Scattering

Feb 25, 2009

Goal

* Neutron Scattering + sum rules = single particle spectrum

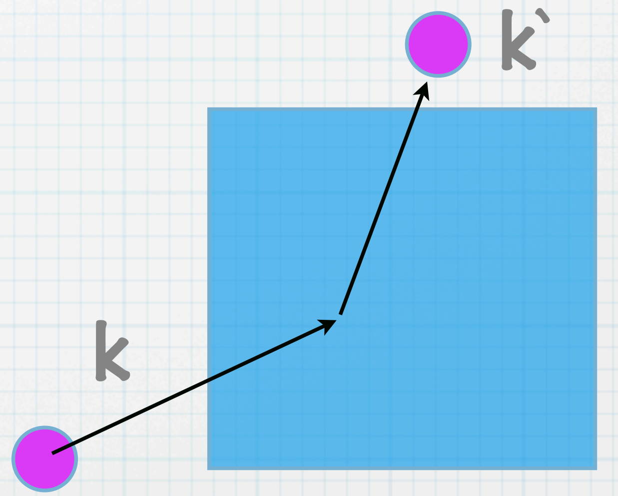
Neutron Scattering in Helium

"fast" neutrons: atoms do not have time to move

Neutron sees potential:

$$V(r) = \int dr' U(r - r') \rho(r')$$

$$V_k = U_k \rho_{-k}$$



Fermi's Golden Rule:

$$\Gamma_{k \to k'} = 2\pi |U_q|^2 \langle \rho_q \rho_{-q} \rangle \delta(\omega)$$

$$q = k' - k$$

$$\omega = \frac{k'^2}{2m} - \frac{k^2}{2m}$$

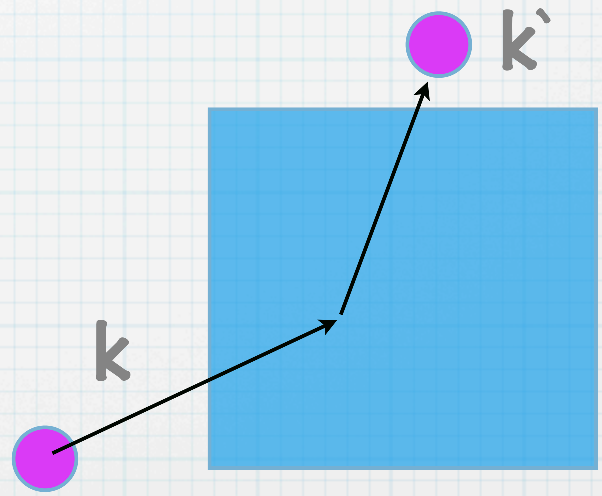
Neutron Scattering in Helium

Static Structure factor

$$S(q)$$

Fermi's Golden Rule:

$$\Gamma_{k \to k'} = 2\pi |U_q|^2 \langle \rho_q \rho_{-q} \rangle \delta(\omega)$$



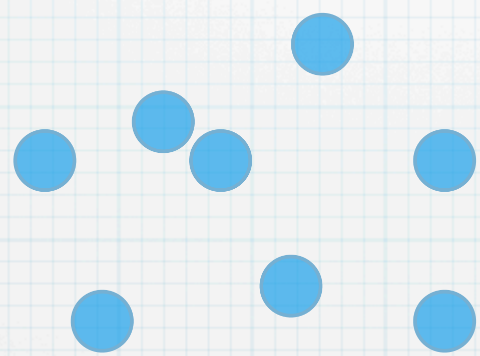
$$q = k' - k$$

$$\omega = \frac{k'^2}{2m} - \frac{k^2}{2m}$$

Helium

Bose Condensate:

Single particle spectrum = phonon spectrum



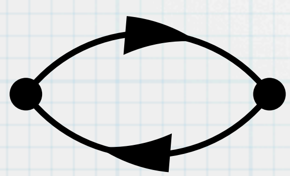
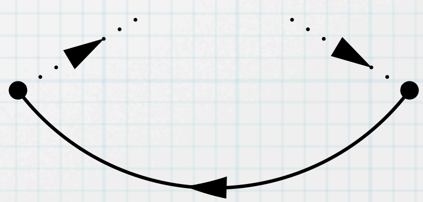
Only long wavelength redistribution of particles = phonons

Helium

Bose Condensate:

Single particle spectrum = phonon spectrum

More formally: single particle spectrum hybridized with phonon spectrum

 has overlap with 

Determining phonon spectrum determines single particle spectrum

Dynamic structure function

Density response function:

$$\chi^R(q,t) = \frac{\theta(t)}{i}\langle[\rho_q(t),\rho_{-q}(0)]\rangle$$

$$= \frac{\theta(t)}{i}\left[S(q,t) - S(-q,-t)\right]$$

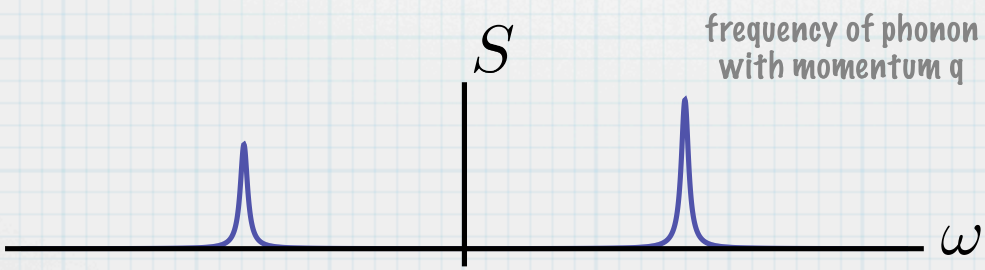
$$S(q) = S(q, t = 0)$$

Meaning of dynamic structure factor

$$S(q,\omega) = \frac{1}{V}\int d^3r \int d^3r' \int dt e^{-ik(r-r')+i\omega t}\langle \rho(r,t)\rho(r',0)\rangle$$

Measures density fluctuations at frequency omega and wave vector q

Detailed Balance: $S(q,\omega) = e^{\beta\omega} S(q,-\omega)$

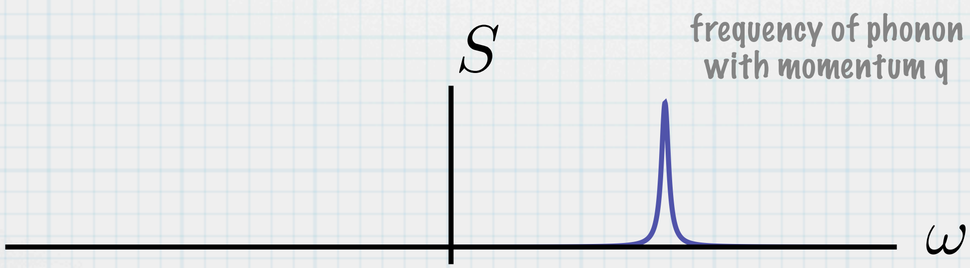


Zero T

$$S(q,\omega) = \frac{1}{V}\int d^3r \int d^3r' \int dt e^{-ik(r-r')+i\omega t}\langle \rho(r,t)\rho(r',0)\rangle$$

Measures density fluctuations at frequency omega and wave vector q

Detailed Balance: $S(q,\omega) = e^{\beta\omega} S(q,-\omega)$



Sum Rules

$$2\mathrm{Im}\chi^R(q,\omega) = S(q,\omega) - S(-q,-\omega)$$

Zero T

$$2\mathrm{Im}\chi \approx 2\pi A_k \left[\delta(\omega-\omega_k) - \delta(\omega+\omega_k)\right]$$

$$\int_0^\infty 2\mathrm{Im}\chi \frac{d\omega}{2\pi} = \int_{-\infty}^{\infty} S(k,\omega)\frac{d\omega}{2\pi} = S(k)$$

$$\int_{-\infty}^{\infty} i\omega\, 2\mathrm{Im}\chi\, \frac{d\omega}{2\pi} \approx 2i\omega_k S(k) \quad = \langle[\dot\rho_k, \rho_{-k}]\rangle$$

f-sum rule

$$\rho_k = \sum_q \psi^\dagger_{k+q}\psi_q$$

$$\dot{\rho}_k = \frac{1}{i}\sum_q \left(\frac{q^2}{2m} - \frac{(k+q)^2}{2m}\right)\psi^\dagger_{k+q}\psi_q$$

$$[\dot{\rho}_k, \rho_{-k}] = i\frac{k^2}{m}N$$

$$\omega_k = \frac{Nk^2}{2mS_k}$$

[S often defined with a factor of V -- since it is extensive]

THE

PHYSICAL REVIEW

A journal of experimental and theoretical physics established by E. L. Nichols in 1893

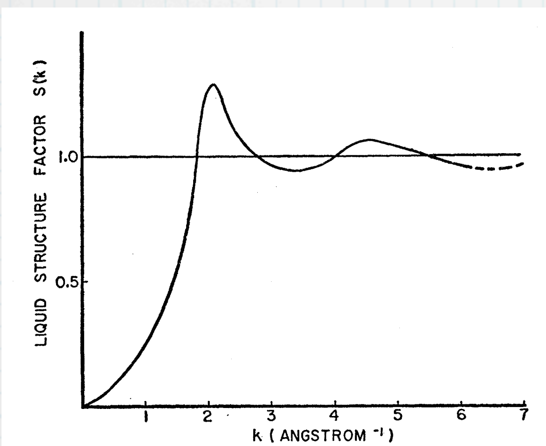
SECOND SERIES, VOL. 102, NO. 5 — JUNE 1, 1956

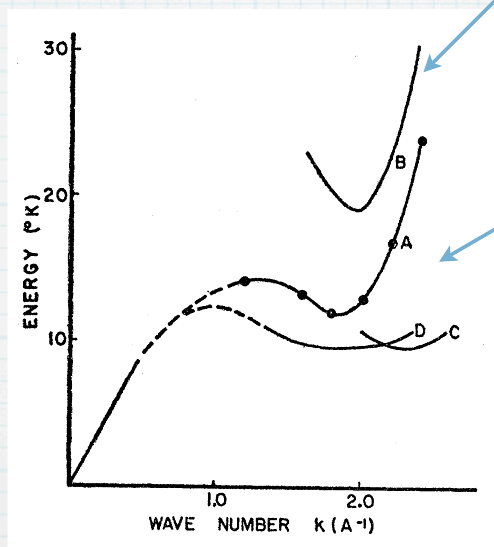
Energy Spectrum of the Excitations in Liquid Helium*

R. P. FEYNMAN AND MICHAEL COHEN
California Institute of Technology, Pasadena, California

(Received February 27, 1956)

Result



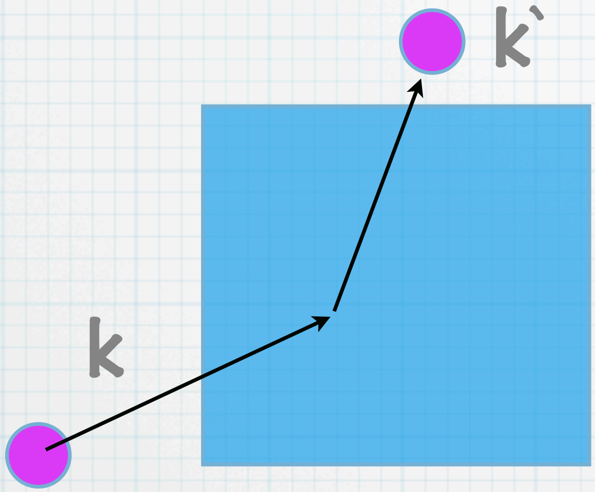


This theory

Better theories

Limited Accuracy: Spectral function has more structure

Inelastic Neutron Scattering



Neutron sees potential:

$$V(r) = \int dr' U(r - r')\rho(r')$$

$$V_k = U_k \rho_{-k}$$

Fermi's Golden Rule:

$$\Gamma_{k \to k'} = |U_q|^2 \sum_f | < f|\rho_{-q}|i\rangle|^2 2\pi\delta(\omega - (E_f - E_i))$$

$$= |U_q|^2 S(q, \omega)$$

$$q = k' - k$$

$$\omega = \frac{k'^2}{2m} - \frac{k^2}{2m}$$

Fluctuation-Dissipation Theorem

$$2\mathrm{Im}\chi^R(q,\omega) = S(q,\omega) - S(-q,-\omega)$$

Dissipation

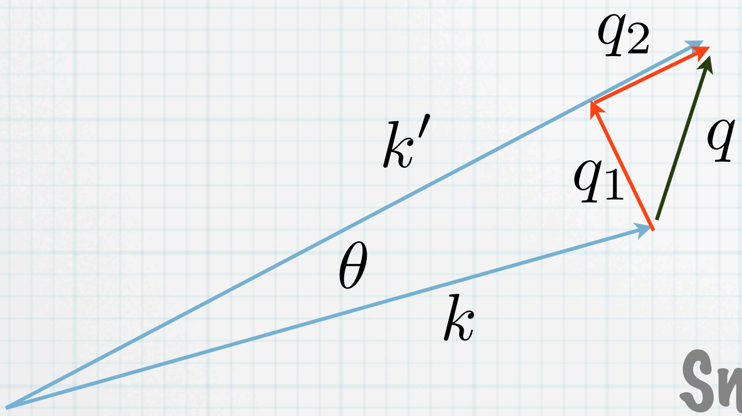
Energy out

Energy in

Collective Mode

Scattering expt

Recovering Static Limit



$$\mathbf{q} = \mathbf{k}' - \mathbf{k}$$

$$\omega = \frac{k'^2}{2m} - \frac{k^2}{2m}$$

Small angles:

$$q_1 \approx k\theta \qquad \omega \approx \frac{kq_2}{m}$$

$$\Gamma_{k\to k'} = |U_q|^2 \sum_f \underline{|<f|\rho_{-q}|i\rangle|^2 2\pi\delta(\omega - (E_f - E_i))}$$

zero unless $\omega \sim cq$

$$q = k\theta\sqrt{1 + \left(\frac{m\omega}{k^2\theta}\right)^2} \approx k\theta\left(1 + \mathcal{O}(c/v)^2\right)$$

Recovering Static Limit

$$\Gamma_{k\to k'} = |U_q|^2 \sum_f |<f|\rho_{-q}|i\rangle|^2 2\pi\delta(\omega - (E_f - E_i))$$

$$q \approx k\theta$$

Integrating over all momentum transfers and energies reduces to

$$\Gamma_\theta \approx \int d\omega\Gamma \longrightarrow S(q)$$