INFORMAL REPORT**MASTER**FOURIER TRANSFORM OF INELASTIC NEUTRON SCATTERED INTENSITY
FOR SOLID $^4\text{He}^\dagger$

by

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I. Introduction

In recent years solid helium has received a great deal of attention in the physics community. This is because, among other things, the lattice dynamics of solid helium provides a testing ground for quantum statistical mechanics. Solid helium is a quantum crystal, that is a crystal in which the motion of the atoms even when the temperature is reduced toward absolute zero remains large compared with the interatomic spacing. Helium is the most extreme example of the quantum solids because of its very light atomic mass and the very weak Van der Waals interatomic forces. Yet these forces are well understood and theoretical calculations can be made with no adjustable parameters. The agreement of experiment and these calculations can thereby be used to judge the principles of the calculation.

In this experiment we use the inelastic scattering of neutrons to find out more about solid helium. We use Fourier transform to determine the probability density of the helium atoms.

II. Inelastic Scattering of Neutrons from Solid ^4He

The method of inelastic neutron scattering is, perhaps, the only way of determining all of the information about the lattice dynamics of solid. In the following discussion we will use the jargon of the physicist. A "phonon" means one of the normal modes of vibration for the collection of atoms in the system. Thus each type of phonon, like the modes of vibration, has a characteristic energy and a characteristic wavelength associated with it. The lattice dynamics of the crystal is completely determined when we know the relationship between the energy and the wavelength of each kind of phonon; this relation is known as the "dispersion relation". The physicist consider these phonons as particles, or more accurately quasiparticles, in his sample and uses the momentum rather than the wavelength (they are related to one another through the quantum mechanical expression, $\hbar q = h/\lambda$ where $\hbar q$ is the momentum, q is referred to as the wave vector, and λ is the wavelength and h is Planck's constant, and $\hbar$ is $h/2\pi$).

To determine the relation of the phonon energies to their momentum by inelastic neutron scattering the experimentalist prepares a neutron with a given momentum and directs it to his sample. This can be done by using Bragg scattering. In this type of scattering the neutron is deflected from a set of atomic planes with a known spacing d_0 through a known angle 2θ as shown in the diagram below. Bragg's Law then tells us that the neutrons reflected have a wavelength of λ where

$$\lambda = \frac{2d_0 \sin \theta}{m}$$

$$m = 1, 2, 3, \dots$$

Thus the direction of the scattered neutron is determined and its momentum is known to be equal to

$$\hbar q = \hbar 2\pi/\lambda = \hbar/x$$

and, since the neutron is a free particle its energy is only its kinetic energy,

$$E_k = \hbar^2 q^2 / 2m_n$$

where m_n is the mass of the neutron equal to $(1.67474 \pm 0.00010) \times 10^{-24}$ gm.

When these neutron impinge on the sample the neutrons scattered through a particular angle are collected and these scattered neutrons are analyzed for their energy by again using a Bragg reflection as described above. In Diagram 2 the complete path of the neutron is schematically shown. Now we can see why the quasiparticle concept of the phonons is useful. It is because there are conservation of momentum and conservation of energy relations for the phonon and the neutron in which the phonon can be considered to be particle like. These relationships are

$$Q = q_i - q_f$$

$$\hbar\omega(Q) = E_{k_i} - E_{k_f} = \hbar^2 (q_i^2 - q_f^2) / 2m_n$$

Now because the experimental apparatus (called a three crystal spectrometer because the neutron scatters from three crystals) is computer controlled, the angles θ_1 , θ_2 and θ_3 can be adjusted such that the Q is held constant. In this "constant Q mode" the intensity of the neutrons can be plotted as a function of that energy and, with some corrections, this is the experimental

determination of the "dynamic response function" $S_p(Q, W)$ of the system under study. An example of such experimental data is shown in Diagram 3.

III. Sum-rules for Inelastic Neutron Scattering from Solids

The scattered intensity as measured on the three crystal spectrometer operated in the constant-Q mode, the mode used in the experiments in question, is proportional to the so-called "scattering law", $S(Q, w)$. There are some general properties of the scattering law that are completely independent of the nature of the properties, the dynamical or the structural, of the scattering sample. One of these is the first-moment sum-rule originally due to Placzek.⁽¹⁾

$$(2\pi)^{-1} \int_0^\infty d\omega \omega S(Q, \omega) = Q^2 / 2M$$

$M = \text{atomic mass}$

Ambegaokar, Conway, and Baym² have shown that the part of the total scattering law $S(Q, w)$ that is due to one-phonon scattering $S_1(Q, w)$, also obeys a similar first moment sum-rule. It is

$$(2\pi)^{-1} \int_0^\infty d\omega \omega S_1(Q, \omega) = (Q^2 / 2M) e^{-2W(Q)}$$

where e^{-2W} is the familiar Debye-Waller factor encountered in X-ray Bragg scattering, and discussed in more detail below. This last equation allows us to determine the effective Debye-Waller factor by integrating the experimental

Diagram

$Q^2 [A^{21}]$

8

10

12

1000

2

4

8

10

12

bec He^4

21100 cm/mole

2

Δ 5145

Δ 5145

Δ 5147

Δ 5205B

1000

Δ 5147

Δ 5147

Δ 5201A

5147 5149

5201A 5201C

5201A 5201C

Δ 5205C

5205F 5205B

5208

10

5205B

5205B

5205C

5205B

5202B

5202E

5205A

$\frac{1}{(0.5)^2}$

4

$$Q^2[A^{22}]_6$$

8

10

12

14

$$\text{bcc He}^4$$
 $21.09 \text{ cm}^3/\text{mole}$

2

data as indicated. For solid He we will find that W will not be simply proportional to Q^2 as it is in classical solids but will be of a more complicated form.

IV. The Debye-Waller

The Debye-Waller factor is defined quantum mechanically as

$$e^{-2W(Q)} = |\langle i | e^{-iQ \cdot r} | i \rangle|^2 = \left| \int \psi^* e^{-iQ \cdot r} \psi dr \right|^2 \quad (1)$$

since

$$\begin{aligned} \psi^*(r) \psi(r) &= \text{probability of finding the particle at point } r, \\ &\quad \text{the probability density} \\ &= p(r) \end{aligned}$$

we will use the semi-classical expression

$$\left[e^{-2W(Q)} \right]^{\frac{1}{2}} = e^{-W(Q)} = \int p(r) e^{-iQ \cdot r} dr \quad (2)$$

in the remainder of this work. Note that this expression relates the atomic (actually the nuclear) probability density to $e^{-W(Q)}$ through the three dimensional Fourier transform.

For most materials the atomic motion is "harmonic" and leads to

$$W(Q) = B(Q/4\pi)^2 \quad (3)$$

where B is a constant. In order to obtain some understanding of the more complicated case for Helium this simpler calculation will be reviewed here.

The Harmonic Potential

From elementary mechanics we have known that the acceleration of an object of mass m is equal to the applied force on the object divided by m . Let us consider an object of mass m attached to a spring such that the force is proportional to the displacement of the object from the origin. If we constrain the motion of the object to the x direction we have

$$F = ma = m \frac{d^2x}{dt^2} = -Kx \quad (4)$$

Now we can demonstrate that such a system will have simple harmonic motion (5), that is

$$x = A \sin (wt).$$

By direct substitution we have

$$x = A \sin wt,$$

$$\frac{dx}{dt} = (A \cos wt) w,$$

$$\frac{d^2x}{dt^2} = A \sin wt \ w^2.$$

Going back to equation (1) we get

$$-A \sin wt (mw^2) = -K A \sin wt,$$

or

$$w^2 = \frac{K}{m}$$

We can understand the motion of this object by considering the energy relationships. Since we have not accounted for any dissipation the total energy E will be conserved. Thus $E = K.E. + P.E.$ where $K.E.$ is the kinetic energy and $P.E.$ is the potential energy which is

$$P.E. = - \int_0^x E \, dx = \frac{K}{2} x^2$$

Therefore

$$E_0 = \text{K.E.} + \text{P.E.}$$

$$= \frac{m}{2} \dot{x}^2 + \frac{K}{2} x^2$$

$$= \frac{m}{2} \omega^2 A^2 \cos^2 \omega t + \frac{K}{2} A^2 \sin^2 \omega t$$

$$= \frac{K}{2} A^2 = \frac{m\omega^2}{2} A^2$$

As in any classical system we can always tell what the potential and kinetic energy is by measuring where the particle is

Now we can determine the probability of finding the particle at point x at some arbitrary time, $p(x)$. It is just

$$p(y) dy = p(y(x)) \left| \frac{dx}{dy} \right| dx$$

$$x = A \sin y$$

$$p(y) = K$$

$$\left[\frac{K}{\pi \sqrt{1-x^2/A^2}} \right] dx = \frac{K}{A \cos x}$$

$$\begin{aligned} \int_{-A}^A p(x) dx &= 1 \\ 1 &= \int_{-A}^A \frac{K dx}{A \sqrt{1-x^2/A^2}} = \frac{K}{A} \left(\sin^{-1} \frac{x}{A} \right) \Big|_{-A}^A \\ &= K \pi / A \\ \therefore p(x) &= \frac{1}{\pi \sqrt{1-x^2/A^2}} \end{aligned}$$

The following diagram shows what is expected, the particle spends most of its time near the limits of its travel, $x = \pm A$.

In Quantum Mechanics the problem is more difficult. Because of the uncertainty principle the particle can not be localized as in the classical example. In fact one finds that the particle has a finite probability of being found at the point where its P.E. is greater than its total energy! One finds for the three dimensional harmonic potential

$$V(r) = Kr^2$$

the probability of finding the particle at r is

$$p(r) = \frac{1}{[2\pi\langle r^2 \rangle]^{3/2}} e^{-r^2/2\langle r^2 \rangle}$$

in its lowest energy state, the zero-point state, where $\langle r^2 \rangle$ is the mean-square-displacement. Thus $p(r)$ is

which is quite different from the classical $p(x)$ illustrated above.

$$\frac{1}{2} = e^{-r^2/2\langle r^2 \rangle}$$

$$\ln 2 = r^2/2\langle r^2 \rangle$$

$$r = \pm \sqrt{2 \ln 2} \langle r^2 \rangle^{1/2}$$

V. Fourier Transform

Shown below are a few useful examples of the Fourier transforms that are commonly used by the physicist.

$$A/ \quad f(x) = e^{-\frac{(x-r_0)^2}{2\sigma^2}}$$

$$\begin{aligned} F(Q) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\left[\frac{(r-r_0)^2}{2\sigma^2} + iQr\right]} dr \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{2\sigma^2} [(r-r_0)^2 + 2i\sigma^2 Qr]} dr \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{2\sigma^2} [r^2 - 2rr_0 + r_0^2 + 2i\sigma^2 Qr]} dr \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{2\sigma^2} [r^2 - 2(r_0 - i\sigma^2 Q)r + r_0^2]} dr \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{2\sigma^2} \{[r - (r_0 - i\sigma^2 Q)]^2 + [r_0 - (r_0 - i\sigma^2 Q)]^2\}} dr \\ &= \frac{1}{\sqrt{2\pi}} \left(e^{-i r_0 Q - \frac{Q^2 \sigma^2}{2}} \right) \int_{-\infty}^{\infty} e^{-\frac{1}{2\sigma^2} [r - A]^2} dr \\ &= \frac{1}{\sqrt{2\pi}} e^{-\frac{Q^2 \sigma^2}{2}} e^{-i r_0 Q} \quad \frac{(\sqrt{2\sigma^2})}{\sqrt{2\pi}} \int e^{-u^2} du \quad A = r_0 - i\sigma^2 Q \\ &= \sqrt{2} \sigma^2 e^{-\frac{Q^2 \sigma^2}{2}} e^{-i r_0 Q} \end{aligned}$$

$$B/ \quad f(x) = \frac{1}{r^2 + (x-r_0)^2}$$

$$\begin{aligned}
 F(Q) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{r^2 + (r-r_0)^2} e^{-iQr} dr \\
 &= \frac{1}{\sqrt{2\pi}} \left[\int_{-\infty}^{\infty} \frac{\cos Qr}{r^2 + (r-r_0)^2} dr + i \int_{-\infty}^{\infty} \frac{\sin Qr}{r^2 + (r-r_0)^2} dr \right] \\
 &= \frac{1}{\sqrt{2\pi}} \left[\frac{\pi}{r} e^{-Qr} \cos(Qr) + \frac{\pi}{r} e^{-Qr} \sin(Qr) \right]
 \end{aligned}$$

C/ $f(x) = \delta(r-r_0)$

$$\begin{aligned}
 F(Q) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(r-r_0) e^{-iQr} dr \\
 &= \frac{1}{\sqrt{2\pi}} (e^{-iQr_0})
 \end{aligned}$$

D/ $f(x) = 1$

$$\begin{aligned}
 F(Q) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} 1 \cdot e^{-iQr} dr \\
 &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (\cos Qr - i \sin Qr) dr \\
 &= \frac{1}{\sqrt{2\pi}} \left[\int_{-\infty}^{\infty} \cos Qr dr - i \int_{-\infty}^{\infty} \sin Qr dr \right] \\
 &= \frac{1}{\sqrt{2\pi}} \left[\sin Qr \Big|_{-\infty}^{\infty} - i \cos Qr \Big|_{-\infty}^{\infty} \right] \\
 &= \sqrt{2\pi} \delta(Q)
 \end{aligned}$$

$$E/ \quad f(x) = \sin (px)$$

$$F(q) = \frac{1}{\sqrt{2\pi}} \int \sin (px) e^{-iqx} dx$$

$$= \frac{1}{2\sqrt{2\pi}} \int_{-\infty}^{\infty} [e^{-i(p-q)x} - e^{-i(p+q)x}] dx$$

$$= \frac{\sqrt{2\pi}}{2i} \frac{1}{2\pi} \int_{-\infty}^{\infty} [e^{i(p-q)x} - e^{-i(p+q)x}] dx$$

$$= \frac{\sqrt{2\pi}}{2i} [\delta(p-q) - \delta(p+q)]$$

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VI. Fourier Inversion of Experimental Data

As shown in the discussion above the Debye-Waller factor is associated with the Fourier transform of the probability function $p(r)$. For materials for which the harmonic potential is a good approximation - most all materials except solid helium - one knows that at low temperatures

$$p(r) = \frac{e^{-r^2/2\langle r^2 \rangle}}{[2\pi\langle r^2 \rangle]^{3/2}}$$

and as we have shown in the previous section

$$\begin{aligned} f(Q) &= \int p(r) e^{i\mathbf{Q} \cdot \mathbf{r}} d\mathbf{r} \\ &= e^{-\frac{\langle r^2 \rangle Q^2}{2}} \end{aligned}$$

For the case for helium the experiments have measured $f(Q)$ and we desire to calculate $p(r)$. If we assume that $p(r)$ is spherically symmetric though not necessarily Gaussian in shape then Eq. (1) becomes

$$\begin{aligned} f(Q) &= e^{-w}_{\text{eff}} = \int p(r) \cos(\mathbf{Q} \cdot \mathbf{r}) d\mathbf{r} \\ &= 2\pi \int_0^\pi \int_0^\pi p(r) \cos(|\mathbf{Q}||\mathbf{r}| \cos \theta) r^2 \sin \theta d\theta dr \end{aligned}$$

let $dx = -\sin \theta d\theta$

$$f(Q) = -2\pi \int_0^\pi \int_0^\pi \cos(Qrx) r^2 dx p(r)$$

let $y = Qrx$

$dy = Qrdx$

$$\begin{aligned} f(Q) &= 2\pi \int_0^\infty \int_{-Qr}^{Qr} \frac{\cos(y)}{Q} dy p(r) \\ &= 2\pi \int_0^\infty \frac{dr}{Q} [\sin(Qr) + \sin(+Qr)] p(r) \\ f(Q) &= 4\pi \int_0^\infty r^2 dr \frac{\sin(Qr)}{Qr} p(r) \end{aligned} \quad \text{DTF}$$

Now using the Fourier theorem we can invert this equation and obtain the probability density function from the experimental data.

$$Qf(Q) = 4\pi \int_0^\infty p(r)r \sin(Qr) dr$$

Multiplying both sides of the equation by $\sin(Qr')$ and integrating on Q we have

$$\begin{aligned} \int_0^\infty Qf(Q) \sin(Qr') dQ \\ &= 4\pi \int_0^\infty dr p(r)r \int_0^\infty \sin(Qr') \sin(Qr) dQ \\ &= 4\pi \int_0^\infty dr p(r)r \frac{1}{2\pi} \delta(r-r') \\ &= 2\pi^2 r' p(r') \end{aligned}$$

F10

VII. Computer Programs

Programs were written to do the calculations described in the equations DTF³ (Density To F-function Transform). The Fourier Transform was performed using the algorithm developed by Filon.⁴ The DTF routine also punches its out put in a form appropriate for input to FTD thus allowing a consistency check between these programs. Table DTF is a listing of DTF and Table FTD is a listing of FTD. Table Filon is a listing of the Transform program used by these routines.


```
PROGRAM FTCD(INPUT,OUTPUT,PUNCH,TAPE11)
DIMENSION A(200), B(200),L(10) ,QQ(200)
COMMON TITLX(3), TITLY(3)
CALL PLCTS(D1,D2,11)
1 PI=3.14158
READ 10,(L(I), I=1,4)
10 FORMAT(6A10)
READ 100, GD, QM
100 FORMAT(5F10,4)
IF(GD.NE,0.0) GOTO 101
PUNCH 10,(L(I), I=1,4)
D=0.0
PUNCH 100,D
CALL FIN
STOP
101 IA= IFIX(QM/GD+0.1)+1
READ 100, (A(I), I=1,IA)
AC=A(1)
DO 200 I=1,IA
200 A(I)=A(I)/AC
PRINT 300
300 FORMAT(1H1,*TABULATED EXPERIMENTAL DATA*)
PRINT 310, (L(I), I=1,4)
310 FORMAT(1H0,6A10)
DO 320 I=1,IA,2
G1=GD*(I-1)
G2=GD*I
QQ(I)=Q1
QQ(I+1)=Q2
G12=Q1**2
G22=Q2**2
320 PRINT 360, Q1,Q12,A(I), Q2,Q22,A(I+1)
360 FORMAT(/,2(F20,3, 2F15,5))
READ 390, (TITLY(I),I=1,3)
READ 390, (TITLX(I),I=1,3)
CALL FPLT (QC,A,0.,IA,1,2)
390 FORMAT(3A10)
C
C COMPUTE (Q*EXP(-K))EFFECTIVE
C
DO 400 I=1,IA
C=QC*(I=1)
400 A(I)=Q*SQRT(A(I))
C
C
READ 100, RD, RM
IB=IFIX(RM/RD+0.1)+1
DO 600 I=1,IB
R=RC*(I-1)+0.0000010
600 B(I)=100.*FILCN(A,0.0,GD,IA,R,0)/(2.0*R*PI**2)
PRINT 700, (L(I), I=1,3)
700 FORMAT(1H1,/* THE DENSITY FUNCTION FOR *, 3A10)
S=0.00
DO 800 I=1,IB,2
R1=RD*(I-1)
R2=RD*I
QQ(I)=R1
```

```

      QQ(I+1)=R2
      R12=R1**2
      R22=R2**2
      RD1=4.*PI*R12*B(I)
      RD2=4.*PI*R22*B(I+1)
      S=S+RD1+RD2
800 PRINT 810, R1,R12,B(I),RD1, R2,R22,B(I+1) ,RD2
810 FORMAT(/,2(F20,3,3F12,4))
      ERHO=S*RD/100,0
      PRINT 830, ERHO
830 FORMAT(/, * THE INTEGRATED DENSITY IS=, F6.3)
      READ 390, (TITLY(I),I=1,3)
      READ 390, (TITLX(I), I=1,3)
      B(1)=0,0
      CALL FPLT (QQ,B,0,,13,1,2)
      PUNCH 840, (L(I), I=1,3)
840 FORMAT(* DENSITY FUNCTION FOR * , 3A10)
      PUNCH 100,RD,RM
      PUNCH100,(B(I),I=1,1B)
      PUNCH 100,QQ,QM
      GOTO 1
      END

```

```

      FUNCTION FILCN(F,XI,D,N,T,I)
      SINE-COSINE INTEGRAL TRANSFORMATION
      BY FILCN$S METHOC, HANDBOOK OF MATH FUNCTIONS,
      P 890.
      F=VECTOR CONTAIN TABULATED F
      FOR X=XI, XI+D, XI+2*D,...,XI+N*D,
      N=MLST EE ODC
      T=CCNJUGATE VARIABLE TO X
      I=0 IMPLIES SIN TRANSFORM
      1 IMPLIES COS TRANSFORM

```

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      DIMENSION F(N)
      S=T*D
      AL=(1.0*(SIN(2.*S)/2.+2.*(SIN(S)+2)/S)/S
      BT=2.*(1+COS(S)+2*SIN(2.*S)/S)/(S**2)
      GM=(4./S**3)*(SIN(S)-S+COS(S))
      CD=0,0
      M=N-1
      CE= (F(N)*SC(1,T*(XI+M*D))+F(1)*SC(1,T*XI))/2,
      DC 100 J=2,M,2
      CD=CD+F(J)*SC(1,T*(XI+(J-1)*D))
100 CE=CE+F(J-1)*SC(1,T*(XI+(J-2)*D))
      SCS=AL*(F(N)*SC(1+1,T*(XI+M*D))+F(1)*SC(1+1,T*XI))
      IF (1,EG,0)SCS=SCS
      FILCN=D*(SCS+BT*CE+GM*CD)
      RETURN
      END

```

```

      FUNCTION SC(I,X)
      SC=SIN(X)
1 IF(1,EG,1)SC=COS(X)
      RETURN
      END

```

```

SUBROUTINE FFLT(X,Y,DEV,NP,IG1,IG2)
DIMENSION X(200),Y(200),DEV(200),TITLE(6),YL(200)
COMMON TITLX(3),TITLY(3)

```

```

IF(IG1)2,1,2

```

```

C SCALE X + Y ARRAYS FOR MAX AND MIN VALUES, IF X-SCALING HAS BEEN

```

```

C 1 DONE JUST SCALE Y ARRAY

```

```

2 CALL SCALE(X,10,,NP,1)

```

```

XMIN=X(NP+1)

```

```

CX=X(NP+2)

```

```

1 CALL SCALE(Y,10,,NP,1)

```

```

YMIN=Y(NP+1)

```

```

CY=Y(NP+2)

```

```

PRINT10,XMIN,DX,YMIN,DY

```

```

10 FORMAT(1H1,* XMIN=*F10,3,5X*DX=*F10,3,5X*YMIN=*F10,3,5X*DY=*F10,3)

```

```

C NOW PLOT EITHER DATA POINTS WITH THEIR ERRORS, JUST DATA, OR LOG

```

```

C 1 DATA

```

```

CALL AXIS(0,,0,,TITLX,,30,10,,0,,XMIN,DX)

```

```

IF(IG2,EQ,3)GO TC 5

```

```

CALL AXIS(0,,0,,TITLY,30,10,,90,,YMIN,DY)

```

```

PRINT30

```

```

30 FORMAT(/,8X*X*10X*X=INCHES*10X*Y*10X*Y=INCHES*10X*DEV*)

```

```

GO TO(3,4)IG2

```

```

C PLOTTING DATA WITH DEVIATION,

```

```

3 DO 6 I=1,NP

```

```

DV=DEV(I)

```

```

XP=(X(I)-XMIN)/CX

```

```

YP=(Y(I)-YMIN)/CY

```

```

CALL SYMBOL(XP,YP,,14,4,0,,=1)

```

```

Y1=(Y(I)+ DV-YMIN)/DY

```

```

Y2=(Y(I)- DV-YMIN)/DY

```

```

CALL PLCT(XP,Y1,3)

```

```

CALL PLCT(XP,Y2,2)

```

```

CALL SYMBOL(XP,Y2,,15,13,90,,=1)

```

```

CALL SYMBOL(XP,Y1,,15,13,90,,=1)

```

```

PRINT20,X(I),XP,Y(I),YP,DV

```

```

20 FORMAT(5(F10,5,5X))

```

```

6 CONTINUE

```

```

C DRAW X AND Y AXES

```

```

C PUT LABEL ON GRAPH

```

```

C READ 10,TITLE

```

```

C CALL SYMBOL(,5,10,,,2,TITLE,0,,80)

```

```

GO TO 99

```

```

C PLOT ARRAY R A T VS, Q

```

```

4 CALL LINE(X,Y,NP,1,-1,4)

```

```

GO TO 99

```

```

C PLOTTING LOG(SCP) VS Q-SQUARED, NEED TO RESCALE X AND Y AXIS, USE SUB

```

```

C TC DRAW Y-AXIS

```

```

5 CALL YLAX(YLMIN,YLMAX)

```

```

DO 7 I=1,NP

```

```

7 YL(I)=ALOG(Y(I))

```

```

DLY=(YLMAX-YLMIN)/10,

```

```

YMIN=EXP(YLMIN)

```

```

YMAX=EXP(YLMAX)

```

```

PRINT50,(YL(I),I=1,NP)

```

```

50 FORMAT(/,/* LOGY*/,/E12,4))

```

```

PRINT30

```

```

DO 8 I=1,NP

```

```

ROUTINE FFLT(X,Y,DEV,NP,IG1,IG2)
  SICH X(200),Y(200),DEV(200),TITLE(8),YL(200)
  IN TITLX(3),TITLY(3)
  1)2,1,2
  X + Y ARRAYS FOR MAX AND MIN VALUES, IF X-SCALING HAS BEEN
  JUST SCALE Y ARRAY
  SCALE(X,10,,NP,1)
  X(NP+1)
  NP+2)
  SCALE(Y,10,,NP,1)
  Y(NP+1)
  NP+2)
  10,XMIN,DX,YMIN,DY
  T(1H1,* XMIN=*F10,3,5X+DX=*F10,3,5X+YMIN=*F10,3,5X+DY=*F10,3)
  LOT EITHER DATA POINTS WITH THEIR ERRORS, JUST DATA, OR LOG
  AXIS(0,,0,,TITLX,-30,10,,0,,XMIN,DX)
  2.EQ,3)GO TC 5
  AXIS(0,,0,,TITLY,30,10,,90,,YMIN,DY)
  30
  T(//RX*X+10X*X=INCHES+10X*Y+10X*Y=INCHES+10X*DEV*)
  (3,4)IG2
  ING DATA WITH DEVIATION,
  I=1,NP
  V(I)
  (I)-XMIN)/DX
  (I)-YMIN)/DY
  SYMBOL(XP,YP,,14,4,0,,=1)
  (I)+ DV-YMIN)/DY
  (I)- DV-YMIN)/DY
  PLCT(XP,Y1,3)
  PLCT(XP,Y2,2)
  SYMBOL(XP,Y2,,15,13,90,,=1)
  SYMBOL(XP,Y1,,15,13,90,,=1)
  20,X(I),XP,Y(I),YP,DV
  T(5(F10,5,5X))
  NUE
  X AND Y AXES
  LABEL ON GRAPH
  10,TITLE
  SYMBOL(,5,10,,2,TITLE,0,,80)
  99
  ARRAY R A Y VS, 0
  LINE(X,Y,NP,1,-1,4)
  99
  LOG(SCP) VS Q-SQUARED, NEED TO RESCALE X AND Y AXIS, USE SUB, YLAX
  Y=AXIS
  PLAX(YLMIN, YLMAX)
  =1,NP
  ALOG(Y(I))
  LMAX=YLMIN)/10,
  XP(YLMIN)
  XP(YLMAX)
  Q,(YL(I),I=1,NP)
  (//+ LCGY*/(E12,4))
  0
  =1,NP

```

2

```

XP=(X(I)-XMIN)/DX
YP=(YL(I)-YLMIN)/DLY
CALL SYMBOL(XP,YP,,14,4,0,,=1)
Y1=Y(I)+DEV(I)
Y2=Y(I)-DEV(I)
YP1=ALOG(Y1)
YP1=(YP1-YLMIN)/DLY
YP2=ALOG(Y2)
YP2=(YP2-YLMIN)/DLY
CALL PLCT(XP,YP1,3)
CALL PLCT(XP,YP2,2)
CALL SYMBOL(XP,YP2,,15,13,90,,=1)
CALL SYMBOL(XP,YP1,,15,13,90,,=1)
PRINT20,X(I),XP,Y(I),YP,DEV(I)
8 CONTINUE
99 CALL CALCMF(XDUM,YDUM,IBL,,=2)
CALL PLCT(15,,0,,=3)
PRINT40,IBL
40 FORMAT(// ' FINISHED PLOT NO. ',I3)
RETURN
END

```

PROGRAM - DTDF(INPUT,OUTPUT,TAPF11)

DIMENSION A(200), R(200), L(10)

,QQ(200)

COMMON TITLX(3), TITLY(3)

CALCULATION OF SCATTERING FUNCTION

NOTE - Q AND R INTERCHANGED

E.G. 3/1/72

CALL PLOTS(D1,D2,11)

1 PI=3.14158

READ 10, (L(I), I=1,6)

10 FORMAT(6A10)

READ 100, QD, QM

100 FORMAT(5F10.4)

IF(QD.EQ.0.0)GOTO 1000

IA=IFIX(QM/QD+0.1)+1

READ 101, (A(I), I=1,IA)

C=A.0

DO 200 I=1,IA

200 S=S+A(I)*((I-1)*QD)**2

S=4.*PI*QD*S

DO 220 I=1,IA

220 A(I)=A(I)/S

PRINT 300

300 FORMAT(1H1,* NORMALIZED TABULATED DENSITY FUNCTION*)

PRINT 310, (L(I), I=1,4)

310 FORMAT(1HC, 6A10)

DO 320 I=1,IA,2

Q1=QD*(I-1)

Q2=QD*I

QQ(I)=Q1

QQ(I+1)=Q2

Q12=Q1**2

Q22=Q2**2

320 PRINT 350, Q1,Q12,A(I), Q2,Q22,A(I+1)

350 FORMAT(7,2(F20.3, 2F15.5))

READ 390, (TITLY(I), I=1,3)

READ 390, (TITLX(I), I=1,3)

CALL FPLT (QQ,A,0.,IA,1,2)

390 FORMAT(3A10)

DO 400 I=1,IA

400 A(I)=A(I)*QQ(I)

A(IA+1)=A(IA+2)=0.0

READ 100, RD, RM

IB=IFIX(RM/RD+0.1)+1

DO 600 I=1,IB

R=RD*(I-1)+0.000010

600 B(I)=(FILON(A,0.0,QD,IA,R,0))*4.*PI/(R)**2

PRINT 700

700 FORMAT(1H1,/* THE EFFECTIVE DEBYE-WALLER FACTOR*)

PRINT 310, (L(I), I=1,4)

IB=IB-1

DO 800 I=1,IB,2

R1=RD*(I-1)

R2=RD*I

QQ(I)=R1

QQ(I+1)=R2

R12=R1**2

R22=R2**2

RD1=R12*B(I)

RD2=R22*B(I+1)

800 PRINT 310, R1,R12,B(I),RD1, R2,R22,B(I+1)

,RD2

```
810 FORMAT(1,2(F20.3,2F12.4))  
  READ 390, (TITLY(I), I=1,3)  
  READ 390, (TITLX(I), I=1,3)  
  CALL FPLT (Q0,8,0.,IP,1,2)  
  GOTO 1  
1000 CALL FIN  
  STOP  
  END
```

VIII. Fourier Transform of Scattering Function to Probability Density

Below are the tabulated output from program FTD for two guesses of the experimental scattering function.

Fig. 1. 1st attempt at smoothing out the experimental data.

Fig. 2. Calculated density ρ at 1st guess.

Fig. 3. 2nd attempt at smoothing out the experimental data.

Fig. 4. Calculated density ρ at 2nd guess.

TABULATED EXPERIMENTAL DATA

1ST GUESS AT F

0,000	0.00000	1,00000
,200	,04000	,99375
,400	,16000	,99062
,600	,36000	,93750
,800	,64000	,85000
1,000	1.00000	,71875
1,200	1.44000	,53750
1,400	1.96000	,37500
1,600	2.56000	,20000
1,800	3.24000	,10312
2,000	4.00000	,10312
2,200	4.84000	,17500
2,400	5.76000	,27500
2,600	6.76000	,20000
2,800	7.84000	,01687
3,000	9.00000	,02125
3,200	10.24000	,03063
3,400	11.56000	,02125
3,600	12.96000	,00406
3,800	14.44000	,00437
4,000	16.00000	,00188
4,200	17.64000	,00025
4,400	19.36000	,00031
4,600	21.16000	,00015

,100	,01000	,99687
,300	,09000	,98750
,500	,25000	,98125
,700	,49000	,93125
,900	,81000	,78750
1,100	1,21000	,61875
1,300	1,69000	,48750
1,500	2,25000	,33750
1,700	2,89000	,16250
1,900	3,61000	,09687
2,100	4,41000	,12187
2,300	5,29000	,21250
2,500	6,25000	,24375
2,700	7,29000	,05625
2,900	8,41000	,01712
3,100	9,61000	,02937
3,300	10,89000	,02781
3,500	12,25000	,01187
3,700	13,69000	,00288
3,900	15,21000	,00612
4,100	16,81000	,00032
4,300	18,49000	,00032
4,500	20,25000	,00030
4,700	22,09000	,00010

THE DENSITY FUNCTION FOR 1ST GUESS AT F

0,000	0,0000	60,5343	0,0000
,100	,0100	24,8202	3,1265
,200	,0400	24,0257	12,0766
,300	,0900	22,6576	25,6251
,400	,1600	20,8552	41,9318
,500	,2500	18,7198	58,8097
,600	,3600	16,3663	74,0392
,700	,4900	13,9145	85,6786
,800	,6400	11,4796	92,3239
,900	,8100	9,1642	93,2800
1,000	1,0000	7,0522	88,6205
1,100	1,2100	5,2043	79,1326
1,200	1,4400	3,6563	66,1620
1,300	1,6900	2,4196	51,3858
1,400	1,9600	1,4642	36,5568
1,500	2,2500	,8225	23,2561
1,600	2,5600	,3547	12,6964
1,700	2,8900	,1542	5,5987
1,800	3,2400	,0530	2,1561
1,900	3,6100	,0459	2,0824
2,000	4,0000	,0540	4,7261
2,100	4,4100	,1665	9,2251
2,200	4,8400	,2412	14,6702
2,300	5,2900	,3046	20,2488
2,400	5,7600	,3502	25,3464
2,500	6,2500	,3768	29,5925
2,600	6,7600	,3867	32,8527
2,700	7,2900	,3840	35,1736
2,800	7,8400	,3725	36,7007

.050	.0025	25,0979	.7885
.150	.0225	24,5210	6,9331
.250	.0625	23,4015	18,3794
.350	.1225	21,8048	33,5658
.450	.2025	19,8222	50,4411
.550	.3025	17,5628	66,7618
.650	.4225	15,1453	80,4106
.750	.5625	12,6881	89,6869
.850	.7225	10,3012	93,5264
.950	.9025	8,0784	91,6183
1,050	1,1025	6,0924	84,4067
1,150	1,3225	4,3915	72,9826
1,250	1,5625	2,9992	58,8888
1,350	1,8225	1,9157	43,8724
1,450	2,1025	1,1214	29,6291
1,550	2,4025	.5822	17,5762
1,650	2,7225	.2540	8,6906
1,750	3,0625	.0891	3,4282
1,850	3,4225	.0403	1,7320
1,950	3,8025	.0652	3,1155
2,050	4,2025	.1288	6,8012
2,150	4,6225	.2046	11,8838
2,250	5,0625	.2749	17,4867
2,350	5,5225	.3298	22,8868
2,450	6,0025	.3658	27,5894
2,550	6,5025	.3836	31,3463
2,650	7,0225	.3867	34,1227
2,750	7,5625	.3791	36,0259
2,850	8,1225	.3646	37,2168

2,900	8,4100	,3557	37,5885
3,000	9,0000	,3353	37,9231
3,100	9,6100	,3120	37,6735
3,200	10,2400	,2850	36,6798
3,300	10,8900	,2534	34,6772
3,400	11,5600	,2158	31,3501
3,500	12,2500	,1715	26,4028
3,600	12,9600	,1205	19,6322
3,700	13,6900	,0639	10,9884
3,800	14,4400	,0034	,6126
3,900	15,2100	-.0583	-11,1522
4,000	16,0000	-.1183	-23,7795
4,100	16,8100	-.1733	-36,5990
4,200	17,6400	-.2204	-48,8522
4,300	18,4900	-.2572	-59,7532
4,400	19,3600	-.2818	-68,5476
4,500	20,2500	-.2930	-74,5635
4,600	21,1600	-.2905	-77,2525
4,700	22,0900	-.2746	-76,2214
4,800	23,0400	-.2461	-71,2563
4,900	24,0100	-.2066	-62,3417
5,000	25,0000	-.1581	-49,6767
5,100	26,0100	-.1031	-33,6867
5,200	27,0400	-.0442	-15,0290
5,300	28,0900	,0153	5,4148
5,400	29,1600	,0725	26,5628
5,500	30,2500	,1241	47,1790
5,600	31,3600	,1673	65,9433
5,700	32,4900	,1997	81,5433
5,800	33,6400	,2195	92,7806
5,900	34,8100	,2256	98,6817

2,950	8,7025	,3459	37,8238
3,050	9,3025	,3240	37,8784
3,150	9,9225	,2990	37,2843
3,250	10,5625	,2599	35,8239
3,350	11,2225	,2354	33,1990
3,450	11,9025	,1945	29,0946
3,550	12,6025	,1468	23,2527
3,650	13,3225	,0928	15,5404
3,750	14,0625	,0340	6,0002
3,850	14,8225	-,0275	-5,1251
3,950	15,6025	-,0887	-17,3972
4,050	16,4025	-,1466	-30,2113
4,150	17,2225	-,1980	-42,8456
4,250	18,0625	-,2402	-54,5203
4,350	18,9225	-,2711	-64,4582
4,450	19,8025	-,2891	-71,9404
4,550	20,7025	-,2935	-76,3523
4,650	21,6225	-,2842	-77,2198
4,750	22,5625	-,2618	-74,2364
4,850	23,5225	-,2276	-67,2855
4,950	24,5025	-,1834	-56,4568
5,050	25,5025	-,1312	-42,0617
5,150	26,5225	-,0739	-24,6413
5,250	27,5625	-,0143	-4,9670
5,350	28,6225	,0444	15,9752
5,450	29,7025	,0992	37,0189
5,550	30,8025	,1469	56,8760
5,650	31,9225	,1850	74,2178
5,750	33,0625	,2113	87,7747
5,850	34,2225	,2243	96,4473
5,950	35,4025	,2235	99,4140

47

[illegible]

0,000	0.00000	1,00000
,200	.04000	,99375
,400	.16000	,99062
,600	.36000	,93750
,800	.64000	,85000
1,000	1.00000	,71875
1,200	1.44000	,53750
1,400	1.96000	,37500
1,600	2.56000	,21875
1,800	3.24000	,13750
2,000	4.00000	,12187
2,200	4.84000	,17500
2,400	5.76000	,27500
2,600	6.76000	,20000
2,800	7.84000	,01687
3,000	9.00000	,02125
3,200	10.24000	,03063
3,400	11.56000	,02125
3,600	12.96000	,00406
3,800	14.44000	,00437
4,000	16.00000	,00188
4,200	17.64000	,00025
4,400	19.36000	,00031
4,600	21.16000	,00015
4,800	23.04000	,00007

,100	,01000	,99687
,300	,09000	,98750
,500	,25000	,98125
,700	,49000	,93125
,900	,81000	,78750
1,100	1,21000	,61875
1,300	1,69000	,48750
1,500	2,25000	,33750
1,700	2,89000	,15937
1,900	3,61000	,12500
2,100	4,41000	,13750
2,300	5,29000	,21250
2,500	6,25000	,24375
2,700	7,29000	,05625
2,900	8,41000	,01712
3,100	9,61000	,02937
3,300	10,89000	,02781
3,500	12,25000	,01187
3,700	13,69000	,00288
3,900	15,21000	,00612
4,100	16,81000	,00032
4,300	18,49000	,00032
4,500	20,25000	,00030
4,700	22,09000	,00010
4,900	24,01000	,10000

THE INTEGRATED DENSITY IS 1.058

THE DENSITY FUNCTION FOR 2ND GUESS AT F

0,000	0,0000	61,7350	0,0000
,100	,0100	25,3737	3,1885
,200	,0400	24,4900	12,3099
,300	,0900	23,0769	26,0993
,400	,1600	21,2185	42,6621
,500	,2500	19,0217	59,7581
,600	,3600	16,6074	75,1297
,700	,4900	14,1003	86,8226
,800	,6400	11,6194	93,4481
,900	,8100	9,2692	94,3486
1,000	1,0000	7,1337	89,6439
1,100	1,2100	5,2718	80,1594
1,200	1,4400	3,7167	67,2547
1,300	1,6900	2,4762	52,5873
1,400	1,9600	1,5369	37,8548
1,500	2,2500	,8686	24,5586
1,600	2,5600	,4297	13,8242
1,700	2,8900	,1735	6,3020
1,800	3,2400	,0529	2,1543
1,900	3,6100	,0247	1,1186
2,000	4,0000	,0523	2,6269
2,100	4,4100	,1074	5,9506
2,200	4,8400	,1700	10,3424
2,300	5,2900	,2279	15,1490
2,400	5,7600	,2746	19,8795
2,500	6,2500	,3084	24,2253
2,600	6,7600	,3300	28,0356
2,700	7,2900	,3413	31,2651
2,800	7,8400	,3442	33,9086

,050	,0025	25,5989	,8042
,150	,0225	25,0021	7,0692
,250	,0625	23,8450	18,7277
,350	,1225	22,1971	34,1697
,450	,2025	20,1550	51,2881
,550	,3025	17,8339	67,7922
,650	,4225	15,3578	81,5385
,750	,5625	12,8496	90,8282
,850	,7225	10,4222	94,6244
,950	,9025	8,1703	92,6603
1,050	1,1025	6,1659	85,4241
1,150	1,3225	4,4548	74,0349
1,250	1,5625	3,0575	60,0332
1,350	1,8225	1,9705	45,1283
1,450	2,1025	1,1713	30,9465
1,550	2,4025	,6233	18,8188
1,650	2,7225	,2818	9,6404
1,750	3,0625	,0991	3,8140
1,850	3,4225	,0297	1,2774
1,950	3,8025	,0334	1,5982
2,050	4,2025	,0778	4,1096
2,150	4,6225	,1387	8,0571
2,250	5,0625	,2001	12,7288
2,350	5,5225	,2529	17,5472
2,450	6,0025	,2932	22,1131
2,550	6,5025	,3207	26,2019
2,650	7,0225	,3368	29,7235
2,750	7,5625	,3437	32,6605
2,850	8,1225	,3430	35,0056

2,900	8,4100	.3401	35,9437
3,000	9,0000	.3297	37,2918
3,100	9,6100	.3131	37,8059
3,200	10,2400	.2898	37,2851
3,300	10,8900	.2595	35,5080
3,400	11,5600	.2222	32,2755
3,500	12,2500	.1783	27,4528
3,600	12,9600	.1289	21,0000
3,700	13,6900	.0755	12,9886
3,800	14,4400	.0198	3,6015
3,900	15,2100	-.0360	-6,8768
4,000	16,0000	-.0899	-18,0771
4,100	16,8100	-.1399	-29,5604
4,200	17,6400	-.1842	-40,8293
4,300	18,4900	-.2209	-51,3348
4,400	19,3600	-.2486	-60,4824
4,500	20,2500	-.2658	-67,6439
4,600	21,1600	-.2715	-72,1813
4,700	22,0900	-.2647	-73,4897
4,800	23,0400	-.2454	-71,0574
4,900	24,0100	-.2139	-64,5415
5,000	25,0000	-.1714	-53,8473
5,100	26,0100	-.1199	-39,1973
5,200	27,0400	-.0623	-21,1756
5,300	28,0900	-.0021	-.7310
5,400	29,1600	.0569	20,8657
5,500	30,2500	.1108	42,1152
5,600	31,3600	.1559	61,4221
5,700	32,4900	.1892	77,2538
5,800	33,6400	.2089	88,3010
5,900	34,8100	.2140	93,6195

2,950	8,7025	.3357	36,7113
3,050	9,3025	.3222	37,6647
3,150	9,9225	.3023	37,6887
3,250	10,5525	.2755	36,5671
3,350	11,2225	.2417	34,0840
3,450	11,9025	.2010	30,0679
3,550	12,6025	.1543	24,4284
3,650	13,3225	.1026	17,1802
3,750	14,0625	.0478	8,4514
3,850	14,8225	-.0082	-1,5225
3,950	15,6025	-.0633	-12,4127
4,050	16,4025	-.1155	-23,8132
4,150	17,2225	-.1629	-35,2548
4,250	18,0625	-.2036	-46,2136
4,350	18,9225	-.2360	-56,1170
4,450	19,8025	-.2586	-64,3514
4,550	20,7025	-.2701	-70,2798
4,650	21,6225	-.2697	-73,2742
4,750	22,5625	-.2567	-72,7675
4,850	23,5225	-.2311	-68,3226
4,950	24,5025	-.1939	-59,7109
5,050	25,5025	-.1466	-46,9890
5,150	26,5225	-.0917	-30,5569
5,250	27,5625	-.0323	-11,1834
5,350	28,6225	.0278	10,0131
5,450	29,7025	.0848	31,6331
5,550	30,8025	.1346	52,1106
5,650	31,9225	.1742	69,8612
5,750	33,0625	.2008	83,4445
5,850	34,2225	.2133	91,7180
5,950	35,4025	.2112	93,9609

.50

1.00

1.50

2.00

2.50

3.00

3.50

LONG VECTOR (0.0 1)

IX. Fourier Inversion of Model Densities to Obtain the Scattered Intensity.

Here we have used the program DTF to calculate the scattered intensity from density functions. Primarily we have investigated the effects of truncating the density function calculated by FTD. Figures 5 and 6 show this density function with the zeroes of the function labeled. Figure 7 is this density function inverted to $r = 10\text{\AA}$. Evidence of the termination-of-series error is seen for Q less than $0.7\text{\AA}^{-1}$. Figures 8 and 9 show the effects of terminating at the 3rd and 1st zeroes, respectively.

Figure 10 is the density function calculated by Jean-Paul Hanson using Monte Carlo methods.⁶ Figure 11 is the Fourier transform of this density function.

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Figure 10

Figure 11

Figure 11

.50 1.00 1.50 2.00 2.50 3.00 3.50

WAVE VECTOR, $Q(A-1)$

2

X. Conclusion

In this work we have obtained the probability density for He^4 in the bcc phase of solid helium by applying the Fourier transform to the integrated intensity obtained in an inelastic neutron scattering experiment. We find that the atoms appear to diffuse more rapidly to the neighboring lattice sites more readily than was expected.

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