SYMMETRISED DYNAMICAL STRUCTURE FACTOR
AND WELL'S DATA

FROM WELL'S THESIS

(1)
$$\underbrace{S(k,\omega)}_{\substack{\text{SYSTEM}\\ \text{ABSORB}\\ \text{ENERGY}\\ \text{= NEUTRONS}\\ \text{LOSES}\\ \text{ENERGY}}} = e^{\beta\hbar\omega}\,\underbrace{S(k,-\omega)}_{\substack{\text{SYSTEM GIVES}\\ \text{AWAY ENERGY}\\ \text{TO NEUTRONS}}}$$

WELL DEFINE

(2)
$$\tilde{S}(k,\omega) = \exp\left[-\frac{1}{2}\beta\hbar\omega + \underbrace{\frac{\hbar^2 k^2 \beta}{2M}}_{\substack{\text{ROBERT SAY WE}\\ \text{CAN IGNORE THIS ONE}}}\right] S(k,\omega)$$

so

$$= e^{-\frac{1}{2}\beta\hbar\omega}\, S(k,\omega)$$

LIKEWISE SETTING $\omega = -\omega$ IN ABOVE FORMULA WE HAVE

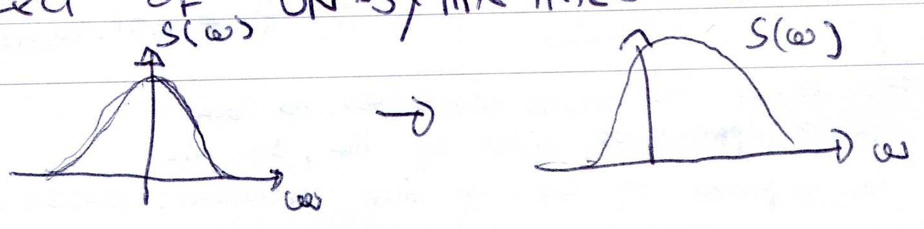
(3)
$$\tilde{S}(k,-\omega) = e^{\frac{1}{2}\beta\hbar\omega}\, S(k,-\omega)$$

INSERTING (2) AND (3) INTO (1) GIVES

$$\cancel{e^{\frac{1}{2}\beta\hbar\omega}}\,\tilde{S}(k,\omega) = \cancel{e^{\frac{1}{2}\beta\hbar\omega}}\,\tilde{S}(k,-\omega)$$

SO IF WE PLOT $\tilde{S}$ ABOUT $\omega = 0$ WE SHOULD SEE THAT IT IS SYMMETRIC!

NOTE THE EFFECT OF UN-SYMMETRIES WOULD BE SOMETHING LIKE



WELL'S DATA GO OUT TO ABOUT

$$\omega = 2 \times 10^{13}\,s^{-1} \xrightarrow{\text{TRANSLATES TO}} 13\,meV$$

AT $T = 120K$ WE HAVE

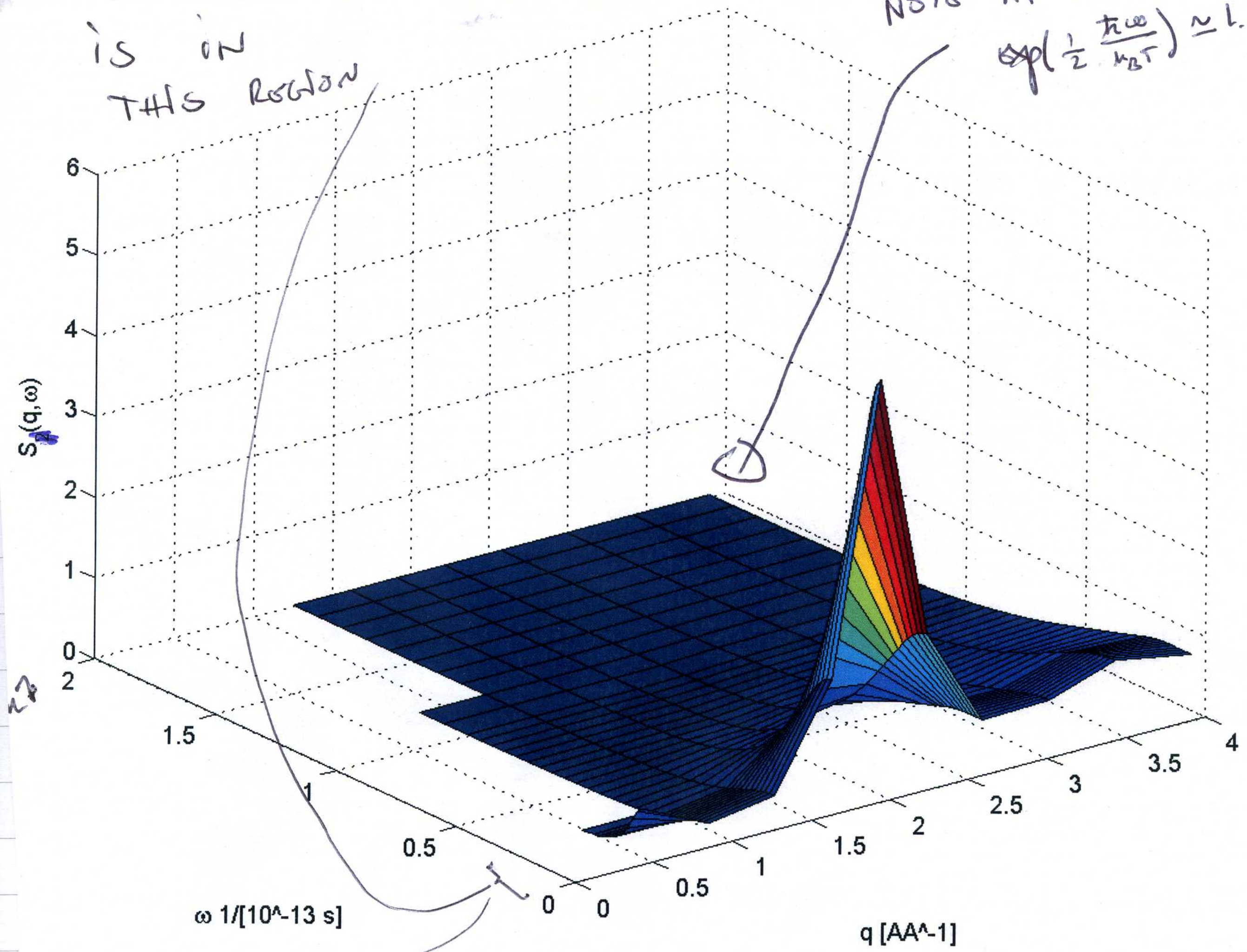
$$k_B \approx \frac{1}{11\,604.505}\ \frac{eV}{K}$$ < GOT FROM WIKIPEDIA ELECTRONVOLT

$\therefore$

$$\frac{1}{\beta} = k_B T \overset{T=120K}{=} 10.3408\ meV$$

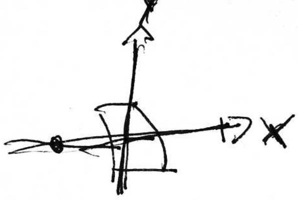
SO IF WE LOOK AT WELL'S, THEN MOST OF THE ACTION IS IN THIS REGION

NOTE AT $\omega = 2$ $\exp\left(\frac{1}{2}\frac{\hbar\omega}{k_B T}\right) \simeq 1.89$



i.e. $0 \to 2.5\,meV$ HENCE WE CAN CONCLUDE $\tilde{S}$ AND S WILL NOT LOOK TOO DIFFERENT.

FROM
A.A. VAN WELL'S THESIS
ON LIQUID AR



wavelengths of the incident and scattered neutrons (λ_f is proportional to the TOF of the neutron from the sample to the detector), $\hbar$ Planck's constant divided by 2π, m the mass of the neutron, σ_b the bound atom cross section; $\mathbf{k}$ and ω are the momentum and energy transfers in units of $\hbar$:

$$\mathbf{k} = \mathbf{k}_0 - \mathbf{k}_f , \quad \omega = (E_0 - E_f)/\hbar \ . \tag{3}$$

Here $E_i = \hbar^2 k_i^2/2m$ $(i = 0,f)$ is the energy of the neutron with momentum $\hbar\mathbf{k}_i$, and $k_i = |\mathbf{k}_i| = 2\pi/\lambda_i$.

S(k,ω) satisfies the detailed balance condition

$$S(k,\omega) = e^{\beta\hbar\omega} S(k,-\omega) \ , \tag{4}$$

with $\beta = 1/k_BT$, k_B being Boltzmann's constant.

Since liquid argon can in first approximation be considered a classical system, we will present most of our results in the form of the symmetrized dynamic structure factor

$$\tilde{S}(k,\omega) = \exp\left[-\tfrac{1}{2}\beta\hbar\omega + \frac{\hbar^2k^2\beta}{8M} \right] S(k,\omega) \ , \tag{5}$$

with M the mass of one particle of the system. Eq.(5) gives a quasi-classical approximation of $S(k,\omega)$[14] that is exact for an ideal gas.

We will also consider the longitudinal current correlation function $C_\ell(k,t)$, defined by

$$C_\ell(k,t) = -\frac{1}{k^2} \frac{d^2}{dt^2} F(k,t) \ , \tag{6}$$

and its frequency spectrum

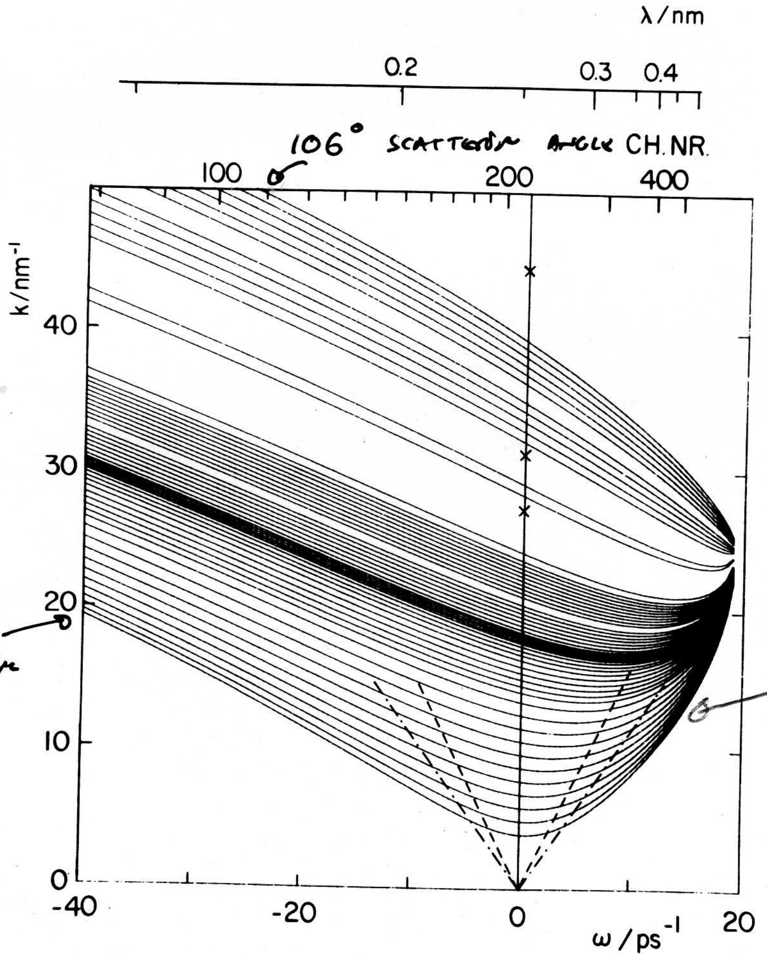
$$C_\ell(k,\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt\, e^{-i\omega t} C_\ell(k,t) = \frac{\omega^2}{k^2} S(k,\omega) \ . \tag{7}$$

FOR THE MDMC CODE
BETTER TO USE S
THAN $\tilde{S}$

WHERE TO EXPECT TO SEE SCATTERING IN Q AND ω SPACE

FROM A.A. VAN WELL AR THESIS

The TOF resolution (for ω=0) of the spectrometer was determined from the elastic scattering of a vanadium sample (see Secs.III.B.2 and IV.C). The relative TOF resolution measured at the detectors (FWHM), Δt/t, varied from 2.7 % to 3.8 %. This resulted in an absolute frequency resolution, Δω, as shown in Fig.1(b).



9° SCATTERING ANGLE

SINGLE CURVE DETERMINED BY

$Q^2 = k_0^2 + k_f^2 - 2k_0 k_f \cos\theta$

$\hbar\omega = E_0 - E_f = \frac{\hbar^2 k_0^2}{2m} - \frac{\hbar^2 k_f^2}{2m}$

INCOMING NEUTRON LOSS ENERGY

Fig.2. The kinematic region for the experiment. TOF channel numbers, scattered neutron wavelengths, and frequency transfers, are indicated. Crosses represent the aluminium Bragg peaks. The dashed and dashed-dotted lines are the sound "dispersion" curves, $\omega_s = c_s k$, for measurements a and d respectively.

SCAT. ANGLE

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