$$

In the IA q and ω are no longer independent variables

Any scan in q, ω space which crosses the line $\omega = q^2/(2M)$ gives the same information in isotropic samples

Detectors at all angles give the same information for isotropic samples

Data Analysis

$$C(t) = 2\left(\frac{2}{m}\right)^{1/2} \frac{E_0^{3/2}}{L_0} I(E_0) D(E_1) \sum_M N_M \frac{d^2 \sigma_M}{d\Omega dE_1} d\Omega$$

$$\frac{d^2 \sigma_M}{d\Omega dE_1} = b_M^2 \sqrt{\frac{E_1}{E_0}} \frac{M}{q} J_M(y_M)$$

$$y_M = \frac{M}{q} \left(\omega - \frac{q^2}{2M} \right)$$

$$J_{M}(y_{M}) = \frac{1}{\sqrt{2\pi w_{M}^{2}}} \exp\left(\frac{-y_{M}^{2}}{2w_{M}^{2}}\right)$$

Strictly valid only if(1) Atom is bound by harmonic forces(2) Local potential is isotropic

Spectroscopy shows that both assumptions are well satisfied in ZrH2

Spectroscopy implies that w_H is 4.16 ± 0.02 Å⁻¹

VESUVIO measurements give





ZrH₂ Calibrations

		W _H	A _H /A _{Zr}
3356	Sep 2008	4.15	21.8
3912	Nov 2008	4.13	21.3
4062	Dec 2008	4.11	21.9
4188	May 2009	4.16	20.8
4642	Nov 2009	4.15	21.5
5026	Jul 2010	4.13	21.5

Expected ratio for $ZrH_{1.98}$ is 1.98 x 81.67/6.56 = 24.65

Mean value measured is 21.5 ± 0.2

Intensity shortfall in H peak of $12.7 \pm 0.8\%$

Momentum Distribution of proton





Measured p²n(p) for ZrH₂



Lecture 3.

What can we learn from a measurement

of the momentum distribution n(p).

Bose-Einstein condensation

Bose-Einstein Condensation $T>T_B$ $0 < T < T_B$ $T \sim 0$



D. S. Durfee and W. Ketterle Optics Express 2, 299-313 (1998).

BEC in Liquid He4



T.R. Sosnick, W.M Snow P.E. Sokol Phys Rev B **41** 11185 (1989)

f =0.07 ±0.01

Kinetic energy of helium atoms. J. Mayers, F. Albergamo, D. Timms Physica B **276** (2000) 811



Macroscopic Quantum Effects



http://cua.mit.edu/ketterle_group/



Quantised vortices in ⁴He and ultra-cold trapped gases

Interference between separately prepared condensates of ultra-cold atoms

Neutron-diffraction study of the static structure factor and pair correlations in liquid ⁴He

E. C. Svensson, V. F. Sears, A. D. B. Woods,* and P. Martel Atomic Energy of Canada Limited Research Company, Chalk River, Ontario, Canada KOJ 1JO (Received 3 December 1979)



High-Resolution Study of Excitations in Superfluid ⁴He by the Neutron Spin-Echo Technique

F. Mezei Central Research Institute for Physics, H-1525 Budapest 114, Hungary, and Institut Laue-Langevin, F-38042 Grenoble, France (Received 28 December 1979)



Line width of excitations in superfluid helium is zero as $T \rightarrow 0$. Why?



Basis of Lectures

J. Mayers	J. Low. Temp. Phys	109 135 109 153	(1997) (1997)
J. Mayers	Phys. Rev. Lett.	80 , 750 84 314 92 135302	(1998) (2000) (2004)
J. Mayers,	Phys. Rev.B	64 224521, 74 014516,	(2001) (2006)
J Mayers	Phys Rev A	78 33618	(2008)

Quantum mechanical expression for n(p) in ground state

$$n(\mathbf{p}) = \int d\mathbf{r}_2 \dots d\mathbf{r}_N \left| \int \Psi(\mathbf{r}_1, \mathbf{r}_2, \dots \mathbf{r}_N) \exp(i\mathbf{p} \cdot \mathbf{r}_1) d\mathbf{r}_1 \right|^2$$

Ground state wave function

$$\mathbf{r} = \mathbf{r}_{1} \qquad \mathbf{s} = \mathbf{r}_{2}, ..\mathbf{r}_{N}$$

$$\mathbf{\nabla}$$

$$n(\mathbf{p}) = \int d\mathbf{s} \left| \int \Psi(\mathbf{r}, \mathbf{s}) \exp(i\mathbf{p}.\mathbf{r}) d\mathbf{r} \right|^{2}$$

What are implications of presence of peak of width \hbar/L for properties of Ψ ?



$$\psi_{\mathbf{s}}(\mathbf{r}) = \Psi(\mathbf{r},\mathbf{s}) / \sqrt{P(\mathbf{s})}$$

$$P(\mathbf{s}) = \int \left| \Psi(\mathbf{r}, \mathbf{s}) \right|^2 d\mathbf{r}$$

$$n(\mathbf{p}) = \int P(\mathbf{s}) n_{\mathbf{s}}(\mathbf{p}) d\mathbf{s}$$

$$n_{\mathbf{S}}(\mathbf{p}) = \frac{1}{\hbar^3} \left| \int \psi_{\mathbf{S}}(\mathbf{r}) \exp(i\mathbf{p}\cdot\mathbf{r}/\hbar^3) d\mathbf{r} \right|^2$$

$|\Psi(\mathbf{r}, \mathbf{s})|^2$ is pdf for N coordinates r,s $P(\mathbf{s}) = \int |\Psi(\mathbf{r}, \mathbf{s})|^2 d\mathbf{r}$ is pdf for N-1 coordinates s



 $\int \left| \psi_{\mathbf{S}}(\mathbf{r}) \right|^2 d\mathbf{r} = 1$

$\Psi_{s}(\mathbf{r})$ is "conditional wave function"

$$n(\mathbf{p}) = \int P(\mathbf{s}) n_{\mathbf{s}}(\mathbf{p}) d\mathbf{s}$$
$$n_{\mathbf{s}}(\mathbf{p}) = \frac{1}{\hbar^3} \left| \int \psi_{\mathbf{s}}(\mathbf{r}) \exp(i\mathbf{p} \cdot \mathbf{r} / \hbar^3) d\mathbf{r} \right|$$

2

What are implications of presence of peak of width \hbar/L for properties of ψ_s ?

 $\psi_{\text{S}}(\textbf{r})$ must be delocalised over length scales ~L







Delocalized, BEC

Localized, No BEC

Feynman - Penrose - Onsager Model

 $\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_N) = 0$ if $|\mathbf{r}_n - \mathbf{r}_m| < a$ a=hard core diameter of He atom

 $\Psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_N) = C$ otherwise



J. Mayers PRL **84** 314, (2000) PRB**64** 224521,(2001)



Periodic boundary conditions. Line is Gaussian with same mean and standard deviation as simulation. f ~ 8% O. Penrose and L. Onsager Phys Rev **104** 576 (1956)



 $\psi_{\rm s}({\bf r})d{\bf r}$

Has same value for all possible **s** to within terms $\sim 1/\sqrt{N}$ 65

Macroscopic Single Particle Quantum Behaviour (MSPQB)

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) = \prod_{n=1}^N \eta(\mathbf{r}_n)$$

 $\eta(\mathbf{r})$ is non-zero over macroscopic length scales

Coarse grained average

$$\overline{\left|\Psi(\mathbf{r}_{1},\mathbf{r}_{2},...\mathbf{r}_{N})\right|^{2}} = \frac{1}{\Omega^{N}} \int_{\Omega(\mathbf{r}_{1})} d\mathbf{r}_{1}^{\prime} ... \int_{\Omega(\mathbf{r}_{N})} d\mathbf{r}_{N}^{\prime} \left|\Psi(\mathbf{r}_{1}^{\prime},\mathbf{r}_{2}^{\prime},...\mathbf{r}_{N}^{\prime})\right|^{2}$$

Smoothing operation – removes structure on length scales of inter-atomic separation. Leaves long range structure.

Coarse Grained

average over

volume Ω

containing

 N_{Ω} atoms



$$\overline{\psi_{\mathbf{S}}(\mathbf{r})} = \frac{1}{\Omega} \int_{\Omega(\mathbf{r})} \psi_{\mathbf{S}}(\mathbf{r}') d\mathbf{r}' = f(\mathbf{r}) \pm \sim 1/\sqrt{N_{\Omega}}$$

$$\overline{F[\psi_{\mathbf{S}}(\mathbf{r})]} = \frac{1}{\Omega} \int_{\Omega(\mathbf{r})} F[\psi_{\mathbf{S}}(\mathbf{r}')] d\mathbf{r}' = F(\mathbf{r}) \pm \sim 1/\sqrt{N_{\Omega}}$$

$$\overline{\left|\psi_{\mathbf{S}}(\mathbf{r})\right|^{2}} = \frac{1}{\Omega} \int_{\Omega(\mathbf{r})} \left|\psi_{\mathbf{S}}(\mathbf{r}')\right|^{2} d\mathbf{r}'$$

$$\overline{\left|\psi_{\mathbf{S}}(\mathbf{r})\right|^{2}} = \left|\eta(\mathbf{r})\right|^{2} \pm \sim 1/\sqrt{N_{\Omega}}$$



$$\rho(\mathbf{r}) = N \int P(\mathbf{s}) d\mathbf{s} |\psi_{\mathbf{s}}(\mathbf{r})|^2$$

Density at r

$$\left|\eta(\mathbf{r})\right|^2 = \rho(\mathbf{r}) \pm \sim 1/\sqrt{N_{\Omega}}$$

$$\frac{1}{\Omega^N} \int_{\Omega(\mathbf{r}_1)} d\mathbf{r}_1' .. \int_{\Omega(\mathbf{r}_N)} d\mathbf{r}_N' |\Psi(\mathbf{r}_1', \mathbf{r}_2', ... \mathbf{r}_N')|^2$$

$$= \frac{1}{\Omega^{N-1}} \int_{\Omega(\mathbf{r}_N)} P(\mathbf{s}) d\mathbf{r}_2 ... d\mathbf{r}'_N \frac{1}{\Omega} \int_{\Omega(\mathbf{r})} |\psi_{\mathbf{s}}(\mathbf{r})|^2 d\mathbf{r}$$

$$\rho(\mathbf{r}) = N \int P(\mathbf{s}) d\mathbf{s} |\psi_{\mathbf{s}}(\mathbf{r})|^2 \quad \text{Density at } \mathbf{r}$$

$$= \frac{1}{\Omega^{N-1}} \int_{\Omega(\mathbf{r}_N)} P(\mathbf{s}) d\mathbf{r}_2 ... d\mathbf{r}'_N \overline{\rho}(\mathbf{r}) \pm \sim 1/\sqrt{N_\Omega}$$

$$\left|\Psi(\mathbf{r}_{1},\mathbf{r}_{2},...\mathbf{r}_{N})\right|^{2} = \overline{P(\mathbf{r}_{2}..\mathbf{r}_{N})}\overline{\rho}(\mathbf{r}_{1})\pm \sim 1/\sqrt{N_{\Omega}}$$
$$= \overline{P(\mathbf{r}_{1},\mathbf{r}_{3}..\mathbf{r}_{N})}\overline{\rho}(\mathbf{r}_{2})\pm \sim 1/\sqrt{N_{\Omega}}$$
$$= \overline{P(\mathbf{r}_{1},\mathbf{r}_{2},\mathbf{r}_{4}..\mathbf{r}_{N})}\overline{\rho}(\mathbf{r}_{3})\pm \sim 1/\sqrt{N_{\Omega}}$$

. .

$$\overline{\left|\Psi(\mathbf{r}_{1},\mathbf{r}_{2},...\mathbf{r}_{N})\right|^{2}}\cong\prod_{n=1}^{N}\overline{\rho}(\mathbf{r}_{n})$$

Provided only properties which are averages over regions of space containing N_Ω particles are considered $|\Psi|^2$ factorizes to ~1/ $\sqrt{N_\Omega}$

Schrödinger Equation (Phys Rev A 78 33618 2008)

$$\frac{\hbar^2}{2m} \frac{\partial^2 \eta(\mathbf{r_n})}{\partial \mathbf{r_n}^2} + \left[V_{eff}(\mathbf{r_n}) + \Xi(\mathbf{r_n}) \right] \eta(\mathbf{r_n}) \cong \varepsilon \eta(\mathbf{r_n})$$
$$\left| \eta(\mathbf{r}) \right|^2 = \overline{\rho}(\mathbf{r}) \qquad V_{eff}(\mathbf{r}) = \varepsilon [\overline{\rho}(\mathbf{r})]$$

Weak interactions

$$\mathcal{E}[\rho(\mathbf{r})] = c\rho(\mathbf{r}) = c |\eta(\mathbf{r})|^2$$
 Gross-Pitaevski Equation

 η (**r**) is macroscopic function. Hence MSPQB.

Quantised vortices, NCRI, macroscopic density oscillations.

Depends only upon

(a) $\psi_{s}(\mathbf{r})$ is delocalized function of \mathbf{r} – must be so if BEC is present

(b) $\psi_{s}(\mathbf{r})$ has random structure over macroscopic length scales – liquids and gases.

NOT TRUE IN ABSENCE OF BEC, WHEN $\psi_{s}(\mathbf{r})$ IS LOCALIZED

Summary T=0

BEC implies $\psi_s(\mathbf{r})$ is delocalized function of \mathbf{r} non-zero over macroscopic length scales

Delocalization implies integrals of functionals of $\psi_s(\mathbf{r})$ over volumes containing N_{Ω} atoms are the same for all **s** to within ~1/ \sqrt{N}_{Ω}

Hence BEC implies MSPQB
Finite T

At T=0 only ground state is occupied.

Unique wave function $\Psi_0(r_1, r_2...r_N)$

At Finite T many occupied N particle states

Measured properties are average over occupied states

$$U(T) = \sum_{i} B_{i}(T)E_{i}$$
$$B_{i}(T) \propto \exp(-E_{i}/T)$$
$$E_{i} = \int \Psi_{i}^{*}(\mathbf{r}_{1}, \mathbf{r}_{2}...\mathbf{r}_{N})\hat{H}\Psi_{i}(\mathbf{r}_{1}, \mathbf{r}_{2}...\mathbf{r}_{N})d\mathbf{r}_{1}d\mathbf{r}_{2}...d\mathbf{r}_{N}$$

Consider one such "typical" occupied state with wave function $\Psi(r,s)$



Typical occupied state $\Psi(r,s)$ must change from localised to delocalised function as T is reduced below T_{B.}









Delocalized

Localized

 $\Psi(\mathbf{s},\mathbf{r}) = \alpha(T)\Psi_D(\mathbf{s},\mathbf{r}) + \beta(T)\Psi_L(\mathbf{s},\mathbf{r})$

α(T) =1 at T=0

 $\alpha(T) = 0$ at $T=T_B$

$$\psi_{\mathbf{S}}(\mathbf{r}) = a_{\mathbf{S}}(T)\psi_{D\mathbf{S}}(\mathbf{r}) + b_{\mathbf{S}}(T)\psi_{L\mathbf{S}}(\mathbf{r})$$

$$\Psi_D(\mathbf{s},\mathbf{r}) = \Psi_0(\mathbf{s},\mathbf{r}) \longrightarrow \Psi_{DS}(\mathbf{r}) = \Psi_{0S}(\mathbf{r})$$

$$\int \left| \psi_{\mathbf{S}}(\mathbf{r}) \right|^2 d\mathbf{r} = \int \left| \psi_{D\mathbf{S}}(\mathbf{r}) \right|^2 d\mathbf{r} = \int \left| \psi_{L\mathbf{S}}(\mathbf{r}) \right|^2 d\mathbf{r} = 1$$

 $T \to 0 \quad a_{\mathbf{s}}(T) \to 1 \qquad T \to T_{B} \quad a_{\mathbf{s}}(T) \to 0$





$$\int_{\Omega(\mathbf{r})} \left| \psi_{\mathbf{S}}(\mathbf{r}') \right|^2 d\mathbf{r}' = \left| a_{\mathbf{S}} \right|^2 \int_{\Omega(\mathbf{r})} \left| \psi_{D\mathbf{S}}(\mathbf{r}') \right|^2 d\mathbf{r}' + \left| b_{\mathbf{S}} \right|^2 \int_{\Omega(\mathbf{r})} \left| \psi_{L\mathbf{S}}(\mathbf{r}') \right|^2 d\mathbf{r}' + CT$$

$$CT = a_{\mathbf{S}}^{*} b_{\mathbf{S}} \int_{\Omega(\mathbf{r})} \psi_{D\mathbf{S}}^{*}(\mathbf{r}') \psi_{L\mathbf{S}}(\mathbf{r}') d\mathbf{r}' + CC$$

$$\psi_{LS}(\mathbf{r})$$
 Localised within $\Omega(\mathbf{r}) \frac{CT}{\int_{\Omega(\mathbf{r})} |\psi_{LS}(\mathbf{r}')|^2 d\mathbf{r}'} \sim \frac{1}{\sqrt{N}}$

 $\psi_{LS}(\mathbf{r})$ Localised outside $\Omega(\mathbf{r})$ CT=0

Contribution of CT is at most ~1/ \sqrt{N}

Two fluid behaviour

$$\rho(\mathbf{r}) = N \int \left| \psi_{\mathbf{s}}(\mathbf{r}) \right|^2 P(\mathbf{s}) d\mathbf{s}$$

$$\overline{\rho}(\mathbf{r}) = \frac{1}{\Omega} \int_{\Omega(\mathbf{r})} \rho(\mathbf{r}') d\mathbf{r}'$$

$$\overline{\rho}(\mathbf{r}) = \overline{\rho}_D(\mathbf{r}) + \overline{\rho}_L(\mathbf{r}) \pm \sim 1/\sqrt{N}$$

$$\mathbf{F}(\mathbf{r}) = \int P(\mathbf{s}) \frac{\hbar}{m} |\psi_{\mathbf{s}}(\mathbf{r})|^2 \nabla \theta_{\mathbf{s}}(\mathbf{r}) d\mathbf{s}$$

Fluid
$$\overline{\mathbf{F}}(\mathbf{r}) = \overline{\mathbf{F}}_D(\mathbf{r}) + \overline{\mathbf{F}}_L(\mathbf{r}) \pm \sim 1/\sqrt{N}$$

Fluid
flow

Flow of delocalised component is quantised

No such requirement for flow of localised component

Localised component is superfluid

Delocalized component is normal fluid

$\Psi(\mathbf{s}, \mathbf{r}) = \alpha(T)\Psi_D(\mathbf{s}, \mathbf{r}) + \beta(T)\Psi_L(\mathbf{s}, \mathbf{r})$ \downarrow $\bar{\rho}(\mathbf{r}) = \left|\alpha(T)\right|^2 \bar{\rho}_D(\mathbf{r}) + \left|\beta(T)\right|^2 \bar{\rho}_L(\mathbf{r}) \pm \sim 1/\sqrt{N}$

$$\left|\alpha(T)\right|^2 = \rho_s(T)$$

 $\left|\beta(T)\right|^2 = \rho_N(T)$

Superfluid fraction

Normal fluid fraction

 $S(q,\omega)=S_D(q,\omega)+S_L(q,\omega)$ $S(q)=S_D(q)+S_L(q)$

n(p)=n_D(p)+n_L (p)

 $E=E_D + E_L$

overlap between $\,\Psi_{\rm D}$ and $\Psi_{\rm L}$ is ~1/ $\!\!\sqrt{N}$

in any integral of $\Psi(\mathbf{r}_1, \mathbf{r}_2...\mathbf{r}_N)$ over $(\mathbf{r}_1, \mathbf{r}_2...\mathbf{r}_N)$

More generally true that



$$\Psi_D(\mathbf{s},\mathbf{r}) = \Psi_0(\mathbf{s},\mathbf{r}) \longrightarrow f(T) = \rho_s(T)f(0)$$

J. Mayers P*hys. Rev. Lett.* **92** 135302 (2004)







 $S(\mathbf{q}) = \rho_{S} S_{0}(\mathbf{q}) + \rho_{N} S_{L}(\mathbf{q})$

More spaces give smaller pair correlations

As T increases, superfluid fraction increases, pair correlations reduce



$$\alpha(T) = \left\langle \frac{S_T(\vec{q}) - 1}{S_B(\vec{q}) - 1} \right\rangle$$

$$S(\mathbf{q}) = \rho_{S}S_{0}(\mathbf{q}) + \rho_{N}S_{L}(\mathbf{q})$$

$$\downarrow$$

$$\alpha(T) = 1 - \rho_{S}(T)[1 - \alpha(0)]$$

J. Mayers P*hys. Rev. Lett.* **92** 135302 (2004) V.F. Sears and E.C. Svensson, Phys. Rev. Lett. **43** 2009 (1979).



Lattice model

Fcc, bcc, sc all give same dependence on T as that observed

Only true if N/V and diameter d of He atoms is correct

Change in d by 10% is enough to destroy agreement

J. Mayers PRL **84** 314, (2000) PRB**64** 224521,(2001)

Seems unlikely that this is a coincidence

$$S(\mathbf{q},\omega) = \sum_{f} \left| A_{f}(\mathbf{q}) \right|^{2} \delta(\hbar\omega + E_{f} - E)$$

 $A_f(\mathbf{q}) = N \int \Psi^*(\mathbf{r}, \mathbf{s}) \exp(i\mathbf{q} \cdot \mathbf{r}) \Psi_f(\mathbf{r}, \mathbf{s}) d\mathbf{r} d\mathbf{s}$ Identical particles

$$\Psi(\mathbf{s},\mathbf{r}) = \alpha(T)\Psi_0(\mathbf{s},\mathbf{r}) + \beta(T)\Psi_L(\mathbf{s},\mathbf{r})$$

$$\downarrow$$

$$S(\mathbf{q},\omega) = \rho_S S_0(\mathbf{q},\omega) + \rho_N S_L(\mathbf{q},\omega)$$

Only S_0 contributes to sharp peaks



J. Phys Cond Matt (1994)

New prediction

$$\overline{\rho}(\mathbf{r}) = \rho_S \overline{\rho}_0(\mathbf{r}) + \rho_N \overline{\rho}_L(\mathbf{r})$$

 $\overline{
ho}_0({f r})$ Has density oscillations identical to gnd state

 $\overline{
ho}_L({f r})$ Has no density oscillations

Measure density oscillations close to gnd state

Measure superfluid fraction w_D before release of traps

Simple prediction of visibility of density oscillations

Summary

Most important physical properties of BE condensed systems can be understood quantitatively purely from the form of n(p)

Non classical rotational inertia – persistent flow

Quantised vortices

Interference fringes between overlapping condensates

Two fluid behaviour

Anomalous behaviour of S(q)

Anomalous behaviour of $S(q,\omega)$

Amomalous behaviour of density

Lecture 4.

What can we learn from a measurement

of the momentum distribution n(p).

Quantum fluids and solids Protons

Measurement of flow without viscosity in solid helium

E. Kim and M. H. W. Chan Science **305** 2004





Signs of superfluidity. The superfluid fraction $f_i(T)$ inferred from the data in (7) as interpreted by Eq. 1, as a function of temperature for different values of the maximum velocity of the walls. The pressure is 41 bars. [Adapted from (7)]

Measurement of the Kinetic Energy and Lattice Constant in hcp Solid Helium at Temperatures 0.07-0.4 K

M. A. Adams, J. Mayers, O. Kirichek, and R. B. E. Down









Measured hcp lattice spacings

Т (К)	(101)	(002)	(100)
0.115	2.759 (7)		3.1055 (300)
0.400	2.759 (7)		3.1055 (300)
0.150	2.758 (7)		3.1056 (300)
0.070	2.758 (7)		3.1055 (300)
0.075	2.758 (2)	2.934 (4)	3.131 (2)
0.075	2.757 (3)	2.940(3)	3.128 (2)

• No change in KE, no change in vacancy concentration through SS transition.

- Implies SS transition quite different to SF transition in liquid.
- Probably not BEC of atoms
- What is cause??

Kinetic Energy of He3



³He mean kinetic energy, E_{K} as a function of the molar volume: experimental values (solid circles), diffusion Monte- Carlo values (open circles). self-consistent phonon method (dashed line).

Measurements of protons

 $n(\mathbf{p})$ is the "diffraction pattern" of the wave function

$$n(\mathbf{p}) = \left| \int \psi(\mathbf{r}) \exp(i\mathbf{p}\cdot\mathbf{r}) d\mathbf{r} \right|^2$$



If $n(\mathbf{p})$ is known $\psi(\mathbf{r})$ can be reconstructed in a model independent way

In principle $\psi(\mathbf{r})$ contains all the information which can be known about the microscopic physical behaviour of protons on very short time scales.

Potential can also be reconstructed

$$E - V(\mathbf{r}) = \frac{\int e^{i\mathbf{p}\cdot\mathbf{r}} \frac{p^2}{2M} \widetilde{\psi}(\mathbf{p}) d\mathbf{p}}{\int e^{i\mathbf{p}\cdot\mathbf{r}} \widetilde{\psi}(\mathbf{p}) d\mathbf{p}}$$

$$\widetilde{\psi}(\mathbf{p}) = \int \psi(\mathbf{r}) e^{i\mathbf{p}\cdot\mathbf{r}} d\mathbf{r}$$

VESUVIO Measurements on Liquid H₂

J Mavers (PRL **71** 1553 (1993)





$$n(\vec{p}) = \left| \int \psi(\vec{r}) \exp(i\vec{p}.\vec{r}) d\vec{r} \right|^2$$

$$\psi(\vec{r}) = C \exp\left[\frac{-(r-R)^2}{2\sigma^2}\right]$$

$$n(\vec{p}) = \left| \int \psi(\vec{r}) \exp(i\vec{p}.\vec{r}) d\vec{r} \right|^2$$



Puzzle

Fit to data gives R=0.36 σ =5.70

Spectroscopy gives R=0.37 σ =5.58

PHYSICAL REVIEW B

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Deep inelastic neutron scattering from fluid hydrogen and deuterium: From vibrational excitations to the impulse approximation

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QM predicts R=bond length not ½ bond length

R should be 0.74!



Red data H₂ 1991 Black YAP 2008

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Single crystals


Reconstruction of Momentum Distribution from Neutron Compton Profile



Direct Observation of Tunneling in KDP using Neutron Compton Scattering G. F. Reiter

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KDP Potential and Wavefunction



Measurement of the 3D Born-Oppenheimer Potential of a Proton in a Hydrogen-Bonded System via Deep Inelastic Neutron Scattering: The Superprotonic Conductor Rb₃H(SO₄)₂

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FIG. 1 (color online). Proton momentum distribution for $Rb_3H(SO_4)_2$ at 10 K: (a) along the x-axis (solid line), y-axis (dashed line), and z-axis (dotted line), the rms errors are shown in dashed lines, (b) in the yz plane.



Nafion



Proton Coherence in Nafion and Dow 858

Excess of Proton Mean Kinetic Energy in Supercooled Water

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Proton Momentum Distribution of Liquid Water from Room Temperature to the Supercritical Phase

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Proton Momentum Distribution in a Protein Hydration Shell

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Changes in the zero point energy of the protons as the source of the binding energy of water to A phase DNA

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Measurements of n(p) give unique information on the quantum behaviour of protons in a wide range of systems of fundamental importance