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本報告は日本原子力研究所シシマ研究委員委然化202-2 性子胶乱断面積の評価作業の総合報告である。報告は一般的 かれている。評価は非干渉近似の範囲で完全であることを目 の他の関連した諸問題についての研究、評価は相足として加 1968年12月	によいて、1900年~1908年に1749に採行 記述, 評価, 基礎的研究の3つの部分に分 指している. 干渉効果, 多重散乱補正, そ 12た. 日本原子力研究所 シグマ研究委員会 熱化グループ* 0
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1. Introduction

The evaluation of thermal neutron scattering cross sections for neutron moderating materials has been the main research program organized by the Thermalization Group of Japanese Nuclear Data Committee. A'number of codes have been made available for the evaluation purpose. Some of them have been programmed originally by members of the Thermalization Group and the others were kindly offered by several foreign and authors. " One of the main purposes of the numerical analysis of thermal neutron scattering cross sections is to find the most appropriate frequency distribution or spectral density for lattice vibrations of crystals, molecular vibrations and rotations in solids and liquids, i.e., to determine the frequency distribution in the generalized sense which gives scattering laws, kernels, total scattering cross sections and other parameters related to the thermal neutron scattering in good agreement with experimental values. The other purpose is to provide standard' sets of kernels and cross sections for reactor analysis. $\otimes_{i \in M} M_{i} \otimes q$ "Phenomenological frequency distributions for practical purposes have been determined from measured scattering laws by means of the well-known extrapolation and iteration technique on the scattering law. Physical quantities which can be calculated directly from frequency distributions given as input data for codes are listed below. (1), Scattering law S(α, β) (2) • Scattering kernel and its, Legendre moments $\sigma_i (E_0 \rightarrow E)$, $\sigma_i (I=0, 1, 2, 3)$ (/=0, 1, 2, 3) (3) Total scattering cross section $\sigma_s(E)$ (4) Transport cross section $\sigma_{tr}(E)$ and the mean cosine of scattering angle $\bar{\mu}(E)$ (5) • Others (second moments, etc.) Evaluated values of these quantities are given in Chapter 3. Frequency distributions are shown in the form of tables and figures. Some typical kernels are illustrated graphically and numerical values of full kernels are given in the form of the list of output cards from the codes. Scattering laws are shown in figures and compared with experimental values. The total scattering cross section, the transport cross section and $\overline{\mu}$ are given in tables and figures and are discussed in comparison with measurements. Materials for which these quantities have been evaluated are light water, heavy water, graphite, beryllium, Ċ. beryllium oxide and organic moderators. For light water and heavy water 30 energy point kernels for THERMOS, source spectrum and thermal neutron diffusion parameters have been calculated in addition to the quantities (1)-(5) listed above. The evaluation which was partially completed but not to the extent to cover the whole items of (1)-(5) is also included in the present report as the supplement to the evaluation of مريد الإيدانية والمراجع individual scattering materials. Most of the experimental data on the scattering law or the double differential scattering cross section ever published contain, some errors, resulting from the resolution and multiple scattering. The method of multiple scattering correction is explained in Section 2.3 and some applications are illustrated in Chapter 3. Numerical

analysis based on the properly corrected experimental values has to be done and this work is certainly the next step in our evaluation program. In Chapter 4 research works on thermal neutron scattering by our members which have not been introduced in Chapter 3 are presented as progress reports. These works are now in progress or almost completed. Their full descriptions will be published in journals.

$$\begin{array}{c} \textbf{JARRI 1181}\\ \textbf{2. General Description}\\ \textbf{3. General Description}\\ \textbf{3. General loss of the double differential isoattering cross section of neutrons from monatomic substances, normalized the system of the system in the correlation function of the intermediate scattering function of a differential isoattering cross section of neutrons from monatomic substances, normalized the system in the system$$

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varies.
Eq. (1) is applicable only to the nuclear part of the scattering. The assumptions underlying Eq. (1) are that (1) the two-body scattering in the center of mass system is independent of energy and isotropic, (2) Fermi's pseudo-potential and the first Born approximation can be used, and (3) nuclear spins are randomly oriented.
These assumptions restrict the range of validity of Eq. (1). The second assumption above was investigated by NISHIGORI et al.³³. They studied neutron propagation in a scatterer system quantum mechanically and

showed that the correction to the use of the first Born approximation is of the order of magnitude of (nuclear scattering amplitude)/(atomic distance). So the correction will be quite negligible. Main scattering quantities evaluated in the present report are, besides the scattering law, the total cross

section, the transport cross section (or the average cosine of scattering angle) and the Legendre components of scattering kernel for l=0, 1, 2 and 3.

$$\sigma_{tr}(E_0) = \int_{\zeta} \sigma_0(E_0 \to E) dE, \qquad (1)$$

$$\sigma_{tr}(E_0) = \sigma_1(E_0) (1 - \overline{\mu}(E_0)) \qquad (8)$$

$$\overline{\mu}(E_0) = \int_{\zeta} \sigma_1(E_0 \to E) dE/\sigma_1(E_0) \qquad (9)$$

$$\sigma_1(E_0 \to E) = \left(\frac{d^2\sigma}{d\Omega + E} P_1(\cos\theta) d\Omega\right)$$

The neutron source spectrum, which is important for the calculation of thermal neutron spectrum, has also been calculated for light and heavy water. This is

$$\int_{E_c}^{\infty} \sigma_0(E' \to E) \frac{dE'}{dE'}, \quad E \le E_c \qquad (1)$$

where E_c is the cut-off energy.

Ó

In reactor calculations, it is particularly important to predict the correct $\sigma_t(E)$ and $\overline{\mu}(E)$. When sharp peaks (including a narrow accoustical band) exist in the spectral density function, as is usually the case, the scattering kernel also exhibits the corresponding peaks, and these remain finite even at fairly high energy. Thus, the integration in Eq. (7) and Eq. (9) needs a great care.

The scattering law satisfy the well-known conditions for the detailed balance and the moment theorem.

$$S(\vec{r}, \vec{\kappa}, -\omega) = e^{-\frac{\hbar\omega}{T}} S(\vec{\kappa}, \omega)^{0} \text{ for both } S_{s}(\vec{\kappa}, \omega) \text{ and } S_{d}(\vec{\kappa}, \omega)$$

$$(12)$$

$$\int_{-\infty}^{\infty} S_{s}(\vec{\kappa}, \omega) d\omega = 1$$

$$\int_{-\infty}^{\infty} S_{d}(\vec{\kappa}, \omega) d\omega = \sum_{i \neq j} \langle e^{-i\vec{\kappa}\cdot(\vec{r}_{i} - \vec{r}_{i})} \rangle_{T}$$

$$(14)$$

$$\int_{-\infty}^{\infty} S_{s}(\vec{\kappa}, \omega) \hbar\omega d\omega = R_{0}$$

$$\int_{-\infty}^{\infty} S_{d}(\vec{\kappa}, \omega) \hbar\omega d\omega = 0$$

$$(15)$$

Here $R_0 = \hbar^2 \kappa^2 / 2M$ is the free atom recoil energy. Eqs. (13) - (17) state that, at high energy, the distinct term of the scattering vanishes and the total scattering cross section as well as $\overline{\mu}$ (E) tend to those for free atom extractering. PLACZEK³ derived the expressions for the higher moments when atoms move in a potential field. High energy cross section was expressed in terms of these moments as

$$\underbrace{\sigma_1}_{F_0} \underbrace{\sigma_1}_{F_0} \underbrace{\sigma_1}_{F_0} = \sigma_1 \underbrace{(1 + \frac{1}{3} \frac{m}{M} - \frac{\langle K \rangle_T}{E_0} - \frac{1}{32} \mu^2 \frac{m}{M} - \frac{\langle C \rangle_T}{E_0^3} + \cdots}_{F_0^3}$$

where K is the kinetic energy of atom, μ is the reduced mass and $C = \frac{\hbar^2}{3M} (\bar{v}V)^2$. It is seen through the derivation of the above formula that the total cross section at high energy can take arbitrary value if the moment. theorem is violated. The total scattering cross section at very low energy is simply proportional to 1/v. In case of free gas, we can write

$$\vec{v} = \int |\vec{v} - \vec{V}| \sigma_s(v) P(\vec{V}) a\vec{V}$$

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where v_r is the	ne relative velocity and $P(V)$ is the distribution	function of velocity	of target atom.	The right hand	
side of the al	pove equation becomes constant if $v \ll \vec{\nu} $	entre o a company a construction and entre construction of the second second second second second second second	بر اینون کرد بر اینون در اینون اینون در می مسجود این سر	an and have seen as a new of the design strategies and a set of the second second second second second second s	۰۰۰ بر ۲۰۰۰ ور
Spectral De The app	nsity Function y_{μ} roximations usually employed in the calculated	tion of scattering la	w are:	en de la sense de la sense Altra de la sense de la sens Outra de la sense	11
(a) th	e use of incoherent approximation except for	the zero-phonon c	oherent elastic so	cattering,	
(b) th	e Gaussian approximation for time correlation	on function, i. e.,		and a second	
$\chi_s(\kappa, t)$	$=e^{-\kappa^2 w(t)}$	4 ** *		19	
where $w(t)$ is	the width function given by (v is the velocit	y of atom)	ومعتقب والمتعار والمتعار	n Rada Barakan Angelan (Barakan) Angelan (Barakan)	A
¢ S	$w(t) = -i\frac{\hbar}{2M}t + \frac{1}{3} \int_{0}^{t} (t-t') < \vec{v}(o) \cdot \vec{v}(t')$	> _T dt'	- <i>U</i>	(20)	
The real and	imaginary part of the velocity correlation fun	ction are mutually	related by fluctu	ation-dissipation	
theorem. \mathbf{T}_{g}	his allows us to write, by defining the spectr	al density function	as,	$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial t}$	
	$\rho(\omega) = \frac{4M}{3\pi\hbar} \frac{\tanh 2T}{\omega} \int_0^\infty R\vec{e} < \vec{v}(o) \cdot \vec{v}(t) >_T c$	os (<i>wt</i>) <i>dt</i>	с ф	(21)	
that	$\mathfrak{sv}(t) = \frac{\hbar}{2M} (\gamma(o) - \gamma(t))$	a para na pa sing anana na sana	n an an an an an gruppe a saon i an an an an	(22)	1, 194 () ()
where	$\gamma(t) = \int_{0}^{\infty} \frac{\rho(\hat{\omega})}{\omega} \left[(n_{\omega,\zeta} + 1)e^{i\omega t} + n_{\omega}e^{-i\omega t} \right] d\omega$	o 2 ⁰	 The second s	40 - 10 - 10 - 10 - 10 - 10 - 10 - 10 -	ΰ.,
	$n_{\omega} = \frac{1}{2} (\coth \frac{\hbar \omega}{(2T)} - 1)$	na na sina Na sina di Arabiana Na sina di Arabiana Na sina di Arabiana Na sina di Arabiana	0 10		0 : : 0 :
ρ(ω) is sli	own to satisfy the normalization condition.	ا از این کار می باد. ۱۹۹۹ - ۱۹۹۵ - ۱۹۹۵ میلی (کنیدری) از این اینکار میکار میکانیم کار در اینکار این اینکار اینکار ۱۹۹۹ - این اینکار اینکار این اینکار میکار میکار اینکار میکار اینکار اینکار اینکار اینکار اینکار اینکار اینکار ا	and a second sec	n - 1975 Alexandro actual anti-anti-anti-anti-anti-anti-anti-anti-	
The approxit	mation (a) is almost always a good approximation	ation to calculate th	e integral scatter	ing quantities of	1
()-(10)	. It is also expected to give the scattering la	w with reasonable	accuracy when th	ne structures due	u, Er
to coherent in	nelastic scattering are smeared. The discrepa	ancy may arise in th	e case of the scat	tering from solid	ig in i i F
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The approximation (a) is almost always a good approximation to calculate the integral scattering quantities of Eqs. (7)-(10). It is also expected to give the scattering law with reasonable accuracy when the structures due to coherent inelastic scattering are smeared. The discrepancy may arise in the case of the scattering from solid at low incident energy. CASSELS⁴⁰ has calculated the one-phonon total cross section of iron by the method due to WEINSTOCK⁵⁰ which is based on the Debye dispersion relation with single sound velocity. Cassels' calculation shows that the incoherent approximation gives substantially a lower cross section than the coherent calculation for neutron energies below 5 meV, and the effect is appreciable even for neutron energy about 20 meV. when temperature is high. No effort has ever been directed to the calculation of the total cross section by using the more realistic dispersion relations than Debye type, including in particular the ffect of polarization vectors. The Gaussian approximation (b) is rigorous for harmonic solids. The classical time correlation function

is, according to Schofield,¹⁾

$$\chi_{s}(\kappa, t) = \exp\left[-\frac{1}{2}\kappa^{2} < \eta^{2} > \tau + \frac{1}{4!}\kappa^{4}(<\eta^{4} > \tau - <\eta^{2} > \tau^{2}) + O(\kappa^{6})\right],$$
where
$$\pi = \frac{1}{2}\kappa^{2}(t) = \frac{1}{2}\kappa^{2}(t)$$

where $\kappa \eta = \kappa (\vec{r}(t) - \vec{r}(0))$ The "computer experiment" by RAHMAN⁶⁰ on liquid argon at 94.4°K shows that the maximum separation of $< r^4 > n$ from its Gaussian, value $\frac{5}{9} < r^2 >^2$ is about 13%, occurring at $t \sim 3 \times 10^{-12}$ sec. It falls off to zero at shorter and longer time. Therefore, the Gaussian approximation seems to be valid for most of the reactor moderating materials at normal temperature. Within the above approximations (a) and (b), the evaluation of the spectral density function is of the central importance in the calculation of neutron scattering. For harmonic crystal, $\rho_{\nu}(\omega)$ for the ν -th basis atom can be written approximately as

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$\rho_{\nu}(\omega, \Omega_{\epsilon}) = \frac{1}{N} \sum_{\kappa} \frac{|\vec{\kappa} \cdot C_{\nu}|^{2}}{\kappa^{2}} \tilde{\sigma}(\omega - \omega_{s})$

if the vibrations are anisotropic. Here Ω_{ϵ} is the solid angle subtended by ϵ . The cross section must be averaged over the orientation of microcrystals. The vibrational amplitude of heavier atom in crystal is in general large in low frequency modes and small in high frequency modes. The opposite is true for the lighter atom. Thus, $\rho_{\nu}(\omega)$ of the heavier atom, is softer than that of the lighter atom. The sum of $\rho_{\nu}(\omega)$ over ν divided by the number of basis atoms is just the frequency distribution as the density of normal modes.

The calculation of Eqs. (24) and (25) requires the complete solution of lattice dynamics. As will be discussed in section 3.4, the calculated frequency distributions of beryllium by YOUNG and KOPPEL⁷ on one hand and by RAUBENHEIMER and GILAT⁸) on the other differ considerably from each other. Both were based on the Born-von Karman model fitted to the measured dispersion curves of SCHMUNK *et al.*⁹ This is rather Gurprising since the fitting of dispersion curves seems to be more or less reasonably good in both theories: The lattice #dynamics of beryllium oxide is still more complicated and no firm theory as yet exists. An increasing interest is paid on the dynamics of liquid. Theoretical calculations have been reported for several simple liquid. But

it is practical at the present stage to determine the low frequency part of the generalized frequency distribution "in phenomenological way and the high frequency part by the theory of molecular vibrations and hindered ro- $\frac{1}{2}$ tations.

Experimentally, the spectral density function $\rho(\omega)$ is determined most easily by the extrapolation and iteration procedure first proposed by EgeLSTAff¹:

$$\rho(\beta) = 2\beta \sinh\left(\frac{\beta}{2}\right) \left(\frac{S_{s}(\alpha,\beta)}{\alpha}\right)_{\alpha \to 0}.$$

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For diatomic substance, $\rho(\beta)$ obtained in this way is

 $\rho(\beta) = \rho_1(\beta) + \frac{\langle a_2^2 \rangle}{\langle a_1^2 \rangle} \cdot \frac{M_1}{M_2} \rho_2(\beta),$

where the index 1 refers, for example, to the main scatterer atom. The normalization of $\rho(\beta)$ is therefore,

$$\int_{0}^{0} \rho(\beta) \, d\beta = 1 + \frac{-2^{2}}{-2a_{1}^{2}} - \frac{m_{1}}{M_{2}}$$

As the time correlation function of diatomic substance can not be expressed by a single Gaussian form, $\rho(\beta)$ loses the meaning as the spectral density function. The simplest way of analysis is to assume $-\rho_1(\beta) = \rho_2^*(\beta)$, and to iterate until a reasonable agreement is obtained between the calculated and the measured scattering law, although a careful study of the time Fourier transform of the scattering law will give $\rho_1(\beta)$ and $\rho_2(\beta)$, separately.

In practice, the procedure of extrapolation suffers from the multiple scattering from sample and the coherent scattering at small momentum transfer. \circ The effect of multiple scattering is sometimes significant even at the region of large momentum transfer. It is now generally recognized that the correction for this effect is veryo important for most of the existing experimental data. Theoretical correction (as MUSE code by HONECK10)) is also not free from ambiguity in the point that the calculated correction factor depends on the assumed frequency distribution. Iteration can be performed but with exhaustive work. BRUGGER¹¹⁾ and SCHMUNK¹²⁾ have respectively used the first moment theorem, Eq. (15), as a measure of the experimental check of the effect of multiple scattering on the measured stattering law of aluminum and beryllium. This method is well defined since the first moment is not affected by the presence of coherent scattering (elastic as well as inclastic) and thus will give a good support to the theoretical calculation of the correction factor. Unfortunately, many of the measurements that have been done so far for other types of materials do no cover the sufficiently wide range of β as to allow the direct calculation of the first moment.

The effect of coherent scattering on the scattering law becomes prominent at intermediate and small momentum transfer. This makes one to suspect if he has extrapolated the scattering law data correctly through $\alpha_2=0$. The calculation has been performed of the one-phonon coherent scattering from polycrystals of aluminum¹³⁾ and graphite. Fig. 1 shows the comparison of the calculated scattering law for aluminum with the

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measured one for $|\hbar\omega|/T=0.5$ and T=23 °C. As seen from the figure, the coherent effect is significant up to many reciprocal lattice zones away from the center. This is because that $|h\omega|$ is small, the corresponding |q|is also small and therefore the contributions from different zones are well separated. The coherent scattering fluctuates around the self term of the scattering except for very small κ . Thus, the incoherent approximation will be fairly accurate if the coherent effect is smeared. The coherent calculation on graphite will be described in section 3. 3. 2.

Method of Computation

In the present evaluation, the Fortran IV programs UNCLE, ES, NELKER, FREE, GASKET-FLANGE and UNCLE-TOM have been used. The last code calculates the zero-phonon clastic scattering of crystals of f. c. c., b. c. c and hexagonal structures. ES is based on the method of EgelSTAFF and SCHOFIELD,14) and cantreat diffusive motion together with bound motion and optical levels. As an integral check of the kernel calculation, the diffusion parameter code DIP was also used. - More details of these codes will be described in (1) following sections.

To facilitate the presentation of later sections, some basic formulae of scattering kernel calculation are given below. UNCLE and ES calculate the scattering cross section/by the method of phonon expansion when κ is small and by the short time expansion when κ is large.^{1), 15} Namely,

$$S_{s}(\kappa,\omega) = e^{-2W} \sum_{N=0}^{\infty} \frac{(2W)}{n!} G_{n}(\omega), \quad \text{for } 2W \le 6$$

$$= \frac{\hbar}{\sqrt{4\pi R_{0} T_{eff}}} e^{-\frac{(\hbar\omega - R_{0})^{2}}{4R_{0} T_{eff}}} \left(1 + O\left(\frac{1}{\sqrt{2W}}\right)\right), \quad \text{for } 2W \ge 6.$$
(27)

Here $h_{tw} = E_0 - E$, R_0 is the free atom recoil energy, 2W is the Debye-Waller factor and T_{eff} is the effective temperature.

$$2W = \frac{\hbar\kappa^2}{2M} \int_{0}^{\infty} \frac{\rho(\omega)}{\omega} \operatorname{coth} \frac{\hbar\omega}{2T} d\omega, \qquad (2)$$

$$T_{eff} = \frac{1}{2} \int_{0}^{\infty} \overline{\rho(\omega)} \hbar \omega \operatorname{coth} \frac{\hbar\omega}{2T} d\omega. \qquad (30)$$

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 $G_n(\omega)$ is the term for the process involving *n* real phonons, defined by and satisfying,

 $G_{n}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} \left(\frac{\gamma(t)}{\gamma(o)}\right)^{n} dt = \int_{-\infty}^{\infty} G_{1}(\omega - \omega') \quad G_{n-1}(\omega') \quad d\omega', \quad \int_{-\infty}^{\infty} G_{n}(\omega) d\omega = \frac{1}{2} \int_{-\infty}^{\infty} G_{$ When n is sufficiently large, it follows from the central limiting theorem of statistics that $G_n(\omega)$ tends to the normal distribution.

$$G_n(\omega) = \frac{1}{\sqrt{\frac{2\pi n\kappa_2}{2\pi n\kappa_2}}} e^{-\frac{(\omega-n\kappa_1)^2}{2n\kappa_2}} \left(1 + O\left(\frac{1}{\sqrt{n}}\right)\right)$$

where.

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$$\kappa_1 = \langle \omega \rangle = \int_{-\infty}^{\infty} \omega G_1(\omega) d\omega,$$

$$\kappa_2 = \langle (\omega - \langle \omega \rangle)^2 \rangle = \int_{-\infty}^{\infty} (\omega - \langle \omega \rangle)^2 G_1(\omega) d\omega$$

ES code can handle the diffusive motion of atoms. Splitting the spectral density function into the diffusive part and the bound part, the scattering law is calculated as

$$S(\kappa,\omega) = \int_{-\infty}^{8} S_{diff}(\kappa,\omega-\omega') S_{b}(\kappa,\omega') d\omega'$$

The diffusive part of the spectral density function is, following after EGELSTAFF and SCHOFIERD,

$$\rho_{\text{diff}}(\beta) = \frac{2d}{\pi} \frac{\sinh \beta/2}{\beta/2} \sqrt{c^2 + \frac{1}{4}} \beta K_1 \left(\sqrt[4]{c^2 + \frac{1}{4}} \beta \right), \qquad (41)$$

$$\int_{-\infty}^{\infty} \rho_{\text{diff}}(\beta) = \frac{d}{c}, \qquad (41)$$

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where K_1 (x) is the modified Bessel function of the second kind, d is related to the diffusion constant by D =

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 $\frac{\hbar}{M}d$, and c is the relaxation time (divided by $\frac{\hbar}{T}$) for atom to start to diffuse. For water at room temperature, c~10² and d~10⁻². So $\rho_{ditt}(\beta)$ is sharply localized near $\beta \equiv 0$. While the diffusive motion is only a very small part of the total freedom of atomic motion₀ the convolution integral of Eq. (40) has to be done very carefully. In the actual calculation the diffusive motion has been neglected and replaced by the free translation of a molecule as a whole. GASKET and FLANGE codes were used to this calculation.

Finally, UNCLE code has been used to calculate the interference scattering from atoms in heavy water molecule in liquid with minor modification of the code. The device is as follows. As in Butler's calculation,¹⁶⁾ by approximating the average of the products over the orientation of the molecule by the product of averages, the time correlation function for a pair of the ν -th and ν' -th atoms in a molecule may be written as,

The polarization vector
$$\vec{C}_{\nu}^{(1)} = \frac{\sin \alpha}{\kappa R_{uv}} e^{-\frac{\hbar \alpha}{4} \left(\frac{\pi w(0)}{M_{u}} + \frac{\pi w'(0)}{M_{u}}\right)} e^{\frac{\hbar \alpha}{2} \frac{\pi w'(0)}{M_{u}} + \frac{\pi w'(0)}{M_{u}}} e^{\frac{\hbar \alpha}{2} \frac{\pi w'(0)$$

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Comparison of the coherent calculation with measurement by Brugger et al. for $|\varepsilon|/T=0.5$. The arrows at the bottom of the figure indicate the position of reciprocal lattice points. The solid line is the calculation based on the dispersion curves and the frequency, spectrum obtained by Walker. Multi-phonon terms were treated in the incoherent approximation. The dotted line is the calulation in the incoherent approximation.

2.2 **Codes Used in Evaluation**

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The codes which have been used for the evaluation of thermal neutron cross sections are listed below. NEUKER: A program for bound hydrogen and deuterium based on Nelkin's formulation. This program computes (1) the seattering law, (2) the scattering kernel and its Legendre moments up to order 3, (3) the total scattering cross section and the transport cross section and produce punched card outputs of full kernels. ES2): A program for general purpose based on Egelstaff-Schofield's formulation? By the use of theoretical or phenomenological frequency distributions or spectral densities for bound motions (including lattice vibrations), molecular vibrations and rotations and parameters for diffusive motion, scattering cross sections for crystals and molecules (solids and liquids) can be computed with this program. Anisotropic crystals, however, can not be handled with the ES code. A frequency distribution with continuous and discrete parts can be used 0 as input data. The program computes (1) the scattering law, (2) the scattering kernel and its Legendre moments up to order 3, (3) the total scattering cross section, its Legendre moments and the transport cross section, (4). the source spectrum and produces punched card outputs of full kernel. UNCLE³: A program for anisotropic and isotropic polycrystalline materials.==:A frequency distribution=== with discrete parts can not be used as input data. The discrete levels have to be approximated, for example, by triangular distributions when they are to be used as input data for UNCLE? The program computes in the incoherent approximation (1) the scattering law, (2) the scattering kernel and its Legendre moments up to order 3, (3) the total scattering cross section, its Legendre moments and the transport cross section and produces a palahing ang Kanalang katang kat punched card outputs of full kernels. \mathcal{L} UNCLE-TOM⁴): A program to compute coherent and incoherent elastic scattering cross sections for polycrystalline materials. Materials which can be handled with this program are those belonging to hexagonal, face centered cubid and body centered cubic lattices. The calculation for the anisotropic crystal is also possible. Main outputs from the program are incoherent and coherent total elastic scattering cross sections, ά the transport cross section and Legendre moments. 12 GASKET⁵⁾: A unified program to compute scattering laws for any moderators (gases, molecules, solids and liquids) in the incoherent approximation. This program evaluates the intermediate scattering cross section and does Fourier inversion to obtain $S(\alpha, \beta)$. Provision has been made in the program for the following

dynamical modes and different combinations of modes:

 (1) Free translation, (2) -Diffusive motion, (3) * Harmonic isotropic vibrations with continuous frequency distribution, (4) Harmonic isotropic vibrations with discrete frequency distribution. The coding, however, has been completed only for combinations of modes (1), (3) and (4). The punched card output of S(α, β) can be obtained in ENDF FORMAT, which can be used for FLANGE. FLANGE⁶: A program which accepts as input the scattering law (calculated with GASKET, for and computes (1) the double differential scattering cross section, (2) the angular distribution, (3) the s kernel and its Legendre moments up to order 3, (4) the total scattering cross section and its Legendre norment. This program punches scattering kernels in ENDF FORMAT and also prepares an input tape for which does multiple scattering corrections. Other codes : Some other*codes were used for the evaluation. These codes have been program special purposes The explanations of codes such as MUSE, DIP, UNCLE-DISTINCT, etc. will in the following sections. NELKER: A Code of Scattering Kernel Calculation for Bound Hydrogen" (were applied on the following section). 	as input example) scattering moments MUSE, o amed for be given
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SUMMIT code originally developed by J. BELL at Gulf-General Atomics The revision was	made by
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the Elastic Scattering Cross Sections for Poly-Crystals" (written in Japanese), unpublished.	المحمد من المحمد من معالم المحمد المحمد المحمد المحمد
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Multiple scattering effect may be the most ill-natured one among errors which cause inacuracy to the cross section determined by experiment. The reason for this situation is firstly due to the fact that to avoid this effect is difficult in present experimental procedures since we are obliged to use relatively thick sample by the limited intensity of source neutron. Therefore necessity of the correction seems obvious. Secondly to perform this multiple scattering correction needs essentially the knowledge of cross section which we are going to measure. Therefore we should assume a theoretical cross section to perform this correction. C

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The reliability of the correction depends partly on the exactness of this assumed cross section: If one can extract the generalized phonon frequency distribution from experimental data, though this data contain b 10 Evaluation of Thermal Neutron Scattering Cross Sections for Reactor Moderators – JAERI 1181 multiple scattering, the kernel which is constracted by this frequency distribution may be used as the assumed --cross section: --Similarly-one-can extract, the generalized phonon frequency distribution from the corrected data, and constract the kernel from this distribution to use for the correction. "By the interation procedure we can obtain a kernel which is free from multiple scattering and also independent of the theoretical model employed. A number of methods for this correction based on different approximations have been developed. In the present report we employed the method developed by HONECK^D. This method employed in the computer code MUSE treats the scattering kernel rather exactly.

The assumptions in the procedure are:

(1) The geometry of the sample is slab with infinite extent.

(2) The scattering kernel $\sigma_*(E_0 \rightarrow E, \theta)$ is assumed to be represented by P₃ terms. Legendre moments up to order 3.

(3) The sample is thin so that the flux distribution across the sample can be expressed by a few space meshes.

(4) A theoretical scattering kernel is used.

The integral transport equation is solved by the direct and numerical procedure. Experimental arrangements are shown in Fig. 1. A neutron enters the sample on the x-z plane. Before a neutron escapes the sample it may make single or multiple collisions in the sample. Neutron detectors are assumed to be placed on the x-z plane, therefore, only the neutron which can escape the slab can reach the detectors.

The basic equations for the neutron transport are,

$$\phi(z, E, \overline{\Omega}) = \frac{1}{\mu} \int_{0}^{z} dz' H(z', E, \overline{\Omega}) e^{-\Sigma(E)\left(\frac{z-z}{\mu_{\Omega}}\right)}, \text{ of for } \mu > 0 \text{ and } z > z',$$
$$= -\frac{1}{\mu} \int_{z}^{a} dz' H(z', E, \overline{\Omega}) e^{-\Sigma(E)\left(\frac{z-z'}{\mu_{\Omega}}\right)}, \text{ for } \mu < 0 \text{ and } z < z',$$

 $H(z', \underline{E}, \underline{\vec{D}}) = \left\{ d \, \underline{\vec{D}}' \left\{ dE \, \Sigma_s(E, \rightarrow E, \mu_0) \, \phi(z_1, \underline{E}, \underline{\vec{D}}'), -\mu_0 \equiv \underline{\vec{D}} \cdot \underline{\vec{D}}', -\mu_0 \equiv \underline{\vec{$

where $\mu = \cos \theta$, and θ is the angle between the neutron vector and the z axis. $\phi(z, E, \overline{\Omega})$ is the neutron flux. The advantage of the use of Eqs. (1) and (2) is that we can obtain the neutron flux according to its order of collisions, that is one iteration corresponds to one scattering order. Thus, inserting the flux of uncollided neutrons into Eq. (2), we can obtain the first collision source. Inserting this source into Eq. (1), we can obtain the first collision flux. Repeating the same procedure we can obtain the higher order collided neutron flux. The uncollided neutron flux in the sample is,

(3)

 $\Psi^{0}(\boldsymbol{z}, \boldsymbol{E}, \boldsymbol{\vec{\Omega}}) = e^{-\Sigma(\boldsymbol{E})\boldsymbol{z}/\boldsymbol{\mu}} \, \hat{\boldsymbol{\partial}} \, (\boldsymbol{E} - \boldsymbol{E}_{1}) \, \hat{\boldsymbol{\partial}} \, (\boldsymbol{\vec{\Omega}} - \boldsymbol{\vec{\Omega}}_{1})''$

where E_1 and $\vec{\Omega}_1$ are the incident energy and solid angle of neutron velocity. As the first collision neutron flux, one can write, inserting Eq. (3) into Eqs. (1) and (2),

$$\psi'(z, E, \hat{\Omega}_1) = \Sigma_s(E_1 \to E_2, \mu_0) \frac{1}{\mu_0} \int_a^z dz' e^{-\Sigma(E_2) \frac{z-z'}{\mu} - \frac{\Sigma(E_1)}{\mu_0}} dz' e^{-\Sigma(E_2) \frac{z-z'}{\mu_0} - \frac{\Sigma(E_1)}{\mu_0}}$$

$$= \frac{z}{\mu_2} \underbrace{\stackrel{e^{-x_1} - e^{-x_2}}{x_2 - x_1}}_{\mathcal{O}} \Sigma_s(E_1 \rightarrow E_2) \ \mu_0$$

od
$$\underbrace{\stackrel{e^{-x_1}}{x_2 - x_1}}_{\mathcal{O}} \Sigma_s(E_1) \qquad \underbrace{\stackrel{e^{-x_2}}{x_2 - x_1}}_{\mathcal{O}} \Sigma_s(E_2)$$

for $y \ge 0$ and $x_1 = \frac{z}{\mu_1} \Sigma(E_1), \quad x_2 = \frac{z}{\mu_2}$

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For the calculation of higher order collided flux, angular dependence of flux and kernel is expressed as the constraint erms of the spherical harmonics, and energy and spatial variables are put into discrete meshes so that the integrals are replaced by the summation.

By the use of the flux of higher order collisions calculated by the MUSE code, the multiple scattering correction factor becomes,



Fig. 1 Geometry of neutron scattering experiment.

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Fig. 2 Multiple scattering correction factor on vanadium sample.



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2. General Description
2.4 Diffusion Parameters (DIP Code)
The method used to calculate the diffusion parameters of various moderators is based essentially
on CALANE's⁶ formalism. The solution
$$\phi(B,E,\mu,t)$$
 of the spatially Fourier transformed, homogeneous
Boltzmann equation for a non-multiplying medium in plane geometry, viz.
 $\left[\frac{1}{2}, \frac{1}{6}, t-lB\mu+\Sigma_1(E)\right]\phi(B,E,\mu)$ of (B,E,μ',t) (1)
is assumed to be of the form
 $\phi(B,E,\mu) = \phi(E,E,\mu)$ exp(-20).
(2)
where B is the Fourier Transform variable, E is the neutron energy, μ is the angular variable, and λ the time
decay constant.
The insertion of Eq. (2) into Eq. (1) yields
 $\left[-\frac{2}{\pi}, -lB\mu+\Sigma_2(E)\right]\phi(B,E,\mu)$
 $= \int_{-1}^{1} d\mu' \int_{0}^{\pi} dE' \Sigma_2(E', \mu' \to E, \mu) \phi(B,E',\mu')$.
(3)
The angular dependence of $\phi(E,E,\mu)$ and $\Sigma_n(E',\mu' \to E, \mu)$ is expanded in Legendre=polynomials
 $\phi(B, E_n^{\dagger}, \mu) = \sum_{m=0}^{\infty} \frac{2l+1}{2} \Sigma_n(E' \to E) P_1(\mu_0)$,
 $\mu' (E, \mu' \to E, \mu) = \sum_{m=0}^{\infty} \frac{2l+1}{2} \Sigma_n(E' \to E) P_1(\mu_0)$,
 $\mu' (B, E_n^{\dagger}, \mu') = (B, E, E) (B, E, D)$
 $= \int_{-1}^{2} d\mu' (S) = (B, E, D) (B, E, D) (B, E', D)$
 $\mu' (B, E_n^{\dagger}, \mu) = \sum_{m=0}^{\infty} \frac{2l+1}{2} \Sigma_n(E' \to E) P_1(\mu_0)$,
 $\mu' (B, E_n^{\dagger}, \mu) = \sum_{m=0}^{\infty} \frac{2l+1}{2} \Sigma_n(E' \to E) P_1(\mu_0)$,
 $\mu' (B, E_n^{\dagger}, \mu) = \sum_{m=0}^{\infty} \frac{2l+1}{2} \Sigma_n(E' \to E) P_1(\mu_0)$,
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 $\mu' (B, E_n^{\dagger}, \mu) = \sum_{m=0}^{\infty} \frac{2l+1}{2} \Sigma_m(E' \to E) P_1(\mu_0)$,
 $\mu' (B, E, E) = \frac{2}{2} (B, E, E) (B, E', D) = \frac{2}{2} (B, E, D) (B, E', D)$
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 $\mu' (B, E', E) (B, E', E)$

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The solution of above equations is obtained successively as follows: (1)	
By integrating the both sides of Eq. (9) over energy and using relation	ang tan Mananan Bata ang kananan ang kananan ang tanta
$\sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \sum_{i$	ý 8 sj
$(\underline{\omega}_{s}(\underline{E}) - \underline{\omega}_{s0}(\underline{E}) - \underbrace{)}_{0} \underline{\omega}_{s0}(\underline{E} - \underline{E}) \underline{\omega}_{0},$	tak A
one obtains	an a a n an a
$\int_0^\infty \left[\Sigma_a(E) - \frac{\alpha_0}{v} \right] \phi_{0,0}(E) dE = 0.$	δαα ΑΟ α ([])
In case the absorption is inversely proportional to the velocity, Eq. (9) has an eigenvalue	
$\alpha_0 = \omega_0 v_0$, α_0 , ω_0	μα _ο
For (9) with this eigenvalue is written as	i ann i Que i i
$O_{\mathbf{a}} = \sum_{\mathbf{a}} (E) \varphi_{\mathbf{a},0} (E) = \int_{0} \mathcal{L}_{\mathbf{a}} (E \to E) \varphi_{\mathbf{a},0} (E \to E) \varphi_{0,0} (E \to E) \varphi_{0,0,0 (E \to E) \varphi_{0,0$	(19)
It is well known that Eq. (13) has an eigenvector x_0	
$\phi_{0,0}(E) = M(E)$	ניין ענון . אראעידא ההענוגריד 100 בי רדי 10
with $M(E)$ the Maxwellian flux spectrum.	2000 - 2000 - 2000 - 2000 - 2000 - 2000 - 2000 - 2000 - 2000 - 2000 - 2000 - 2000 - 2000 - 2000 - 2000 - 2000 -
$\mathbf{J} = \mathbf{U}, \mathbf{M} > \mathbf{U}$	an ta' an Indian 1929. Ang ing ing ing ing ing ing ing ing ing i
The equation, $\sum_{i} (E) \phi_{i} (E) = \begin{cases} \infty \sum_{i} (E' \rightarrow E) \phi_{0} = (E') dE' = \frac{m}{m} \phi_{0} = 1(E). \end{cases}$	(15)
2m+1 -	
is solved for $\phi_{0,m}(B)$. The solution is enected by writing the equation at discrete energy po	$\lim_{n \to \infty} \mathbf{L}_n \text{ and } \mathbf{\underline{\Gamma}}_{\mathbf{C}}^{-}$
placing the integral by a numerical quadrature formula, to obtain	
$\Sigma_{\mathfrak{s0}}(E_i)\phi_{0,\mathfrak{m}}(E_i) - \sum \Sigma_{\mathfrak{sm}}(E_j \to E_i)\phi_{0,\mathfrak{m}}(E_j) dE_j = \frac{m}{2m+1}\phi_{0,\mathfrak{m}-1}(E_j).$	(16)
in a general second	and a second
1 his equation is written in matrix form	
$A_{m}\phi_{0,m} = \frac{m}{2m+1}\phi_{0,m-1},$	(17)
where A_m is a matrix defined as	an manga ang ang ang ang ang ang ang ang ang
$A_{r}(i,j) = \sum_{so}(Ei) \ \hat{o}_{ij} - \sum_{sm}(E_j \to E_i) \ \Delta E_j.$	
Eq. (17) is solved, a metrically by a matrix inversion routine.	n an
c) $n=1, m=0$	en de la contra de la contra de Marine de la contra d
Eq. (10) has a form in this case $\int_{-\infty}^{\infty} dx = \int_{-\infty}^{\infty} $	$\frac{\Delta u_{\rm ext}}{\Delta t} = \frac{1}{2} \frac{1}{2$
$\Sigma_{\mathfrak{s0}}(E) \phi_{2,0}(E) + \frac{\alpha_2}{v} \phi_{0,0}(E) - \phi_{0,1}(E) = \int_0^\infty \Sigma_{\mathfrak{s0}}(E' \to E) \phi_{2,0}(E') dE'$	(19)
$D_0(=\alpha_2)$ is determined by numerically integrating Eq. (19) over energy	$\mathcal{L}_{\mathcal{A}}$
$D_0 = \alpha_2 = \int_0^\infty \phi_{0,1}(E) dE \Big/ \int_0^\infty \frac{1}{v} \phi_{0,0}(E) dE.$	(20)
ϕ The equation which determines $\phi_{2,0}(E)$ is, in matrix form,	. Й
$A_0 \phi_{2,0} = \phi_{0,1} - \frac{\alpha_2}{v} \phi_{0,0}.$	(21)
This is not solvable by the straightforward matrix inversion method, because A_0 is not a	normal matrix.
SHIBA ²⁾ showed that the rank of A_0 is N-1 (N being the dimension of A_0) and one additional con	ndition is neccs-
sary to solve Eq. (21). The additional condition is obtained from the fact that $\phi_{2,0}(E)$ does	not contribute
to the net neutron density ³⁾ , viz.,	
$\int_{0}^{\infty} \frac{1}{v} \phi_{2,0}(E) dE = 0$	(22)
d) Higher components	E.
The same procedure is repeated to obtain $C(=\alpha_4)$ and $F(=\alpha_6)$. It should be noted that	t the Legendre
components of the scattering kernel with <i>l</i> up to 2 are necessary for the calculation of diffusion	parameters D_0 ,
. 이번 동안에 있는 것이다. 이번 것이 가슴을 가지 않는 것이다. 이번 것이 같은 것은 것이라는 것은 것은 것이다. 것이다. 가슴이 가슴 것이 가슴을 가지 않는 것이다. 것이다. 가슴이 가슴을 가 같은 것은 것이 같은 것이다. 이번 것이 같은 것이 같은 것이다. 이번 것이다. 것이 같은 것이 같은 것이 같은 것이다. 것이 같은 것이 같은 것이 같은 것이다. 것이 같은 것이 같은 것이 같은 것이 같은 것이 같은 것이 같은 것이 같은 것이 같은 것이 같은 것이다. 것이 같은 것이	

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An example of the eigenfunction calculation is shown in Fig 1. In Table 1 are shown some results of diffusion parameter calculations for H2O at 20°C. Experimental results are included in the table for the sake of comparison. From Table 1 one can see that the maximum energy of 0.625 eV is sufficient but 50 energy points are required for the calculation of diffusion parameters. Scattering kernels were computed by using GAKER and NELKER codes, both of which are based on the Nelkin's model. Table 11 shows that the slight difference in methods to calculate scattering kernels leads to a rather large difference in calculated diffusion parameters. The fects of the scattering model on diffusion parameters will be discussed in more details in Chapter 3.%

The thermal diffusion length L in Table 1 was calculated from the following equation: $L^{2} = \frac{D_{0}}{2\alpha_{0}} \left[1 + \sqrt{1 + \frac{4\alpha_{0}C}{D_{0}^{2}}} \right],$ which is known to be correct to order B^{4} .

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ő		.u	Tab	le 1. Re	sults of d	iffusion pera	meters of H	20 at 20°C	لينتشي	ø H	
1	NO.	Maximum energy (eV)	NO. of groups	NO. of angle Pts.	Max. I	Code used	D (cm ² . sec ⁻¹)	C (cm ¹ . sec ⁻¹)	F (cm ⁶ . sec ⁻¹)	L 2	
SE,	1# 2	0.900 0.900	"30 30	11 ['] 24	(b 1	GAKER	38016.5 38017.0	3114.2 3120.0	161.6 163.2	7.9936 7.9938	4
ne da See generales en e	•3 4	0.625 0.625	25 50	24 ن24 ^ن		And a second sec	3 7515.6,	"3089.2	155.7	7.8897	ni in ni ini ini ni ini ni ini
اندی کیور مراجع	5 6	0.707 0.900	30 30	24 11	1	NELKER	37501.6 37482.1	3072.6 2890.6	153.7 123.2	7.8864	a 9
anna agus Anna agus Anna ag	- 7 8	GHATAK, H Clendenin	oneck (' ('64)	65)	n na sina ang sang sang Sang sang sang sang sang Sang sang sang sang sang sang sang sang s	(Nelkin) (37045 37570	3361 3380	169 210	Entrings Control on the project of the information of the second seco	e •
مید دیند مرد میکند مرد مرد م	9 10	Kallfelz Clendenin	('65) ('64)		Goldman (Rad	-Nelkin) Ikowski)		3350 2730	<u>144</u> 250		mariterezie inc _{are}
100, and 100 a		Kallfelz Glaser ('6	('65) 7)	۵۰ میلورسی این ۱۰۰ ۲۰۰۵ ۱۹۹۰ - ۲۰۰۰ - ۲۰۰۰ ۱۹۹۰ - ۲۰۰۱ - ۲۰۰۱	(l-laywoo (od P(B))	33900 34520	3080 4220	218 363	an agén a mun a sa s	an an train tha an
÷	13 0 14	SPRINGER (Experimen	'64) * * t of Arai	(from	$\sum_{s}(E)$ and $\sum_{s}(E) = \sum_{s}$	nd µ(E))	35300 35630 <u>+</u> 80	3420±170	214±139		
۱ ۱ ۱	15 16	STARR, KOI de Juren, 1	PPEL ('61) Reier ('61)) ()		A 0		0		7.62±0.0 7.701±0.0	16 012

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Table 1. Results of diffusion parameters of H2O at 20°C

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		an an an <mark>it</mark> er an	<i>(</i>)			ана на Стала ф	u u u u u u u u u u u u u u u u u u u
S D			Evaluation	Υν το μου μεταγικότε 1 το το 1	n na sa sa babana — nO -s - na -sa ana - nu - n 0 O O I	se an	· · · · · · · · · · · · · · · · · · ·
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For liquid H₂O a lot of frequency distributions $\rho(\beta)$ have been derived experimentally from neutron scattering laws because scattering by hydrogen is mainly incoherent. Here, frequency distributions of hydrogen \Im in water are argued to fit measured total and differential scattering cross sections. If it is assumed that the rotation of H₂O molecule around its three principal axes of inertia are hindered and can be approximated by a harmonic torsional oscillation and two bond-stretching vibrations of the H₂O molecule are degenerate into one vibrational mode, the frequency distribution of freely recoiling H₂O molecule is expressed as:

(1)

 $\rho(\beta) = \frac{1}{18}\delta(\beta) + \frac{1}{2.25}\delta(\beta - \beta_r) + \frac{1}{6}\delta(\beta - \beta_{r1}) + \frac{1}{3}\delta(\beta - \beta_{r2})$

where β_r , β_{ν_1} , β_{ν_2} are the energies of hindered rotation, bending and stretching vibrations. However water has a broad band of torsional oscillation because of inharmonic potentials and of the collective modes of clustering molecules. As suggested in the literatures, the shape of the rotational band in the frequency spectrum will partly improve the agreements of the calculated total and differential scattering cross sections with experimental data.

Recently the availability of accurate differential and integral cross section measurements for water¹⁾⁻¹ has encouraged the development of more detailed models. Here, two of these, the model modified by KOPPEL⁵ from HAVWOOD's experimental frequency spectrum and the model derived by HAVWOOD⁵ from his experimental data on scattering law are introduced for comparison with ours. Both frequency spectra are shown in Fig. 1. In Koppel model, the frequency distribution near $\beta = 8$ is approximated by a discrete line of the same frequency with a weight of 1/6 in accordance with Eq. (1). At low frequency end, an ω^2 behavior is introduced and the remaining part, which is adjusted to 1/18 of the total area, is treated in the short collision time approximation. The area corresponding to the torsional mode is obtained by cutting off the distributed

^o part of the Haywood's experimental spectrum at 0.165 eV, the energy corresponding to the bottom of the valley between the torsional and first vibrational peaks. The suppressed part is then replaced by an additional discrete line at 0.205 eV with the weight of 1/6 required by Eq. (1).

Although integral and single differential quantities can be well reproduced by these models, small discrepancies in total scattering cross sections are still seen, for example, at energies around 0.045 eV or below 0.001 eV, as shown in Fig. 2, and the calculated average cosine of scattering angle is large compared with the measured value for energies below 0.02 eV. In our models, same as in Koppel model, the assumption of free mass-18 translation was adopted for the evaluations of scattering cross sections so the discrepancy in low energy region is not surprising.

The agreement in this energy region is easily obtained by introducing diffusive mode of water and quasicrystalline frequency spectrum. The discrepancy in the energy range of 0.02 to 0.2 eV is seen in the previous models and this is partly diminished by broadening the rotational band (model-1), although the discrepancy shifts to other energy region. In order to isolate the rotational band from the higher vibrational band, in one of the models (model-2) the high frequency part of the torsional oscillation band is cut off sharply. This brings the calculated results to a good agreement with the experimental data in total cross section, but the average cosine value of scattering angle shift upward at low energy part, as shown in Fig. 3. The difference in average 18 0 a ma Evaluation of Thermal Neutron Scattering Cross Sections for Reactor Moderators JAERI 1181

cosine values at fairly low energy depends on the assumption of free translation. A few typical results of $S(\alpha, \beta)$ values are also shown in Fig. 4. At low energy transfers, Haywood model which takes into consideration the quasi-crystalline structure of water phenomenologically, fits quite well to experimental data. At low $\beta_{(3)}$ the good agreement between Koppel model and the model-2 is observed. As β increases, Koppel model comes close to Haywood model. Also at high β , a fair agreement between the model-2 and the experimental, values is noticed.

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For reference, scattering kernels for the zero-th and the first Legendre moments are shown in Figs. 5 and 6, respectively. The calculated values of diffusion parameters using Koppel model and model-2 are compared in Table 2 with the values derived from pulsed neutron measurements as a integral check of these scattering kernels. Also the spectrum of thermal neutron source from hydrogen in water is shown in Fig. 7. In summarizing the preceding results, we might say that although the present status of the model is satisfactory for calculating each experimental quantity, there is no model at present which fits all the integral and differential data equally well.

9	E (eV)	$\sigma_{ m tot}$ for Koppel model	σ_{tot} for Model-2	$\overline{\mu}$ for Koppel model	μ̃ for Model-2
and the second sec	0.00025	439.8	452.0	$\frac{\partial f_{i}}{\partial t} = \frac{\partial f_{i}}$	n an
4	0.00101	" 248.1 ⁽⁾	252.0	0.0035	0.0038
ر. بر از ماهندی از این اورو ایک ماند. از از افغانی از ایک	0.00228	196.3	198.3	0.0289	0.0328
Barat (1997), and an and an	0.00405	170.9	171.0	0.0495	0.0545
	0.00632	155.6 🥬	(154.1	0.0655	0.0728
a la a cara de	0.00911	143.6	140.8	0.0806	0.0904
n na herri e Na na herri e	0.01240	134.8	130.9	0,0995	c 0.112 "
n Martin on a significant significant si	0.01619	126.5	120.7	0.118	0.134
	0.02049	118.7	113.3	0.136	0.154
ine weeks which and a new an array constant in the fi	0.02530	111.5	105.6	0.155	0.174
	0.03061	105.1	99.0	0.175	0.195
nan a mara yayana ayan tan an ya	0.03643	99.0	92.9	0.193	
2 - 4 - 1 - 2 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1	0.04276	93.6	87.7	0.211	0.232
n na na sana na sana na sana na sana sa	0.04959-	88.8	83.4	0.229	0.248
	0.05692	84.8	79.9	0.245	0.262
i de la constant Antipa de la port	0.06517	, 81.0	76.9	0.260	0.275
	0.07485	77.6	74.3	0.274	0.286 ⁰
	0.08612	74.4	72.0ª	0.287	0.298
	¹ 0.09919	71.7	70.0	0.302	0.311
na an a	0.11398	69.3	68.2	Ö.317	0.325
	0.13123	66.6	66.0	0.329	0.336
ي د ايند معر مير مير مير مير مير مير د از از در د اير اير مير مير مير اير م	0.1525	63.7	63.2	0.342	0.351
e leste a constant a constant de la constant	0.1790	61.5	. 61.3	0.358	0.364 👋
na an an an an an an an an Sina an Sina an Antairte Sina an Angarta an Angarta	0.2124	59.1	59.0	0.377	0.381
۱ بر ا ت	0.2546	57.0	56.7	0.398	o 0.40 1
Q (0.3081	54.8	54.3	0.417	0.420
a si san ang ang ang ang ang ang ang ang ang a	0.3760	52.5	52.1	0.434	
	0.4618	50.2	49.4	0.447	p 0.463
ى ئىرىكى ئىرىيى تەرىپىيە تورىپ	0.5702	48.1	47.1	0.458	0.475
4. 1945 - 1946 - 1946 - 1946 - 1946 - 1946 - 1946 - 1946 - 1946 - 1946 - 1946 - 1946 - 1946 - 1946 - 1946 - 1946 -	0.7067	ົດ 46.6	44.3	* 🚯 0.473	0.498

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6 F JAERI 1181	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Evaluation	αν το το 1940 το
	Toble 2. Diffusion	parameters in H ₂ O at 20°	
D_0 (cm ²	/s)(C(cm ⁴ /s)	F (cm ⁶ /s)	Refs
35,630± 37,516 34,825	-80 3,420±170 3,089 3,232	214±139 156 351,~~	Experimental ^{a)} Nelkin kernel Koppel model
37,125	3,047	240	Model-2
an an an Albert and an an Albert and an an an Albert and an an Albert and an an an Albert and an an an an an an		eferences	
1) HAYWOOD B. C., TH	IORSON I. M. : "The Scat	tering Law for Light and	Heavy Water at 20°C and 150°C,"
⁻²⁰ ß. BNL-719, p. 26, 19	062, HAYWOOD, B.C. : "Con	mparison of the Scattering	Law for Water al 22°C and 150°C,"
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and Liquids, Chal	k River," Vol. 1, p. 359,	IAEA, 1963.	an an an an an ann an an an an an an an
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4) HABUNG O Kas "	Fi2O at 302°K, KAPL-N	frematical Cross Sections of	n ad the Scattering Law for HaO and
$\alpha D_0 O$ at 299°K and	for H ₂ O at 268°K" BN	WL-436 (UC-34), 1967.	
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7) BEYSTER J.R. : Nucl.	Sci. Eng. 31, 254 (1968).	an an an Alain an Ala Alain an Alain an Alai Alain an Alain an Alai	
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	o Fig. 1. Frequency distr	ibutions for room temperatur	e H ₂ O.









Thermal Neutron Scattering by Water Vapou

(1) Introduction

As the most typical model for water scattering kernel such as the Nelkin model¹⁰ assumes the free translational motion of a molecule as a whole, the model for liquid water could be applied to water vapour when the rotational motion is treated appropriately. In the present note we calculate the scattering law and total scattering cross section for water vapour using simple models and compare them with the experimental results, especially paying some attentions to the temperature dependence of the total scattering cross sections. Theoretical models employed here are the free gas model, Krieger-Nelkin model which can be'deduced from Nelkin model by treating the free rotation classically and the spherical top model in which the free rotation is treated quantum mechanically. The assumption of symmetrical top molecule is inadequate for the case of water vapour, but this model gives the reasonable theoretical prediction of scattering law.

The experiments performed on the water vapour are few and there are large and unexplained differences between two total cross section data^{2), 3)}. The scattering law for water vapour which was measured by GLäser⁴⁾ are the only experimental values available. It is desirable that more experiments are performed on water ť vapour.

(2) Calculation

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Models employed here are the free gas model, Krieger-Nelkin model and the spherical top model. In the last two models we have neglected the excitation of vibrational motion.

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24	Evaluation of Thermal Neutron Scat	tering Cross Sections	for Reactor Moderat	ors JAERI 1181
Free aas n	nodel	an a		na a su an an ann an agus ann
This is	the simplest model which neglects the	internal vibration a	nd the rotational r	notion and assumes
the scatterir	by water vapour as the scattering h	v a single proton		notion, and assumes
The set	attering law is	y a single proton.	s e e en ante a se se	provide the second s
		8 - Carlos A. 19	•	20 D
ų,	$S(\alpha,\beta) = \sqrt{\frac{1}{4\pi\alpha}} \cdot e^{-\frac{\alpha^2+\beta^2}{4\alpha}}$		()	сы стана (1) д.
The total sc	attering cross section is,		· · · · · ·	an a
	$\sigma(E) = \sigma_f \left\{ \left(1 + \frac{1}{2E} \right) \operatorname{erf} \left(\sqrt{\frac{E}{T}} \right) + \right\}$	$-\frac{1}{\sqrt{\pi}}\sqrt{\frac{T}{E}} e^{-E/T} \}$	an an an an Arabana	(2)
Krieger-Ne	lkin model ⁵⁾ and a second second second			
This m	odel treats the rotational motion classic	ally, which correspon	nds to the increase	of the effective mass
for translati	ional motion.			
The sc:	attering law is.	475 1	··· k	· · · · · · · · · · · · · · · · · · ·
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n ta getterre an anne.	$S(\alpha,\beta) = \sqrt{\frac{1}{4\pi\alpha}} e^{\frac{-\alpha - rp}{4\alpha}} e^{-2A\gamma T\alpha}$	na independent and an and a second	ningen segen de la sindere en la demokratiere en la demokratie	
where	$\overline{\alpha} = \frac{M_{H}}{M} \alpha$, $\overline{A} = \frac{\overline{M}}{m} = 2.055$			
The total sc	cattering cross section is,		(p) (1) (2) (2) (2) (2) (2) (2) (2) (2) (2) (2	•.3 • • • • • • • • • • • • • • • • • •
where	$\sigma(E) = \frac{2\sigma_{T}\overline{\omega}}{E} \left\{ \operatorname{erf} \left(\sqrt{C} \right) - \sqrt{1-p} \right\}$	e^{-C_p} erf $(\sqrt{C(1-p)})$	$\overline{\mathbf{p}} \left\{ \begin{array}{ccc} \mathbf{a}_{1} & \mathbf{a}_{2} & \mathbf{a}_{3} \\ \mathbf{a}_{2} & \mathbf{a}_{3} \\ \mathbf{a}_{4} & \mathbf{a}_{4} \\ \mathbf{a}_{5} & \mathbf{a}_{5} \\ $	in the second seco
raggio consecutive des en el consecutive de la consecutive de la consecutive de la consecutive de la consecutiv	$\overline{\omega} = \frac{1}{2}, C = \frac{\overline{ME}}{\overline{m}}, p = -\frac{1}{2}$	 Active systems can be used as a second strain second s	ana ang kanalang kan National ang kanalang	na na parte na na mana ang ang ang ang ang ang ang ang ang
S 6	$2m\gamma$ mi $1+$	$\frac{\alpha}{4\beta}$		
ure a calificador A recentration de la composition A recentration de la composition de la composition de la composition de la comp	$\alpha' = \frac{m + \overline{M}}{mT}$	en an an an Alband gean tartha An an ann an Alband geann An Alband Alband	n na sana ang sa	an an an Galdar an an An An An A
an a	$\beta = \frac{2 \overline{M} \gamma}{\overline{T}}$	- A part of the second s	n an an an an an an an an ann an ann an	
n na har e se an har an har ann a Tarl an 1995 ann an 1995 ann an 1995 Tarl ann an 1995 ann an 1995 ann an 1995 Tarl ann an 1995 ann an 19	$T = \sum_{6w}^{-1} (\vec{C}^{(i)})^2 = 0.753 \ eV^{-1}$	n an an ann an Anna an An an Anna an A	an a	ter and the second s
«Spharical **	na film sandar a con transcribentarian and and a son a single and a son a single and a son a single and a si	an a	الي . 1994 - يون ما يون منطقين بالمحمد بالمحمد محمد بالاستان . 1995 - يون ما يون ما يون ما يون ما يون محمد بالاستان .	من من من من من من المن المن من م
Spherical T	op model		1	

of the three components of moment of inertia of a water molecule as the one for a spherical top molecule. The scattering law is, The scattering law is,

$$S(\alpha, \beta) = \sqrt{\frac{1}{4\pi\alpha}} e^{-\frac{\alpha^2 + \beta^2}{4\alpha}} e^{-2MT\gamma\alpha}$$

$$+ \sum_{j} B_T(j) \sum_{j} \frac{2J + 1}{2j + 10} e^{-\frac{U_{jj}}{4\alpha}} \sum_{n=|j-J|}^{|j+J|} j^2_n(\sqrt{2MT\alpha} b)$$
where

wilete E

$$B_{T}(j) = \frac{G(2j+1)\exp\left(-\frac{j(j+1)}{2ITC}\right)}{\sum_{j}(2j+1)^{2}\exp\left(-\frac{j(j+1)}{2IT}\right)},$$

$$U_{jJ} = \left(\frac{S_{jJ}}{T^{2}} - 2\beta \frac{S_{jJ}}{T} - 2\alpha \frac{S_{jJ}}{T}\right),$$

$$S_{jJ} = \frac{j(j+1)}{2I} - \frac{J(J+1)}{2I},$$

j, b : distance from a center of mass to a scattering atom, I : moment of inertia, $j_n(x)$: spherical Bessel function.

3. Evaluation

The total scattering cross section for this model has not been calculated.

(3) – Results and Comparison

In Fig. 1 the total cross sections at 100°C are compared with theories. According to HEINLOTH, the total cross sections of two different phase of water differs about 30 barns, which is close to the difference between the calculated values by the liquid model and the free gas model. This difference can not be explained by the Krieger-Nelkin model In Fig. 2 the temperature dependence of the total cross section is shown. The energy gradient of Hofmeyer's experimental results can be predicted by the Krieger-Nelkin model but the experimental data are always larger than the theoretical value by 5 to 10 barns.

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The scattering laws calculated with three models are compared with experiment in Fig. 3. As far as the scattering law data are concerned, the spherical top model can predict most precisely the experiment. This shows that, at least for this molecule the treatment of rotation is essential. Asymmetrical treatment of rotation may give further improvement.

As water vapour is one of the important and simple molecules, more experimental informations are desirable to check the theory or theoretical assumptions. At present, we can conclude that the precise treatment of rotational motion is neccessary for the analysis of the thermal neutron scattering from water vapour.

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a **b 4** Fig. 3 Scattering law for water vapour at 241°C and 25 atm.

		$H = \pm i \epsilon_{\rm eff} \epsilon_{\rm eff}$	u W
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3.2 Heavy Water	anna a chainn an chuir an chui Tha chuir an chuir an Tha chuir an	n an	an a
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3. 2. 1 Heavy Water		2000 - 1990 - 1990 - 1990 - 1990 - 1990 - 1990 - 1990 - 1990 - 1990 - 1990 - 1990 - 1990 - 1990 - 1990 - 1990 -	ст
(1) Introduction	•		4. 1
We present here the spectral de	nsity function for heavy water w	which can predict successf	fully, to some
extent, the experimental results on the	ermal neutron scattering propertie	es. Although the formul	ation is essen-
tially based on the coherent scattering	g which will be discussed in the	next chapter, the calculat	ion is limited
within the frame of the incoherent so	attering approximation. In near	r future, coherent scatteri	ng calculation
is planned.	en na santa sa santa mana sa santa na sa	e anna an an an an Albana an Albana. B' Albana an Albana an Albana. Albana an Albana an Albana.	· · · · · · · · · · · · · · · · · · ·
Physical interpretation of the pro	esent model will be given in the r	next chapter, so that here	we only give
the results and comparison with expo	riment. Calculation was perform	ned with the UNCLE, C	JASKET and
(2) Spectral Density Euroption	an a		, ana ang ang ang ang ang ang ang ang ang
(2) Spectral density functions for de	teron and oxygen atoms are give	n in Table 1 and also show	vn in Fia. 1
(3) Scattering I aw	v	0	
Scattering law of heavy water in	the incoherent scattering appro	ximation is,	
$S(\alpha,\beta) = \frac{1}{2(A_{\alpha}^{2} + C_{\alpha})}$	$\frac{1}{2} \cdot \sum_{\nu} (A_{\nu}^{2} + C_{\nu}^{2}) S_{\nu\nu}(\alpha, \beta)$	en e	o (1)
	- C L	ania e	
where A_{μ} and C_{μ} are the amplitudes	of concreme and inconcreme scatt	serings - respectively, above	(<i>a</i> , <i>p</i>) is self-
Comparison with experimental	results is performed in the next	t chapter (see Fig. 4 on	n. 41). Con-
tribution of each term of Eq. (1) will	be seen in Fig. 3 on p. 40. Altho	ugh the present spectral de	ensity function
can also fit the scattering law at high	t temperature (423°K), the follow	wing kernel estimation v	vas performed
for only room temperature.	 A second sec second second sec	No.	(a) Second State (State (St
(4)— Scattering-Kernel	and any formation - maintain the province spin - of the track of the stars of the stars of the second of the second of the stars of the second o	n particularitation and the second	0.0
Scattering kernels for deuteron	and oxygen are listed in Append	ix. Typical kernels as the	he function of
final energy are shown in Figs. 2 and 3	ne a service de la service La service de la service de	na na sana ana ana ana ana ana ana ana a	line (line and line a
(5) Total Scattering Cross Secti	on and μ (E) we have a set of the set of	na an a	
Total scattering cross section σ_0	(E) and the first Legendre momentum $225^{\frac{1}{2}}$	ent $\sigma_1(E)$ are listed in T	able 2. Total
at low neutron energy where experi	mental result is low because of	coherent scattering effect	cenent except
In Fig. 5. $\overline{u}(E)$ is compared wi	th experiments. ¹⁾ , ²⁾ The reason	n of fluctuation of calcu	lated $\overline{\mu}(E)$ at
higher energy is due to $\sigma_1(E)$, whose	e oscillatory values depend on the	e mesh of energies as she	own in Fig. 6.
This indicates the necessity of employ	ring the fine energy mesh up to hi	gh energy region to calcul	ate the reliable
scattering kernels.	4 V		a a a a a a a a a a a a a a a a a a a
(6) Conclusion	and a second second A second secon	n <mark>de senta de la 1865 de la constanción de la Constanción de la constanción de la cons</mark>	
Further check for the kernel was	performed using the DIP code.	Diffusion parameters us	ing up to $l =$
l kernels are compared with experir	nent (Table 3). Agreement betwee	een theory and experimen	t for diffusion
constant is fairly good. The calcula	ted diffusion cooling constant C	falls between the largest :	and the lowest
experimental data. Therefore, the p	resent model can be used for the	e calculation for neutron	thermalization
properties of neavy water.			en U ran en

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1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		Table 1. Spectral density for D_2O			J ₂ O	©		
n na		4.4 	ε (eV)	$ ho_{\rm DD}(E)$	ρ ₀₀ (E)	· · · · ·	()	
	6 .	See And Sec	0.004	3.855	30.84	n An An An An A		
		n an	0.008	4.426	35.41	n 1977 e la service de la companya d		
0			0.012	3.534	28.27	г		
 Signer March March State (1997) ■ 	e la companya	lan (Secondarian)	0.016	3,462	27.70		· · · · · · · · · · · · · · · · · · ·	
<u>й</u> - 1		ρ ^{ac} (E)	0.020	3.248	25.98			
and the second	алан алан алан алан алан алан алан алан	-16	0.024	2.868	22.94	1	in	
9	a diserta da este a compositoria de la compositoria de la compositoria de la compositoria de la compositoria de		0.028	2.320	18.56		en en ser en La ser en ser	
0		07.	0.032	୍ୟ 1.25 8	10.28		2	
9			0.036	0.0	0.0		. 8	
a service and a service of the servi			0.048	0.4560	0.08801	$e_1,\ldots,e_{i_1},\ldots,e_{i_{i_1}},\ldots,e_{i_{i_{i_1}},\ldots,e_{i_{i_{i_{i_1}}},\ldots,e_{i_{i_{i_{i_{i_{i_1}}}},\ldots,e_{i_{i_{i_{i_{i_{i_{i_{i_{i_1}}}}},\ldots,e_{i_{i_{i_{i_{i_{i_{i_{i_{i_{i_{i_{i_{i_$		
	Ø	Discrete	0.146	0.1483	0.03779	e se en la traditionat	1. N. C	
an and the first state of the state	andraa ta baba Afrika artaita	levels ¹⁴	0.3385	0.2957	0.07419	n an	n an	
n an	n alger 14 an an <mark>an</mark> Charl an Ann an An	ang	a a the second secon	.	in the second	All Sec.	na a an an an an an an an an	

Table 1. Spectral density for D₂O

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n an	Table 2a. $\sigma_0(E)$	and σ_1 (E) for a deu	teron atom in D ₂ O	<u> </u>
Energy (eV)	σ_0 (E) Inelastic (barns)	σ ₀ (E) Elastic (barns)	$\sigma_1(E)$ Inelastic (barns)	σ ₁ (E) Elastic (barns)
0.00025	7.35424	7.61268	-0.47783	0.06136
0.00101	4.07890	7.07109	-0.51006	0.23591
0.00228	3.32483	6.27711	-0.57322	0.47147
0.00405	3.16337	5.36353	0.62579	0.71042
0.00632 🥨	3.41166	4.44778		0.90572
0.00911	3.65728	3.60964	-0.66711	1.03208
0.0124	3.87995	2.90158	-0.62020	1.08442
0.01619	4.08775	2.33212	-0.49586	1.07547
0.02049	4.10182	1.88712	-0.38066	1.02436
0.0253	4.10377	1.54478	⁽³⁾ -0.22056	0.94964
0.03061	4.00668	1.28234	-0.10249	0.86582
0.03643	3.93824	1.07918	0.03925	0.78203
0.04276	3.82206	0.91990,	0.11290	0.70334
0.04959	3.85635	0.79333	0.20793	0.63209
0,05692	3.89565	0.69119	0.25966	0.56876
0.06517	3.95897	0.60370	0.35486	0.51029
0,07485	3.92689	0.52563	., 0.41185	0.45481
0.08612	3.89598	0.45684	0.48971	0.40335
0.09919	3.86129	0.39665	0.55340	0,35632
0.11398	3.84385	0.34518	0,61645	0.31464
0.13123	3.80278	0.29980	0.66934	0.27677
0.1525	3.71867	0.25799	0.69205	0.24093
0.179	3.75000	0.21980	0.81672	0.20741
0.2124	3.63327	0.18523	0.81567	0.17644
0,2546	3.64271	0.15453	0.91251	0.14841
0.3081	3.6453 0 ⁰	0.12770	0.99618	Ö.12352
0.376	3.33586	0.10464	0.81679	0.10183
0.4618	3.33074	0.08520	0.867549	0.08334
0.5702	3.41785	0.06900	0.98934	0.06778
0.7067	3.35372	0.05567	0.97983	0.05488
a a a a a a a a a a a a a a a a a a a	Table 2b. σ_0 (E) and σ_1 (E) for a oxy	gen atom in D₂O	
---------------------------------------	----------------------------	---------------------------------	----------------------------	-------------------------------
Energy (eV)	$\sigma_0(E)$ Inelastic	$\sigma_0(E)$ Elastic	$\sigma_1(E)$ Inelastic	σ ₁ (E) Elastic
	(barns)	(barns)	(barns)	(barns)
0.00025	4.14745	4.1267	-0.21392	0.03554
0.00101	2.38256	3.82150	-0.22393	0.13288
0.00228	2.06147	3.37637	-0.23928	0.26425
0.00405	2.01648	2.86811	-0.26+23	0.39560
0.00632	2.20873	2.36345	a – 0.29403	0.50056
0.00911	2.40502	1.90647	-0.32834	0.56575
0.01240	2.63148	1.52462	-0.34849	0.58960
0.01619	2.84181	1.22066	-0.34400	0.058027
0.02049	2.98850	0.98522	-0.32589	0.54895
0.02530	3.10295	0.80529	-0.29740	0.50601
0.03061	3.19887	0.66798		0.45924
0.03643	3.26980	0.56197	-0.23991	0.41333
0.04276	3.32079	0.47897	-0.20176	0.37073
0.04959	3.36560	0.41304	-0.17416	0.33249
0.05692	3.40278	0.35986	-0.15071	0.29870
0.06517	3.43552	0.31431	-0.12496	0.26765
0.07485	3.47059	0.27366	-0.09427	0.23829
0.08612	3.49140	10.23785 no	-0.07271	0.21113
0.09919	3.51470	0.20651	-0.05172	0.18637
0.11398	3.54401	0.17971	0.02819	0.16446
0.13123	3.55847	0.15609	-0.91271	0.14458
0.15250	3.56949	0.13432	0.00463	0.12580
0.17900 faile	3.58685	0.11443	0.02925	0.10825
0.2124	3.58208	0.09644	0.03694	0.09205
0.2546	3.57486	0.08045	0.04008	0.07740
0.3081	9 3.56259	0.06648	0.03030	0.06440?
0.3760	3.55780	0.05448	0.02632	0.05308
0.4618	3.56530	0.04356	0.01541	0.04343
0.5702 jj	3.56980	0.03592	0.00763	0.03531

	Table 2c. σ_0 (E), σ_1 ((E) and $\overline{\mu}$ (E) for D ₂ O	ала с на начени укредски сула на И се с 1944 г
Encity (eV)	σ ₀ (E) (barns)	$\sigma_1(E)$ (barns)	7 (E)
0.00025	38.208	-1.01132	-0.02462
0.00101	28.504	-0.63935	-0.02243
0.00228	24.642	-0.17853	-0.007245
0.00405	21.938	0.30063	0.013704
0.00632	20.291	0.68465	0.03374
0.00911	18.845	0.96725	0.05133
0.0124	17.719	1.16955	0.06600
0.01619	16.902	1.39549	0.08256
0.02049	15.9596	1.5105	0.09465
0.0253	15.205	1.6567	0.10895
0.03061	14.445	1.7221	0.11922
0.03643	13.866	1.8160	0.13097
0.04276	13.284	1.8015	0.13561
0.04949	13.078	1.8384	0.14057
0.05692	12.936	1.8048	0.13952
0.06517	12.875	1.8729	0.14547
0.07485 🗢	12.649	1.8773	0.14841
0.08612	12.435	1.9245	0.15476
0.09919	12.237	1.9541	0.15969
0.11398	12.102	1.9985	0.16513
0.13123	11.919	2.0241	0.16982
0.1525	11.657 •	1.9964	0.17126
0.179	11.641	2.1858	0.18776
0.2124	11.3155	2.1132	0.18675
0.2546	11.2497	2.2393	0.19905
0.3081	11.1751	2.3341	0.20887
0.376	10.4933	1.9166	0.18265
0.4618	10.4407	o 1.9606	0.18718
0.5702	10.5192	2.1572	0.20391
0.7067	10.2613	2.09937	0.20459



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Fig. 6 Effect of energy mesh points on $\sigma_1(E)$ (inelastic)

3. 2. 2 Heavy Water (Supplement)

Coherent Scattering from Heavy Water

(1) Introduction

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Neutron thermalization in heavy water, which is one of the two liquid moderators for a thermal neutron reactor, is more complicated than in another liquid moderator, i.e. light water. The reasons for this complicacy are:

(i) Deuteron is a coherent scatterer, in contrast with hydrogen which can be treated as an incoherent scatterer. This means that for the scattering from heavy water the contribution from atom pairs can not be neglected.

Free atom cross sections for deuteron and oxygen are comparable, while this is not the case for hydrogeneous moderator because the free atom cross section for hydrogen is usually much greater than those for the other atoms. This means that even if under the incoherent scattering approximation the scattering from oxygen can not be neglected.

Furthermore the scattering property of heavy water has the usual difficulty that may be encountered when one is treating with the thermal neutron scattering by liquid.

From scattering law data it is possible to determine the spectral density function when the scatterer is incoherent and only one type of nucleus contributes to the scattering. But since heavy water does not satisfy these conditions, the spectral density function which is deduced from scattering law data has ambiguity. Therefore, to determine the spectral density function for heavy water, a molecular dynamical treatment is required.

An incoherent scattering model for heavy water was presented by HONECK¹, which is equivalent to the Nelkin's model for light water²). MCMURRY³ presented another incoherent scattering model, extending his MR model⁴ for light water to heavy water. Coherent scattering calculation was performed by BUTLER⁵ for the first time and the structure of the scattering law was explained successfully, which had not been predicted in the incoherent scattering approximation. This model was employed by KOPPEL and YOUNG⁵ to calculate the integral parameters of scattering kernel for heavy water. They showed that in general the coherent scattering terms from the inter- and intra-molecular interference cancel largely each other in the case of total scattering cross section for example.

Recently PUCHER⁷ presented the crystal model which described the translational motion as the mode with the Debye-Einstein frequency spectrum. He also successfully predicted the low energy structure of the total scattering cross section considering the pair distribution function in heavy water.

The different treatment of the coherent neutron scattering from heavy water was proposed by us^s. The calculation is based on the Butler's model with experimentally determined acoustic spectral density for the translational motion of a molecule as a whole. In the present note we will describe the model in some detail and also comment on the effect of the multiple scattering.



 $\int_{-\infty}^{\infty} S_{\nu\nu}, (\vec{k}, \omega) d\omega = \langle e^{i\vec{k}\cdot(\vec{R}, -\vec{R}, \prime)} \rangle_T = \langle \frac{\sin(\kappa R_{\nu\nu})}{\kappa} \rangle_T,$

.

(12)

(1

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(13)

Calculation of Scattering Law (3)

 $\int_{-\infty}^{\infty} S_{\nu\nu}, (\bar{\kappa}, \omega) \hbar \omega d\omega = \frac{\hbar^2 \kappa^2}{2M_{\nu}} \bar{o}_{\nu\nu}.$

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The calculation of $\overline{S}_{\nu\nu}$, $(\vec{\kappa}, \omega)$ can be carried out by the phonon expansion procedure. But, the application of the Sjölander approximation needs some care in the present case. For the self term the validity of the approximation is assured by the central limiting theorem of statistics. For interference scattering, however, $\rho_{\nu\nu}$, (ω) can equally be negative or positive because of the orthogonality, as expressed by Eq. 11). The central limiting theorem is then no longer valid and, in fact, the Sjölander approximation occasionally gives a divergent result. The difficulty can be overcome as follows. We divide $\rho_{\nu\nu}$, (ω) into two parts, positive and negative definite parts. We apply the Sjölander approximation sepatately to each part of the scattering law corresponding to the above division. The final result is obtained by the convolution integral of these two scattering laws.* The short collision time approximation also leads to a divergent result. We can apply the short time expansion only to the scattering part corresponding to the positive definite spectral density, and the negative idefinite part has to be treated by the phonon expansion. The final expression for the calculation is as follows. In the following expressions we drop the subscripts ν and ν' , if net necessary.

a) Phonon expansion

The usual phonon expansion method can be applied to the present case. The scattering law is, by using the notations closely after SUMMIT code,

 $\overline{S}_{uu}(\vec{\kappa},\omega) = \sum_{n} e^{-2W} \frac{1}{n!} (2W)^{n} \phi_{n}(\varepsilon),$ where 9 $2W = \frac{\hbar^2 \kappa^2}{2M} \tilde{\gamma}(0),$ $\tilde{\gamma}(0) = \frac{1}{2} \left\{ \frac{M}{M_{\nu}} \gamma_{\nu\nu}(0) + \frac{M}{M_{\nu}} \gamma_{\nu\nu\nu}(0) \right\},$ $\phi_{\Gamma}(\varepsilon) = \frac{\rho(\omega)}{2\varepsilon \tilde{\gamma}(0) \sinh(\varepsilon/2T)} e^{\varepsilon/2T},$ (1A)(17) $\phi_n(\varepsilon) = \left[\phi_1(\varepsilon - \varepsilon')\phi_n(\varepsilon')d\varepsilon'\right],$ (18) ĺ b) Sjölander expansion As it has been suggested, above, we divide the generalized spectral density as $\rho(\varepsilon) = \rho^{(1)}(\varepsilon) + \rho^{(2)}(\varepsilon),$ (19) $\rho^{(1)}(\varepsilon) \ge 0$ and $\rho^{(2)}(\varepsilon) \le 0$, where The scattering law in Sjölander approximation is, $\overline{S}(\vec{\kappa}, \varepsilon) = \sum_{n} e^{-2W} \left(\frac{\hbar^2 \kappa^2}{2M}\right)^n \sum_{n} f_1 \cdot f_2 \cdot f_{34},$ where $2\pi\kappa_2(n,r)$ $(i) = \frac{\alpha_1(i)}{\alpha_{\nu}(i)}$

* This point was suggested by H. TAKAHASHI.

$$\kappa_{2}^{(i)} = \frac{\alpha_{2}^{(i)}}{\alpha_{0}^{(i)}} - \left(\frac{\alpha_{1}^{(i)}}{\alpha_{0}^{(i)}}\right)^{2},$$

$$\alpha_{0}^{(i)} = \int_{0}^{\infty} \frac{\rho^{(i)}(\varepsilon)}{\varepsilon} \coth\left(\frac{\varepsilon}{2T}\right) d\varepsilon = \gamma^{(i)}(0),$$

$$\alpha_{1}^{(i)} = \int_{0}^{\infty} \rho^{(i)}(\varepsilon) d\varepsilon,$$

$$\alpha_{2}^{(i)} = \int_{0}^{\infty} \rho^{(i)}(\varepsilon) \varepsilon \cosh\left(\frac{\varepsilon}{2T}\right) d\varepsilon.$$

c) Short time expansion

Using the same notation, one can write $\overline{S}(\vec{\kappa}, \vec{\epsilon})$ as

$$\overline{S}(\vec{\kappa}, \varepsilon) = \sum_{n} e^{-2W} e^{\frac{\hbar^2 \varepsilon^2}{2M} \gamma^{(1)}(0)} \frac{1}{n!} \left(\frac{\hbar^2 \kappa^2}{2M}\right)^n (\gamma^{(2)}(0))^n \frac{1}{\sqrt{2\pi x_2^{(n)}}} e^{-\frac{(\varepsilon - x_1)^n}{2x_2^{(n)}}} e^{-\frac{(\varepsilon - x_1)^n}{2x_2^{(n)}}}} e^{-\frac{(\varepsilon - x_1)^n}{2x_2^{(n)}}} e^{-\frac{(\varepsilon - x_1)^n}{2x_2^{(n)}}} e^{-\frac{(\varepsilon - x_1)^n}{2x_2^{(n)}}}} e^{-\frac{(\varepsilon - x_1)^n}{2x$$

where

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(4) Generalized Spectral Densitral for Heavy Water

 $x_{\mu}^{(n)} = \frac{\hbar^{2}\kappa^{2}}{2M} \alpha_{\mu}^{(1)} + n\kappa_{\mu}^{(2)}$

Inserting into Eq.(9) the eigenvectors and the eigen frequencies calculated by BUTLER, we obtain,

$$\rho_{DD}(\varepsilon) = \rho_{DD}^{ac}(\varepsilon) + 0.4560^{3}(\varepsilon - \varepsilon_{1}) + 0.1483^{3}(\varepsilon - \varepsilon_{2}) + 0.2957^{3}(\varepsilon - \varepsilon_{3}),$$

$$\rho_{00}(\varepsilon) = \rho_{00}^{ac}(\varepsilon) + 0.08801^{3}(\varepsilon - \varepsilon_{1}) + 0.03779^{3}(\varepsilon - \varepsilon_{2}) + 0.07419^{3}(\varepsilon - \varepsilon_{3}),$$

$$\rho_{D_{1}D_{2}}(\varepsilon) = \rho_{D_{1}D_{2}}^{ac}(\varepsilon) - 0.1039^{3}(\varepsilon - \varepsilon_{1}) + 0.001003^{3}(\varepsilon - \varepsilon_{2}) + 0.005042^{3}(\varepsilon - \varepsilon_{3}),$$

$$\rho_{D0}(\varepsilon) = \rho_{0D}(\varepsilon) = \rho_{D0}^{ac}(\varepsilon) - 0.1245^{3}(\varepsilon - \varepsilon_{1}) - 0.05203^{3}(\varepsilon - \varepsilon_{2}) - 0.1063^{3}(\varepsilon - \varepsilon_{3}),$$
(2)

 $\epsilon_1 = 0.018 \text{eV}, \ \epsilon_2 = 0.146 \text{eV}$ and $\epsilon_3 = 0.3385 \text{eV}$

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For the acoustic part of the frequency distribution $\rho_{yy}^{ac}(\varepsilon)$, we use the spectral density determined from the slow neutron experiment by LARSSON and DAHLBORG¹⁰⁾. The shape of $\rho_{yy}^{ac}(\varepsilon)$ is assumed to be the same – for every pair of atoms. The normalization is done with the use of Eq.(11) (see Figs. 1 and 2).

(5) Comparision with Experiment

As it will be seen from the discussion in section 3, the UNCLE code¹¹, which is a version of the SUMMIT code¹², is most readily utilized for the numerical calculation of the present problem with minor changes in the input quantities, input processing and formulas for the short collision time approximation. The version, UNCLE-DISTINCT, was prepared for use of IBM 7090 and 7044.

The total scattering law for the molecule is given by

$$S(\vec{\kappa}, \varepsilon) = \frac{1}{2(A_{\nu}^{2} + C_{\nu}^{2})} \sum_{\mu\nu\nu} (A_{\nu\nu\nu}^{2} + \partial_{\mu\nu\nu}, C_{\nu\nu\nu}^{2}) S_{\mu\nu\nu}, (\vec{\kappa}, \varepsilon),$$

(26)

where A_{ν} and C_{ν} are the amplitudes of coherent and incoherent scatterings, respectively.

In Figs. 3, the contributions of the interference scattering terms to the total scattering law are shown, and in Figs. 4 and 5, the calculated scattering laws are compared with the experimental data by HAYWOOD at T=295°K and 423°K¹³). Although $\rho_{\mu\nu}(\varepsilon)$ may be temperature dependent, the spectral density function was assumed to be the same for both temperatures in the present calculations. The contribution from the distinct atom pair becomes less important as β becomes larger and the temperature becomes higher. The agreement between theory and experiment is good on the whole, especially in the range of large α . For small α , the measured scattering law is generally larger than calculated one. A part of this discrepancy may be attributed to the multiple scattering effect. This point will be discussed in the next section. In Fig. 6, Butler's result is compared for $\beta = 0.5$ with the present calculation. Since BUTLER assumed free translational motion of a molecule as a whole, his result failed to agree with measurement except for the large α region.

(6) Effect of Multiple Scattering

As it had been discussed by SLAGGIE¹⁵⁹, the multiple scattering correction for double differential scattering data is a very important factor. We made this correction for the experimental data by HAYWOOD, using the incoherent scattering kernel (see the previous section). SLAGGIE also discussed the model dependence of the multiple scattering correction. Further analysis using a more realistic model for heavy water, for example, a model including the coherent scattering, may be desirable.

The experimental geometry is assumed as shown in Fig. 7. The specimen is a disk of 6 cm diameter and held at 45° to the incident beam. The thicknesses of the samples are, 0.209 cm for $E_0=0.109$ eV and 0.242 cm for $E_0=0.039$ eV¹⁴, where E_0 is the incident neutron energy. The calculation was performed only for room temperature case using the MUSE code.

In Figs. 8 and 9 the multiple scattering correction factors are shown for $E_0=0.11$ eV and $E_0=0.04$ eV. At small angles the multiple scattering correction factor becomes large and strongly dependent of the final energy, for small scattering angle. But for larger angles it tends to be flatter and approaches to unity.

From these results we corrected the multiple scattering for $\beta = 0.5$ and $\beta = 1.0$ (Figs. 10, 11, 12, 13 and 14). Agreement between theory and experiment was considerably improved especially in low α region. The multiple scattering correction seems one of the most important correction for experimental data, and produces some ambiguity when comparison is made between theory and experiment. Therefore it is desirable to establish a reliable method for the multiple scattering correction.

(7) Conclusion

The present model for heavy water can predict well the scattering laws at room and high (423°K) temperatures. The main part of the discrepancy between the present theory and experiment by HAYWOOD may be attributed to the multiple scattering effect.

One of the future problems is the calculation of the scattering kernel including the coherent scattering. By making a comparison with other recent experiments¹⁶ we can develop a more realistic model for heavy

Acknowledgements

water.

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74 y. one dimensional lattice vibration for the particular wave vectors in the directions of symmetry axes and from 16

Frequency distributions of lattice vibrations in graphite have been obtained by YOSHIMORI & KITANOD, YOUNG & KOPPEL²³ and CARVALIIO³⁹. YOSHIMORI & KITANO calculated the frequency distributions for outof-plane and in-plane vibrations by means of the Houston's method. The Houston's method solves the the frequency distributions for one-dimensional lattices the one for three-dimensional lattice is composed analytically. Hence the YKO (YOSHIMORI & KITANO) distribution has spurious singularities inherent in the one dimensional lattice. YOUNG & KOPPEL also used the Yoshimori-Kitano model, but they employed hte root sampling method to obtain the frequency distribution. Thus, YK (YOUNG & KOPPEL) distribution is free from the spurious singularities inherent in the Houston's method. YKO and YK distributions are shown in Fig. 1. CARVALUO performed the extensive measurements on scattering law for graphite at 533°K and determined the frequency distribution by means of the well known extrapolation procedure on $S(\alpha, \beta)/\alpha$. C(CARVALHO) distribution is shown in Fig. 3 in comparison with YK distribution. A remarkable resemblance is seen between them.

Scattering laws for graphite at 22°C calculated from YKO and YK distribution are shown in Fig. 4 in comparison with experimental values compiled by HAYWOOD & SINCLAIR⁵. Agreement with experimental values is better for scattering law calculated from YKO distribution than those from YK. It can not be concluded, however, that YKO distribution is better than YK distribution, because corrections to multiple scattering have not been applied to the experimental scattering law. From the theoretical point of view YK distribution is the best distribution among the available distributions at present.

In Fig. 5 comparisons are made between scattering laws at 300°K calculated from YK and C distribution³). There is seen little difference between them. What is effective in the calculation of the scattering cross section is the gross structure of the frequency distribution and the fine structure is rather irrelevant.

Some typical kernels for graphite at room temperature are shown in Fig. 6. These 30 energy point kernels were calculated from the YK distribution. The arrow on the abscissa indicates the incident energy of neutrons. The incoherent inelastic, elastic (coherent-incoherent) and total scattering cross sections are shown in Fig. 7, together with the total elastic scattering cross section calculated in the incoherent approximation.

In Fig. 8 the transport cross section for graphite at room temperature is illustrated.

Recently PAGE published his experimental data on the scattering law for graphite at 1300°K and 1800°K⁵. PAGE evaluated also the frequency distribution for graphite at 1800°K from the scattering law data⁷. The phenomenological frequency distribution determined by PAGE are compared in Fig. 9 with the YK distribution

for room temperature! In spite of the large difference in temperature, overall qualitative features of these distributions bear a remarkable resemblance, except the higher energy cut in the Page's distribution.

For examining the effect of the temperature dependence of the frequency distribution on the scattering cross section, scattering laws for graphite at 1800°K were calculated from the YK distribution at room temperature. These scattering laws are compared with the experimental values obtained by PAGE in Fig. 10. It should be noticed that resolution and multiple scattering corrections are not applied to the measured scattering law. Agreements between calculated and measured values are guite good. Structures seen in the measured scattering law can be attributed mainly to the one-phonon coherent scattering. It may be said from the results shown in Fig. 10 that the YK distribution can be used with reasonable accuracy in calculating the scattering cross section for graphite at high temperature.

Elastic and inelastic scattering cross sections for graphite at 1800°K are shown in Fig. 11 in comparison with those at room temperature. It is remarkable that the inelastic scattering cross section at 1800°K is considerably large in comparison with that at room temperature and has minimum point around 0.015 eV. The inelastic scattering cross section at 1800°K was calculated with UNCLE code from the averaged isotropic frequency distribution, because the execution time of the IBM-7044 computer was estimated to be more than two hours when the anisotropic frequency distribution was used. As for the elastic scattering cross section, that at room temperature becomes smaller, contrary to the inelastic scattering cross section is not large, but above 0.01 eV it is considerably large. For the neutron energy below the Bragg cut BNL 325 contains data on the total cross section at up to 1040°K.⁶ If these experimental values are plotted as a function of temperature T, they can be fitted with a linear function of T. The calculated value at 1800°K for the energy below



ų. 54 11 ÷6 έĒ. Fig. 2 Frequency distribution for graphite at room temperature, determined by and the second Young and Koppel. р р¹ $\mathbb{V}_{\mathcal{O}} = \overline{\mathbf{0}}$ **4**

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Fig. 3 Comparison between Young-Koppel and Carvalho frequency distributions for graphite at room temperature (in the averaged isotropic form).

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anisotropic Young-Koppel frequency distribution.





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0.2

0.3

0.1



3.3.2 Coherent Inelastic Scattering of Slow Neutrons from Polycrystalline Graphite

Several years ago H. TAKAHASHI made a detailed investigation of one-phonon coherent scattering from graphite by using the root sampling technique. Although the work was reported briefly at the conference on inelastic scattering of neutrons, Nov., 1965, Japan Atomic Energy Research Institute and was published in JAERI 1113 ('66), it is felt worth-while to reproduce his work in greater detail in the present evaluation report. Since he is now at BNL on leave from JAERI, the article is presented by one of the editors (S.I.) with permission of H. TAKAHASHI. The writer was informed that TAKAHASHI recalculated the same problem with the force constants determined by YOUNG and KOPPEL, and is preparing the results for publication.

In this paper we present the results of root-sampling calculation for coherent inelastic scattering of neutrons from graphite at room temperature based on Yoshimori-Kitano theory of lattice vibrations.¹⁰ The unsymmetrized one-phonon scattering law $S(\kappa, \omega)$ per atom for polycrystal is expressed by

$$S(\kappa, \omega) = \frac{1}{4\pi} \int d\Omega_{s} S(\vec{\kappa}, \omega)$$
(1)
$$S(\vec{\kappa}, \omega) = \frac{(2\pi)^{3}}{NV_{0}} \frac{h}{2M} \sum_{\vec{\tau}} \sum_{s} |g_{s}(\vec{\kappa})|^{2} \hat{\vartheta}(\vec{\kappa} + \vec{q} - \vec{\tau}) \frac{1}{\omega_{s}} \cdot [(n_{s} + 1)\hat{\vartheta}(\omega - \omega_{s}) + n_{s}\hat{\vartheta}(\omega + \omega_{s})].$$
(2)

(3)

Here $g_s(\vec{k})$ is the dynamical structure factor;

$$I_{s}(\vec{\kappa}) = \sum_{\nu=1}^{4} (\vec{\kappa}, \vec{C}_{\nu}) e^{i\vec{\kappa}\cdot\vec{r}_{\nu}} e^{-W_{\nu}\vec{\kappa}}$$

 $s = (\lambda, q)$ stands for the index for the normal mode and ν is for the basis atom. $\vec{C}_{\nu} \cdot \vec{r}_{\nu}$ and $2W_{\nu} \cdot \vec{r}_{\nu}$ are, respectively, the polarization vector, the position in a unit cell and Debye-Waller factor for the ν -th basis atom. The symbols have been defined in § 2.1. Eq. (1) was calculated by the root-sampling technique taking 675 wave vector points in an irreducible segment of the first Brillouin zone for the range of $\alpha = \frac{h^2\kappa^2}{2MT} \leq 1.0$ and $\beta = |\hbar\omega|/T \leq 2$. T is the temperature, in energy unit. An IBM-7044 Fortran IV program, ONE PHONON, was programmed for this purpose. In Yoshimoni-Kitaro theory, the one phonon term in Eq. (1) is split into the sum of the parts corresponding to in-plane vibrations and out-of-plane vibrations. $S(\kappa, \omega) = S_{II}(\kappa, \omega) + S_{\perp}(\kappa, \omega)$ (4)

Since in in-plane vibrations the motions of atoms lying on different layers are not coupled, the main physical-7 part of S_{11} (κ , ω), except for Debye-Waller factor, does not depend on κ_z and q_z . Z-axis is taken in the direction of the c-axis.

The calculation proceeds in the following way. A sampling point q is taken in the irreducible segment of the first Brillouin zone. Secular equation is solved to obtain $\omega_{\nu}(\vec{q})$ and $\vec{C}_{\nu}(\vec{q})$. $\vec{C}_{\nu}(\vec{q})$ is then transformed to $\vec{C}_{\nu}(\vec{k})$, where $\vec{k} = \vec{\tau} + \vec{q}$, using crystal symmetry. The range of $\vec{\tau}$ was restricted by $\alpha \leq 1.0$. The intensities of scattering from various τ are collected and classified according to the resulting $|\kappa|$ and ω , with intervals $d\alpha = 0.01$ and $d\beta = 0.1$, respectively. In order to get better statistics, the calculation was done separately for $S_{II}(\kappa, \omega)$ and $S_{\perp}(\kappa, \omega)$. This technique is advantageous, because the out-of-plane vibrations have the higher density of normal modes than that for in-plane vibrations for $\beta \ge 2$, and this implies that a greater number of sampling points are required to calculate $S_{II}(\kappa, \omega)$ with the same accuracy as that for S_{\perp} (x, w). The statistics was improved by using the frequency distribution, the density of normal modes, which were calculated with a larger number of sampling points. With the above technique, the present size of sampling points, 675, was not insufficient to make a meaningful comparison between theory and experiment. Typical results are shown in Figs. 1-4. Plotted together is the multi-phonon contribution calculated in the incoherent approximation using the anisotropic frequency distribution obtained by YOUNG and KOPPEL.²⁾ Figs. 1 and 2 show the structure of typical $S_{II}(\alpha, \beta)$ and $S_{\perp}(\alpha, \beta)$. In the range of β considered here, S_{II} (α, β) exhibits maxima at $\kappa \approx \tau_{1/2}$ and minima at κ in-between $\tau_{1/2}$, where $\tau_{1/2}$ is the projection of τ on hexagonal plane. This behavior is understood in closely analogous way to the case of an isotropic crystal,³⁾ by drawing the momentum conservation diagram in reciprocal lattice space and also by recalling that the density of trans-

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verse vibrations is much higher than that of longitudinal vibrations for acoustic branches $(\beta \le 3)$ (c.f. Fig. 5). The structure of $S_{\perp}(\alpha, \beta)$ is more complicated. When $\beta \sim 0.5$, the minima occur for $\kappa \approx \tau$ and maxima near in-between τ , and the positions of maxima are seen shifted towards larger κ are sincreases. When β exceeds somewhat over 0.6, the diffraction-like structure at small α diminishes abria. Firstly, and, at the same time, the phase of minimum and maximum is reversed. These may be interpreted roughly β follows. Firstly, when β is about 0.5 or less, we are observing the accoustic vibrations. In Yoshimori-Kitano theory, the squared frequency of out-of-plane vibrations can be written as

 $\omega^{2}(q) = (\omega^{(1)}(q_{2}))^{2} + (\omega^{(2)}(q_{1}))^{2}$

The (central) force constant between the adjacent layers is about only 1/50 of the bending force constant of the plane. Assuming Yoshimori-Kitano's force constants, $\omega^{(1)}(q_z)$ is 11meV at the zone boundary and becomes maximum at the next zone center, 16 meV. The $\omega^{(2)}(\bar{q}_{11})$ is about 80meV at (1010) zone boundary. The equifrequency surface is therefore not a sphere, but rather, roughly speaking, a cigar type directed to c-axis. The cigar clongates as β increases. For β , say 0.5, the end of the cigar lies near (0001) zone boundary and the lateral surface lies at less than half way to [1010] zone boundary. The density of the modes is high in the direction of c-axis and low in the direction perpendicular to it. Now, in the case $\kappa \approx \tau$ (002), the constant κ sphere crosses the equi-frequency cigar surface at about the middle part of it. There, the density is low. When κ is about $(\tau (002) + \tau (003))/2$, the κ -sphere glazes the ends of the cigar, where the density is high. This explains the stated results and also the shift of positions of maxima with β . For $\kappa \approx \tau$ (003) and $\approx \tau$ (100), the scattering becomes small either because of the destructive interference or of the orthogonality of \vec{C}_{μ} and $\vec{\kappa}$.

When β exceeds somewhat over 0.6, the equi-frequency surface becomes approximately an infinite cylinder and the bending vibrations (transversal) contribute to the scattering. Since the reciprocal lattice is dense in the direction of c-axis (see Fig. 6 (b)); prominent structure is not expected as κ increases from τ (002) to τ (003). Fig. 6 (a) and (b) also illustrate why the phase of minima and maxima is reversed as β increases from 0.5 to 0.7.

The structure of $S_{\perp}(\alpha, \beta)$ changes rather rapidly as β increases further, and it depends not only on the geometrical structure and the gross feature of dispersion curves, but also on the polarization vectors.

Figs. 3-5 show the comparison of the calculated scattering law with the experimental data by HAYWOOD and SINCLAIR. 'For large α , the agreement is satisfactory. The considerable discrepancy at small α may be attributed to the effect of multiple scattering from the sample.

CARVALHO⁰ calculated the multiple scattering correction for his measurement of graphite at 533 °K. The correction factor was about 0.3 and 0.4 respectively, for $\beta = 2$ and $\beta = 3$ at $\alpha = 0.1$. He also has converted his 533 °K results to room temperature, although the procedure may not be very accurate, to compare with the present calculation. Although the fine structures may have been smeared due to the finite angular resolution in the measurement, the agreement between his results and the present calculation is satisfactory.

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Fig. 3 One-phonon scattering law for graphite at room temperature (1).

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Fig. 5 A schematic drawing of momentum conservation law in reiprocal lattice to illustrate the structure of $S_{\parallel}(\kappa, \omega)$; Dotted semi-circles indicate the constant κ circle. When $\kappa \approx \tau$ (inner circle), transverse vibrations contribute predominantly to $S_{\parallel}(\kappa, \omega)$, while for κ at between τ (outer circle) the longitudinal vibrations are effective. * Solid circle is the equi-frequency surface for in-plane vibrations.



 κ spheres. The outer circle crosses the high density part of equi-frequency surface, thus resulting a large scattering cross section. For the inner circle, the situation is opposite. Fig. 6b shows the same illustration for $\beta \sim 0.7$. The equi-frequency surface becomes practically an infinite cylinder. No prominent structure of $S_{\perp}(\kappa, \omega)$ is expected in this case.

3.4 Beryllium

Frequency distributions of lattice vibrations in beryllium have been obtained by SINCLAIR," YOUNG & KOPPEL²³ and RAUBENHEIMER & GILAT." SINCLAIR measured extensively scattering law for beryllium at 22°C and evaluated the frequency distribution by means of the well known extrapolation procedure on $\hat{S}(\alpha, \beta)/\alpha$ proposed by EGELSTAFF. YOUNG & KOPPEL and RAUBENHEIMER & GILAT obtained frequency distributions theoretically by means of the root sampling method. YOUNG & KOPPEL used the Schmunk's⁴⁹ central force model in which the interactions with up to fifth neighbors are taken into consideration. RAUBENHEIMER & GILAT used the modified axially symmetric model formulated by DEWAMES, WOLFRAN and LEHMAN.⁵⁹ All these frequency distributions are shown in Fig. 1 (Note that the normalizations are different for three distributions).

As can be seen from Fig. 1, theoretical distributions have deep valley around $\nu = 15 \times 10^{12} \text{ sec}^{-1}$, but experimental one does not. Qualitatively, YK (YOUNG & KOPPEL) distribution resembles S(SINCLAIR) distribution closer than RG (RAUBENHEIMER & GILAT) distribution does, in spite of the fact that the theoretical basis for YK distribution is cruder than that for RG distribution. Phenomenological S distribution, however, can not be said to be precisely true, because the extrapolation procedure has some arbitrariness in eliminating the coherent and multiple scattering contributions from measured scattering law. Therefore, it can not be concluded from Fig. 1 that YK distribution is closer to the truth than RG distribution.

Scattering laws calculated from YK and RG distributions are shown in Fig. 2 in comparison with experimental one determined by SINCLAIR.⁶⁾ Agreements are not good for both theoretical values. It may be inferred from Fig. 2 that the true peak in the frequency distribution at the lower frequency exists between the peaks in YK and RG distributions. Scattering laws calculated from S distribution are also shown in Fig. 2. The main peak around $\beta = 2.0$ of the scattering law calculated from S distribution is smaller, whereas those from YK and RG distributions are much larger than experimental values. This may be the reflection of the relative effects of the two main peaks in the frequency distribution. In view of what is said above, experimental data on scattering law were re-evaluated and the final frequency distribution (MOD-2) thus determined is shown in Fig. 3 in comparison with S distribution. MOD-2 distribution is, now, similar to RG distribution qualitatively. This is a reasonable result, since the modified axially symmetric model gives the dispersion relation in excellent agreement with experimental dispersion curve determined by SCHMUNK:ⁿ

Scattering laws calculated from MOD-2 distribution are shown in Fig. 4. Discrepancy between theoretical and experimental values at small α is mainly due to the coherent and multiple scattering. Theoretical values

have been obtained in the incoherent approximation and the multiple scattering corrections have not been applied to experimental data. At large α where the coherent and multiple scattering effects are unimportant, the agreement is quite good.

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Some typical scattering kernels are shown in Fig. 5 for illustration. Numerical values of full kernels are given in Appendices. These 30 energy point kernels were calculated from the MOD-2 frequency distribution.

The incoherent inelastic, elastic (coherent + incoherent) and total scattering cross sections are shown in Figs. 6 and 7. The total elastic scattering cross section calculated in the incoherent approximation is also shown for comparison with the exact elastic scattering cross section. Oscillations seen in the inelastic scattering cross section are due to the structure of the frequency distribution and also dependent upon the energy mesh sizes. If finer energy mesh sizes are used, the amplitudes of the oscillations become smaller and the cross section becomes smoother.

In Fig. 8 the transport cross section for beryllium at room temperature is illustrated. The same explanations as given to the total scattering cross section are also applied to the transport cross section.

Data on thermal neutron scattering from bervillium at high temperature are not available at present. Calculations for beryllium at high temperature have not been performed, because we have no data to compare with calculated cross sections.

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Fig. 1 Frequency distribution for Be at room temperature. Note that normalizations are different for each distribution.





Fig. 3 Evaluated frequency distribution for Be in comparison with Sinclair distribution.







3.5 Beryllium Oxide

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The crystal structure of beryllium oxide is wurtzite type, the lattice parameters being c=4.37 Å, c/a=1.623and the structural parameter u=0.387 at room temperature. The study of lattice dynamics of beryllium oxide is of interest not only because of its use as an important reactor moderator, but also because it is a piczoelectric semiconductor and has a high thermal conductivity and a low electrical conductivity at room temperature. Sinclair has measured the scattering law at 293°K with incident energy of 0.135 eV.¹) Results were given for the ranges $0.25 \le h\omega \le 0.1$ eV and 0.1 Å $<\kappa/2\pi < 1$ Å. The extrapolation, procedure gives the generalized frequency distribution of the form;

$$\rho(\omega) \stackrel{\bigcirc}{=} \rho_{\mathrm{Be}}(\omega) + \frac{\sigma_b^0}{\sigma_b^{\mathrm{Be}}} \frac{M_{\mathrm{Be}}}{M_0} \rho_o(\omega)$$

Since $\rho_{\rm Be}(\omega)$ and $\rho_0(\omega)$ can not be determined separately, the assumption was made that $\rho_{\rm Be}(\omega) = \rho_0(\omega)$ in the analysis of scattering law. The iteration was performed until a reasonable fit was obtained between the = calculation and the experiment. The resulting generalized frequency distribution is tabulated in Table 1. and shown graphically in Fig. 1 (a). Fig. 1 (b) shows the phonon dispersion curves recently measured by OSTHELLER *et al.* by neutron scattering technique for wave vectors in (0001) and (1010) directions.²) Also plotted in Fig. 1 (b) are the *L*-point frequencies incasured by LOH from infrared reflection spectra and Raman scattering.³ The 135 meV LO frequency and 85 meV TO frequency are seen to satisfy Lyddane-Sachs-Teller relation $\omega_{\rm LO}/\omega_{\rm TO} = \frac{1}{2\pi}\sqrt{\varepsilon_0/\varepsilon_{\infty}}$, where ε_0 and ε_{∞} are respectively the static and the high frequency dielectric constants. In comparing Fig. 1 (a) and 1 (b), the critical frequencies are seen to agree well generally in both the generalized frequency distribution and the phonon dispersion curves. The 135 meV LO frequency found by optical measurement has not been observed by neutron scattering measurements. The neutron scattering experiment with a high incident energy or at a high sample temperature will likely to find this mode of vibrations. 'The critical frequency near 50 meV in the generalized frequency distribution may correspond to the frequency of **JAERI 1181**

about 40 meV of single crystal measurement. This deviation is not significant if the ambiguity of the extrapolation procedure is allowed for.

Figs. 2~6 show the comparison between the calculation and the experiment of scattering law. The agreement is fair at intermediate and large values of α . The discrepancy at small α may be attributed to the presence of the multiple scattering from the sample of the experiment. The measured scattering law exhibits considerable structure with respect to α , which may presumably be the coherent effect.

The total cross section was calculated and was compared with BNL-325 values in Fig. 7. The calculation agrees well with BNL-325 value for energies above Bragg cut-off. Pavor and SABINE⁴⁹ measured the total cross section of 5 Å neutrons for the temperature range between 100°K-2000°K³⁰. Their measurement was compared with the present calculation in Fig. 9. In the calculated range of temperature 300°K-1050°K, the agreement between the calculation and the experiment is seen excellent.

Fig. 8 shows the calculated transport cross section at room temperature, from which diffusion coefficient is calculated to give

$$=\frac{2v_0}{\sqrt{\pi}}\int_0^\infty \frac{M(E)}{3\Sigma_{tr}(E)} dE = 1.44 \times 10^5 \text{ cm}^2 \text{ sec}^{-1}$$

for the density 2.79 gr/cm³ and at temperature 20°C. Here $v_0 = \sqrt{2T/m}$. The experimental values measured by pulsed neutron technique are, in the unit of 10⁵ cm²/sec,

 $D_0 = 1.18$ (24°C); 1.36 (80°C); 1.60 (140°C)

by IYENGAR et al.⁵⁾ ('57) for a density 2.96 gr/cm³, and

 $D_0 = 1.56 \pm 0.01$ (20°C)

Da

by ZHEZHERUN et al.⁶¹ ('64) for a density 2.70 gr/cm³.

The present calculated value is sizeably small compared with the experimental value by ZHEZHERUN et al., A part of the discrepancy may be due to the expression of Eq. (1), which is approximate in nature (c. f. section 2.4).

PRYOR and SABINE have measured by neutron diffraction technique the vibrational amplitudes of atoms in beryllium oxide for varying temperatures⁵). Fig. 10 shows the calculation and the experiment of the mean square amplitudes of atoms as functions of temperature. As the present treatment assumes that the frequency distributions are the same for both beryllium and oxygen atoms, the mean square amplitudes of vibrations are given by

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$$\langle \tilde{u}_{\mu}^{2} \rangle_{T} = 3 \cdot \frac{\hbar}{2M_{\mu}} \int_{0}^{\infty} \frac{\rho_{\nu}(\omega)}{\omega} \operatorname{coth} \frac{\hbar\omega}{2T} d\omega$$

Although the measured vibrational amplitudes scatter rather wildly, the calculation definitely underestimates the amplitude of oxygen atom and overestimates that of beryllium, particularly at high temperature. Therefore, the present phenomenological frequency distribution may have to be modified to calculate the high temperature scattering cross section. PRYOR and SABINE calculated the vibrational amplitudes of atoms by assuming Debye-Einstein frequency spectrum, which was determined to fit with specific heat data. They assumed that cation and anion move in unison in acoustic vibrations and move oppositely in optical modes of vibrations. Their result is also plotted in Fig. 6. By using this model, they also calculated the total cross section of 5 Å neutrons, the results plotted in Fig. 5 in comparison with the experiment and with the present calculation.

To conclude, the generalized frequency distribution evaluated in the present report reproduces satisfactorily the observed scattering law and total cross section at room temperature. Theoretical transport cross section uiderestimates the diffusion coefficient by about 8%, although a transport theoretic calculation of diffusion coefficient may be necessary before drawing the conclusion. Theoretical Debye-Waller factor deviated from the observed values at high temperature, indicating the necessity of the lattice dynamical calculation? of spectral density function. This last point will become important in predicting the scattering law at high temperature.

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from the paper by Ostheller. The solid lines were mapped by neutron scattering techniques. The dashed lines are branches which have not been mapped. The solid points at q=0 are the frequencies determined by Loh from optical measurement.










3.6 Santowax and Diphenyl

Santowax is a mixture of ortho-, meta- and para-terphenyls $(C_6H_5)_2 C_6H_4$. The melting points of these isomers are 58°C, 89°C and 213°C, and the boiling points are 332°C, 363°C and 250°C, respectively at normal pressure. Diphenyl, $(C_6H_5)_2$, has melting point of 71°C and boiling point of 254.5°C under the same condition.

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The scattering law for polyphenyls has been measured by BRUGGER¹ and GLÄSER²). Fig. 1 shows the comparison of the measured scattering law for benzene, diphenyl and santowax at room temperature for typical values of β . As seen from the figure, the scattering law per hydrogen atom for diphenyl and santowax are mutually indistinguishable for all the ranges of observed α and β , while the scattering law for benzene is systematically larger than the other two for $0.6 \le \beta \le 2.0$. We, therefore? assume the same spectral density functions for diphenyl and santowax of the form;

$$\rho_{\nu}(\omega, \Omega_{\kappa}) = \rho_{\nu}^{acc}(\omega) + \sum_{\alpha} \frac{|\vec{\kappa} \cdot \vec{C}_{\nu}^{(1)}|^2}{\kappa^2} \delta(\omega - \omega_{\lambda})$$

where ν stands for either hydrogen or oxygen atom, ρ_{ν}^{acc} (ω) is the acoustic part of the spectral density function, and $\vec{C}_{\nu}^{(\mu)}$ and ω_{λ} are respectively the eigenvectors and the frequencies of internal vibrations of a

molecule. $\rho_{a}^{acc}(\omega)$ is determined by extrapolation-iteration procedure from the observed scattering law. Assuming that atoms move isotropically and in unison in this part of frequencies, we have $\rho_{c}^{acc}(\omega)=12 \rho_{H}^{acc}(\omega)$. Table I gives $\rho_{a}^{acc}(\omega)$ determined in this manner. The acoustic part of the spectral density function includes the translation and rotation of a molecule as a whole and also maybe a part of the internal vibrations. The areas are respectively 0.0803 and 0.963 for hydrogen and carbon. Therefore, we expect that the scattering from carbon atom is very much like that from free carbon gas. As the optical vibrations we assume that these are the same as the internal vibrations of a benzene molecule. The eigenvectors and frequencies³³ are tabulated in Table 2. In the actual calculation of the neutron scattering, we have used the isotropic approximation instead of Eq. (1), namely,

$$\rho_{\nu}(\omega) = \rho_{\nu}^{acc}(\omega) + \frac{1}{3} \sum_{\lambda} |\vec{C}_{\nu}^{(\lambda)}|^2 \hat{\sigma}(\omega - \omega_{\lambda}).$$

In using Eq. (2), $\vec{C}_{\nu}^{(\alpha)}$'s were renormalized as to give $\int_{0}^{\infty} \rho_{\nu}(\omega) d\omega = 1$. This renormalization makes the vibrational amplitudes of carbon atoms incorrect, but, this will not cause significant error in the calculated scattering properties of polyphenyl.

(Figs. 3(a)-3(b) show the comparison of the calculated scattering law for santowax at 23°C with the measured values. The agreement between the calculation and the measurement is satisfactory except for small α . Table 3 gives the calculated total cross section and the average cosine of the scattering angle, $\bar{\mu}$ (E), for santowax at 23°C. These were compared with experimental values in Fig. 4 and Fig. 6. The calculated total cross section agrees well with the experimental values by BRUGGER and HOFMYER4) for santowax, but is considerably larger than that by ANTONINI and PAOLETTI⁵⁾ for diphenyl at room temperature. Very recently, Sprevak⁶⁾ calculated the total cross section for liquid diphenyl at 150°C. He assumed a free translation of a molecule as a whole and determined the eigenvectors of internal vibrations of diphenyl molecule by choosing the interatomic force constants so as to give the best fit for the "vibrational frequencies measured by optical techniques. The calculated total cross section was in good agreement with the measured value by ANTONINI et al. Fig. 5 shows the comparison of the present calculation of total cross section (per hydrogen atom) of santowax at 23°C and 267°C with SPREVAR's calculation for diphenyl at 150°C. It is seen that the present calculation yields definitely larger cross sections than SPRFVAK's calculation for the entire range of energy. Since the scattering laws for diphenyl and santowax are indistinguishable as observed previosly, the total cross sections (per-hydrogen atom) for both materials are expected to be nearly the same, particularly at low neutron energy. Further measurement of total cross section will be very helpful in clarifying the point.

Fig. 6 shows the comparison of the calculated average cosine of the scattering angle for santowax at 23° C with the measured values for m-terphenyl at room temperature. The agreement is good except at the experimental point at E=0.0225 eV, where the calculated value is larger than the measured one by 40%.

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Evaluation of Thermal Neutron Scattering Cross Sections for Reactor Moderators JAERI 1181 70

E (eV)	$\sigma_{\rm H}^{(0)}/\sigma_{\rm FH}$	σc ⁽⁰⁾ /σ _{FC}	σ _{tot} (barns)	σ ⁽¹⁾ (barns)	μ. μ
0.001	5.62	1.68	1750	-46.5	-0.0266
0.004	4.21	1.31 (a)	1310	<i>a a</i> 26.8	0.0204
0.009	3.515	o 1.161	1100	73.2	0.0664
0.016	3.13	1.112	988	113	0.114
0.0225	2.87	1.082	910	121.5	0.1335
0.036	2.48	1.050	799	146	0.1825
0.044	2.35	1.051	741	156	0.210
0.060	2.06	1.022	675	156	0.231
0.071	1.95	1.028	644	160	0.248
0.090	1.795	1.033	600	166	0.277
		1.030		169	0.297
0.14	1.553	1.028	531	181	0.341
0.20	1.423	1.034	494	190	0.384
0.25	1.357	1.020	474	193	0.408
0.30	1.310	1.016	460	195	0.424

Table 3. Calculated total cross section and average cosine of scattering angle for santowax at 23°C. $a_{\rm c}$ ⁽¹⁾ is the cross section for the *l*-th Legendre component of angular distribution.

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Fig. 1 Comparison of the measured scattering laws per hydrogen in Benzene, Diphenyl and Santowax at room temperature for typical values of β .



Fig. 3 The scattering law per molecule of Santowax at 23°C. Comparison between calculation and experiment.









JAERI 1181 75 **Research Works** Loy Frequency Spectra of Organic Moderator Molecules T. SEKIYA, K. SAKAMOTO and Y. WATARI Department of Nuclear Engineering, Osaka University, Suita, Osaka (1)Introduction Recently organic materials (usually polyphenyls) are used as moderator and coolant in some types of nuclear reactors by the reason why they have similar number densities of hydrogen to water and low vapor pressure at high temperature. In the light of that, the neutron inelastic scattering data of those organic molecules are growing rapidly^{1~1}. As almost all the organic molecules for reactor use contain benzene rings, one of the aims of our research is to determine interaction potentials between benzene rings. In the simplest case of gaseous biphenyl the intramolecular potential has approximately 4-fold symmetry about c-axis and is represented in a form of $H/2(\cos 4\phi - 1)$. The method to determine the barrier height H will be explained in (2). The results suggest that the low frequency peak in neutron scattering data obtained by GLASER² corresponds 0 83.0 to the hindered rotation. : (z 367 ¹⁰ Recently TARINA³⁰ measured inelastic scattering cross section in the temperature region containing solid-

liquid transition point. To catch the physical meaning of these scattering data, we need to be familiar with the dynamical structure of these materials. As cold neutrons have energies comparable to those for rotational, lattice-vibrational and diffusive motions, it is necessary to consider all the degrees of freedom simultaneously from a standpoint of molecular theory. So-called GF Matrix Method has been developed by many authors⁵⁹ to analyse Raman and infrared spectrum data^{60, 70}. These theories which will be discussed in (3) however, are always limited to solid state. In the temperature range containing solid-liquid transition point, NMR data include not only rotational degrees of freedom but also diffusive one. We will try to connect the results for solid with those for liquid state in (4). In (5) we will discuss results and assumptions, and will give some suggestions for the possible generalizations of conventional methods.

(2) Internal Rotation of Biphenyl Gas⁸⁾

To determine the potential of internal rotation along c-axis of two benzene rings in a biphenyl molecule, we must take into account the competetion between orthogonalizing effect based on H-H repulsions and coplanarizing effect based on π -electrons.

The potential of internal rotation is determined as follows:

In biphenyl molecule shown in Fig. 1 there are two effects competing each other. (a) Orthogonalizing effect caused by the H-H repulsions between two pairs of hydrogen atoms in ortho-positions. The repulsion potential is a function of H-H distance and the tendency may be investigated by using the data for hydro-carbon given by SIMMONS⁹.

(b) Coplanarizing effect caused by π -electrons whose energy has already been evaluated by many authors¹⁰⁾. ^{11), 12)} on the basis of the molecular orbital method.

The H-H repulsion potential curve $R(\phi)$ was calculated by using SIMMONS data, where ϕ is the angle between two planes of benzene rings. The π -electron resonance integral potential curve $S(\phi)$ was calculated by molecular orbital method. As V(0)=0, we also have to assume that S(0)=R(0), we get S(0)=-3 kcal/mol from the calculation¹² based on the molecular orbital method. This value is also consistent with SIMMONS' R(0) corresponding to the H-H distance. In the first approximation we will determine H under the assumption that $S(\phi)$ is given by a cosine function. As $R'(\phi) = V(\phi, H) - S(\phi)$ is a linear function of H we can determine H so as to fit the $R'(\phi)$ to $R(\phi)$ at N positions $\phi_1, \phi_2, \dots, \phi_N$, in the meaning of the least square method.

Such an optimum H may be determined by the following equation:

$$\frac{d}{dH}\sum_{i=1}^{N} \left\{ R'(\phi_i) - R(\phi_i) \right\}^2 = 0$$

Next we define $R_1(\phi)$ and $S'(\phi)$ by the relations

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$$R_{1}(\phi) = \frac{R(\phi) + R'(\phi)}{2},$$

$$S'(\phi) = V(\phi, H_{1}) - R_{1}(\phi), \quad S_{2}(\phi) = \frac{S(\phi) + S'(\phi)}{2},$$

and determine new H_1 so as to fit $S'(\phi)$ to the real $S(\phi)$ in the meaning of the least square method. In practice, it needs only three repetitions to get the optimum value H=0.95(kcal/mol)=0.042(eV) within the error limit of 1%. The result is shown in Fig. 2.

We regard the molecule as a symmetric top, then we can get the eigen-values by the method of KOEHLER and DENNISON.

As the barrier height is more than twice of the thermal energies we may use the harmonic approximation which corresponds to replacing the cosine potential curve by a parabola. The level spacing thus obtained is 0.0037 eV at room temperature and it agrees rather well with peak position in frequency distribution obtained by $GL\ddot{a}SER^{2}$.

(3) Normal Vibration of Crystalline Benzene

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a) Crystal Structure of Solid Benzene

According to Cox's¹³⁾ X-ray analysis of solid benzene, the crystal structure of benzene is orthorhombic bipyramidal and the unit cell contains four molecules which occupy the corners and the face centers of its cell as shown in Fig. 3 The faces of the cell are orthogonal each other and lattice dimensions in a, b, c directions are all different, $a_0 = 7.034$ Å, $b_0 = 9.666$ Å, $c_0 = 7.460$ Å at 270°K. In equilibrium structure all the planes of the rings are approximately parallel to the *b*-axis and they make an angle of about 40° with (100) planes. This crystal has the symmetry elements of *E*, C_2^{a} , C_2^{c} , *i*, σ_a , σ_b , and σ_e . In Table 1° the result of the factor group analysis of the crystal is shown.

n (0)	D _{2h} ¹⁵	$E C_2$	$c^a C_2{}^b$	C2 ^c	i σ_a^{γ}	ς σ _b α	r _c infrared _p	Raman
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Toble 1. Symmetry species and the character table of crystalline benzene.

By using the bond lengths of benzene molecule:

C-C bond length -: 1.397Å

C-H bond length : 1.085Å

and atomic weights

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	l=1.00797, C=12.011	5,	1	
we may evalu	uate the moments of inertia	along three principal axes show	n in Fig. 3:	. U
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b) Norm	al Coordinates and Frequ	Jency Spectrum	9 0. 10 J	te de la companya de
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whose Cartes	sian components are taken a	along coordinate axes fixed on the	ne molecule and the cryst	al respectively.
They are con	nnected with each other b	y the transformation matrix T_{i}	 A Local and the second sec second second sec	e en
s i sista di ini. A	$Y_i = T_i X_i$	and the state of the	a ta	(1)
The kinetic	and the intramolecular po	otential energies are straightfor	wardly expressed by \ddot{X} 's	
an a	$T = 1 \stackrel{4}{\nabla} \dot{\vec{v}} u \dot{\vec{v}}$. 0	ta Aliante de la companya de la company Aliante de la companya	6
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where M and	\mathbf{F}_0 are the diagonal mass m	natrix and the potential energy n	natrix, respectively. The	intermolecular
potential ene	ergy V' is casily expressed	by \tilde{Y} 's:	and the state of the	Active Active
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	$V = \frac{1}{2} \prod_{i,j=1}^{j} I_j F_{ij} Y_j$	$m{m{m{m{m{m{m{m{m{m{m{m{m{$		(4)
By using equ	uations (1), (3), and (4), th	e total potential energy is writh	en as follows:	* 2
		4~		4. ⁶
Maria Arang	$V = V + V' = \frac{1}{2} \sum X_i F_0.$	$\vec{X}_i + \frac{1^{\rm a}}{2} \sum \vec{X}_i \vec{T}_i F'_{ij} T_j \vec{X}_j.$	where the transformation p_{1} is a single straining $\int_{0}^{\infty} \mathbf{u}_{1} \frac{\mathbf{D}}{\mathbf{u}_{1}} \mathbf{u}_{2} $, where $ \mathbf{u}_{2} $ is a $ \mathbf{D} $ is a single straining of the transformation $ \mathbf{u}_{2} $, where $ \mathbf{u}_{2} $ is a single straining of the transformation $ \mathbf{u}_{2} $, $ \mathbf{u}_{2} $ is a single straining of the transformation $ \mathbf{u}_{2} $, $ \mathbf{u}_{2} $ is a single straining of the transformation $ \mathbf{u}_{2} $, $ \mathbf{u}_{2} $ is a single straining of the transformation $ \mathbf{u}_{2} $, $ $	(5)
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$$V = \frac{1}{2} \sum_{i}^{4} \widetilde{\vec{Q}}_{i} \widetilde{\vec{L}}^{T_{R}} \widetilde{\vec{T}}_{i} F'_{ij} T_{j} L^{T_{R}} \widetilde{\vec{Q}}_{j}.$$

Accordingly the eigenvalues and eigenvectors of the 24 dimensional matrix:

 $F^{TR} \equiv (\tilde{L}^{TR} \tilde{T}_i F'_{ij} T_j L^{TR})$

give the frequency spectrum and the vibrational modes of the optically active lattice vibrations. The matrix F^{TR} is further reduced to smaller matrices due to the symmetry of the Bravais cell using the symmetry coordinates given in Table 3.

		lable	3. The symmetry coordi	nates for the	e latt	tice vibrations of benzene.	
•••	Aig	$S_1 = \frac{1}{2} (Q_1)$	$T^{z} + Q_{2}^{Tz} + Q_{3}^{Tz} + Q_{4}^{Tz}$	A ₁₄ 5	S ₁₃	$=\frac{1}{2} \left(Q_1^{Ty} - Q_2^{Ty} + Q_3^{Ty} - Q_4^{Ty} \right)$	
42 1	Ű	$S_2 = \frac{1}{2} (Q)$	$1^{T_x} + Q_2^{T_x} + Q_3^{T_x} + Q_4^{T_x})$	ي • بر مراجع مالي الم	S_{14}	$=\frac{1}{2} \left(Q_1^{k_z} - Q_2^{k_z} + Q_3^{k_z} - Q_4^{k_z} \right)$	دينې د د د د د د د د د د د د
алан А. Алан Ма	. 1 14	$S_3 = \frac{1}{2} (Q)$	$R_{y} + Q_{2}^{R_{y}} + Q_{3}^{R_{y}} + Q_{4}^{R_{y}}$	£	S15	$=\frac{1}{2} (Q_1^{Rx} - Q_2^{Rx} + Q_3^{Rx} - Q_4^{Rx})$	i.
1:	B28	$S_4 = \frac{1}{2} (Q_1)$	$T_{z} - Q_{2}T_{z} + Q_{3}T_{z} - Q_{4}T_{c}$	B24 S	S ₁₆	$=\frac{1}{2} (Q_1^{Ty} + Q_2^{Ty} + Q_3^{Ty} + Q_4^{(Ty)})$	na internet in a sa sa sa
6		$S_5 = \frac{1}{2} (Q_5)$	$T_{x} - Q_{2}T_{x} + Q_{3}T_{x} - Q_{4}T_{x}$		S ₁₇	$= \frac{1}{2} (Q_1^{R_2} + Q_2^{R_2} + Q_3^{R_2} + Q_4^{R_2})_{g_1}$	Та Так
α Παγικά Πάτου θα		$S_6 = \frac{1}{2} (Q_1)$	$R_{y} - Q_{2}R_{y} + Q_{3}R_{y} - Q_{4}R_{y}$	3 A S	S ₁₈	$= \frac{1}{2} (Q_1^{R_x} + Q_2^{R_x} + Q_3^{R_x} + Q_4^{R_x})$	
0. 1 10	B1# 0	$S_7 = \frac{1}{2} (Q_1)$	$T_{z} - Q_{2}T_{z} - Q_{3}T_{z} + Q_{4}T_{z}$	Big S	519	$= \frac{1}{2} \left(\mathbf{Q}_{1}^{Ty} + \mathbf{Q}_{2}^{Ty} - \mathbf{Q}_{3}^{Ty} - \mathbf{Q}_{4}^{Ty} \right)$	en e
4. 	61	$S_8 = \frac{1}{2} (Q_1$	$^{Tx} - \mathbf{Q}_2^{Tx} - \mathbf{Q}_3^{Tx} + \mathbf{Q}_4^{Tx})'$		520	$=\frac{1}{2} (Q_1^{R_2} + Q_2^{R_2} - Q_3^{R_2} - Q_4^{R_2}) $	
4	*2 -	$S_9 = \frac{1}{2} (Q_1)$	$^{Ry}-Q_2^{Ty}-Q_3^{Ry}+Q_4^{Ry}$	0 S	521	$=\frac{1}{2} \left(Q_{1}^{R} + Q_{2}^{R} - Q_{3}^{R} - Q_{4}^{R} \right)$	n an
	B _{3N}	$S_{10} = \frac{1}{2} (Q_1)$	$T^{\tau} + Q_2 T^{\tau} - Q_3 T^{\tau} - Q_4 T^{\tau}$	B _{3g} S	522	$= \frac{1}{2} (Q_1^{Ty} - Q_2^{Ty} - Q_3^{Ty} + Q_4^{Ty})$	
an a	- * - a	$S_{11} = \frac{1}{2} (Q_1)$	$T_{x}+Q_{2}T_{x}-Q_{3}T_{x}-Q_{4}T_{x})$		S ₂₃	$= \frac{1}{2} (Q_1^{R_2} - Q_2^{R_2} - Q_3^{R_2} + Q_4^{R_2})$	en e
ning for the second state of the	, , , , , , , , , , , , , , , , , , , ,	$S_{12} = \frac{1}{2} (Q_1$	$R_y + Q_2 R_y - Q_3 R_y - Q_4 R_y)$		24	$= \frac{1}{2} \left(\dot{Q}_{1}^{3} R_{x} - Q_{2}^{R_{x}} - Q_{3}^{R_{x}} + \dot{Q}_{4}^{R_{x}} \right)$	، المراجع (1999) براج سیمید دورد دیستار (پار ۲۰۱۰)

c) Determination of Rotational Barrier Heights from NMR Data and Calculation of Rotational Frequencies.

In 1953 ANDREW and EADES¹⁴⁾ measured the nuclear magnetic resonance absorption spectrum and the spin-lattice relaxation time of benzene in polycrystalline form between 75°K and 278°K. As the intramolecular contribution of the second moment decreased about one-fourth of the total second moment between 90°K and 120°K they concluded that the reorientations of the molecules about each hexad axis were caused near this temperature. In general the potential barrier hight H of such a hindered rotation of atomic assemblies is given by the following equation;

$$\tau_{c} = \tau_{0} \exp\left(\frac{H}{RT}\right),$$

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where τ_c ; correlation time of thermal motion,⁶

R ; gas constant, 🔿

T; absolute temperature. In solid case the spin lattice relaxation time *T*₁ of such a motion was derived by BLOEMBERGEN¹⁵⁾ and is expressed by ;

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 $\int_{C} \frac{1}{T_1} = C \left(\frac{\tau_e}{1 + \omega^2 \tau_e^2} + \frac{2\tau_e}{1 + 4\omega^2 \tau_e^2} \right),$

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and

where C is a constant and ω is an angular frequency of the magnetic field. So, by measuring the spin lattice relaxation time T_1 , it is possible to decide the H value from the slope of log τ_e against $\frac{1}{T}$. From the data given by ANDREW and EADES, we get two lines (see Fig. 4),-the one between 90°K and 240°K, the other between 240°K and the melting point-whose slopes are decided by the least square method and the resulting barrier heights are;

$H = \begin{cases} 3.7 \pm 0.2 \text{kcal/mol} & (90^{\circ}\text{K} \le T \le 240^{\circ}\text{K}) \\ 10.5 \pm 0.2 \text{kcal/mol} & (240^{\circ}\text{K} \le T \le 270^{\circ}\text{K}) \end{cases}$

(10)

(15)

Er. (16)

The linearity between 90°K and 240°K depends on the decrease of correlation time about hexad axis with temperature increase. On the other hand, it seems that the rotation about two-fold axis which has been interrupted by neighbouring molecules becomes free by the thermal expansion and so τ_c changes its slope abruptly at 240°K. Therefore the former corresponds to hexad axis, rotation and the latter to mainly two-fold ones.

Usually the rotational energy about *m*-fold axis is given by
potential energy;
$$V = \frac{H}{H} \frac{1}{2} (1 - \cos m\varphi)$$
, (11)
kinetic energy ; $u = K = -\frac{\hbar^2}{2I} \frac{d^2}{d\varphi^2}$, (12)

where φ is a rotational angle and I is the moment of inertia. The Schrödinger equation in this case is expressed as follows:

$$\frac{d^2u}{d\varphi^2} + \frac{2I}{\hbar^2} \left\{ E - \frac{H}{2} \left(1 - \cos m\varphi \right) \right\} u = 0 , \qquad (13)$$

where u is the eigenfunction, and E is the eigenvalue. The potential barrier heights determined from NMR data are rather higher than the thermal energies, so we can write approximately Eq. (13) as follows:

$$\frac{d^2u}{d\varphi^2} + (\lambda - \xi^2 \varphi^2) u = 0, \qquad (14)$$

where As (14) is the equation for the well-known harmonic oscillator, wave functions may be expressed by Hermite functions;

$$u_n^{\prime 0} \stackrel{o}{=} \exp\left(-\frac{\xi}{2}\varphi^2\right) H_n\left(\sqrt{\xi\varphi}\right), \quad \lambda = (2n+1)\xi,$$

and the corresponding eigenvalue is

$$E = \left(n + \frac{1}{2}\right) m \hbar \sqrt{\frac{H}{2I}}.$$
(17)
By substituting the values given in a) and c) into Eq. (17) the level energy of hand aris matrice in

to Eq. (17) the level space of hexad axis rotation is By substituting calculated: .0 **σ**ία.

 $\Delta E_6 = (8.2 \pm 0.2) \times 10^{-3} \text{eV}.$

If the second barrier height in Eq. (10) is mainly caused by two-fold axis rotation, the level spacing is: 60 $\Delta E_2 = (6.3 \pm 0.1) \times 10^{-3} \text{ eV}.$

d) Comparison between These Calculated Values and Observed Ones.

	In Table 4 the	frequency spectrum evaluated	from GF	Matrix	Method is	compared	with Raman a	nd
	infrared spectrum.	We also give neutron scattering	ng data in	Table 5.	ast≱, internet 2	e		
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48	So	lid .	р 1. т. на тра м	Liq	uid
t te	GF method by Shimanouchi (—3°C)	Raman spectrum by Fruhling (0°C)	Rot. " } axis	Raman spectrum by Blatz (26°C)	Infrared spectrum by Stanevich (10°C)
Ag	3.5 7.1 9.8	$\begin{array}{c} 4.3 \ (\nu_1) \\ 7.8 \ (\nu_2) \\ \dots \end{array}$	2 y x		· · · · · · · · · · · · · · · · · · ·
	4.1 8.7 12.6	4.3 (v ₁) 13.0(v ₄)	2 7 8 8		
B ₂₈	6.9 8.6 9.4	7.8 (ν ₂) 8.6 (ν ₃)	y W z x	9.3	€
B ₃	7.4 8.9 12.4	8.6 (v3) 13.0 (v4)	у 	 International statements OP OP OP OP OP OP 	
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B _{2µ}	3.8 7.1		G	0 ° a	6.8
B₃₊	5.5		ų	Contraction of the second s	· · · · · · · · · · · · · · · · · · ·

Table 4. Lattice vibrational frequencies of benzene molecule.

(meV)

(j Table 5. Neutron scattering data of liquid benzene. (meV)

Zemlyanov (20°C)	(Glüser (20°C)	Ross (20°C)	cRush (23°C)
0 1.8	n de l'esterie esterie de la composition de la composition de la composition de la composition de la compositio	and the second sec	Anno Annos Anno Annos
3,7 (v1) ⁰			
5.8 (ν2)	≃ 10	° ≃ 7.5	≃ 9.9
(3) 7.6	l a gl¥r i strang a skarta og Sang som som som S ang år som som		la falla siza di segona. Ny s
ο 12.1 [,] (ν ₄)			د میرود و مصحب پرستان کنه می محمد و می معطوم در از ماه در این

Table 6.	Pressure var	iation of rotati	onal relaxatior	time.	ender og en en sender som en en en er som en en er som en er e En er en e	ц ч
Pressure (atm)	1,	200	400	600	700	•
en al al anticipation de la companya	1 44.40		1	10.00		•

$\log_{0} \tau_{c}$	0 -11.14 -11.14	-11.06 11.03
	43	
Toble 7. Extrapõla	ted rotational relaxation time in	Fig. 4.
Temperature (°K)	304.8	278.7
$\log \tau_c$	-11.74	<u>_</u> 11.04

(4) Quasi-crystalline Structure of Liquid Benzene.

Boss and STEJSKAL¹⁶⁾ measured the pressure variation of rotational relaxation time in liquid benzene at 304.8°K. These values are given in Table 6.

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In Table 7 we show the values of $\log \tau_e$ at 304.8°K and at the melting point (278.7°K) by extrapolating the line between 240°K and 270°K in Fig. 4.

By comparing these two tables, we find that, within the limit of experimental errors, $\log \tau_c$ of liquid benzene is just upon the extrapolated straight line of solid benzene in Fig. 4 and by pressurizing the liquid benzene, the relaxation time approaches gradually to that of solid at the melting point. So we may expect that the rotational barrier heights of liquid benzene are approximately equal to those of solid near the room temperature and its rotational structure is nearly the same as solid one.

Moreover self diffusion seems to exist in liquid state. In such a motion NMR spin echo method¹⁷ is very useful to measure the self diffusion coefficient D and to determine the potential barrier height from it using the following equation:

$$D = D_0 \exp(-\beta V_0/V_F) \exp\left(-\frac{H}{RT}\right),$$

where β ; geometrical factor between 0.5 and 1,

 V_0 ; specific volume for closest packing,

V; specific volume,

 $V_F = V - V_0$; free volume.

From this point of view, R. HAUSER, G. MAIER and F. NOACK determined the potential barrier height of self diffusion in liquid benzene from room temperature up to the critical point. We assume here that the potential curve is given by

 $V(X) = \frac{H}{2} \left(1 - \cos \pi \frac{x}{\lambda}\right)$, (λ ; period of the potential curve).

By using the barrier height H=2.0 kcal/mol which is given by above method, we get the level spacing ΔE ;

 $\Delta E = 2.3 \times 10^{-3} \text{ eV}$ ($\lambda_{3} = 6\text{\AA}$)

(5) Discussion and Conclusion

D In (2) we treated intramolecular rotation in biphenyl gas and in (3) we explained the conventional theories which were developed to treat crystalline system; especially solid benzene. We stress here that, by combining above two methods, they may be generalized to treat the biphenyl crystal which include intramolecular rotation. a

(2) As shown in Table 4 BLATZ stressed that, in both cases of Raman and infrared experiments, the average values over all active frequencies except lowest two agree rather well with the peak positions of liquid benzene. Strictly speaking these agreements cannot be accepted straightforwardly, because he compared averages for crystal with the peak positions for liquid. On the contrary we treated solid benzene in (3). c) Our result for hexad axis rotational level from NMR data shows a good agreement with the above-mentioned average value. And this also proves the validity of neglect of two levels.

③ Although it becomes possible to explain the general tendency of inelastic scattering of neutron from above discussions, many problems about fine structure of scattering cross section are remained to be clarified. For example we found that the lowest level 1.8 meV in Table 5 is the same order as our level spacing for diffusion motion obtained in (4). From above discussion we may conclude that in the quasi-crystalline structure of liquid benzene both the degree of freedoms of solid and liquid states coexist.

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1) Z 2) C 3) T 4) F 5) F 6) F	References ZEMLYANOV M.G. and CHERNOPLEKOV H.A. : Atomnaya Energiya 14, 257 (1963). GLÄSER W. : Nucleonik 7, 64 (1965). TARINA V. : J. Chem. Phys., 46, 2273 (1967). Ross D.K., SZABO F.P. and SANALAN Y. : Symposium on Neutron Thermalization and Reactor Spectra SM 96/1 (1967).
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eta meterarria da anticipación de la companya e actividad que esta ومواد المتحول والالا المعادية procession on proceeding and an and the second 7)) Fig. 1 Principal axes of biphenyl molecule.





and

where

Theory of Multiple Scattering of Slow Neutron

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- Suita, Csaka

When the wavelength of a neutron is very long, the neutron interacts with the target system as a whole rather than with the individual atoms, and the effect of multiple scattering becomes important. The Van Hove formula¹⁾ for neutron scattering fails to describe such a process. In the previous paper²⁾, the Van Hove formula is generalized to include the effect of the multiple scattering. On account of the drastic approximations adopted in the paper, however, the formula proposed does not satisfy the condition of detailed balance. The purpose of the present paper is to remedy this defect.

The scattering of a neutron is described by a scattering operator T, which can be rearranged in the following form,

$T = \sum_{\alpha} T_{\alpha} + \sum_{\alpha} \sum_{j \neq \alpha} T_{\alpha} G T_{\beta} + \sum_{\alpha} \sum_{j \neq \alpha} \sum_{\gamma \neq j} T_{\alpha} G T_{\beta} G T_{\gamma} + \cdots ,$	n an s	(1)
$T_a = V_a + V_a G V_a + V_a G V_a G V_a + \cdots$		(2)
$G = \frac{1}{1}$	Ø	 (3)

where G refers to the propagator of the neutron, and H_A and H_n stand for the Hamiltonians of the target atoms and the neutron, respectively. The scattering operator T_a describes the scattering of a neutron by a single atom α in the target system through the interaction potential $V_a = V(r_n - r_a)$, where r_n and r_a are the position operators of the neutron and the atom α , respectively.

In the present formalism, two approximations will be introduced. The first is that the propagators G 5 in the single scattering operator T_a are replaced by that of the free neutron $G_0 = (\varepsilon_i - H_n + i\varepsilon)^{-1}$, although the propagators G in (1) are treated exactly. By virtue of the fact that the propagators G in (1) is retained as it is, the recoil effect to the intermediate neutron is taken into account and the condition of detailed balance is satisfied. The second approximation is

$$\langle k_j | t(\varepsilon_i) | k_l \rangle \simeq -\frac{2\pi l_l^2}{m} a_l$$

where $l(\varepsilon_i)$ is the scattering operator which describes scattering of a neutron by a target atom fixed at the origin and ε_i is the incident energy of the neutron.

Under these two assumptions, we obtain the following expression for the scattering cross section;

$$\frac{d^{2}\sigma}{d\Omega d\varepsilon_{f}} = \sum_{n=0}^{\infty} a^{2} \frac{k_{f}}{k_{i}} \int_{-\infty}^{\infty} \frac{dt}{2\pi \hbar} e^{i(\varepsilon_{f} - \varepsilon_{i})t/\hbar} \int_{-\infty}^{\infty} dt_{1}' \cdots dt_{n}' dt_{1} \cdots dt_{n}$$

$$\times \int d\mathbf{x}_{0}' d\mathbf{x}_{1}' \cdots d\mathbf{x}'_{m} d\mathbf{x}_{i} d\mathbf{x}_{1} \cdots d\mathbf{x}_{n} e^{ik_{f}(\mathbf{x}_{0}' - \mathbf{x}_{0})} e^{-iki(\mathbf{x}_{m}' - \mathbf{x}_{n})}$$

$$\times K_{i}^{(-)}(\mathbf{x}'_{m} - \mathbf{x}'_{m-1}, t'_{m} - t'_{m-1}) \cdots K_{i}^{(-)}(\mathbf{x}_{1}' - \mathbf{x}_{0}', t_{1}' - 0) \cdot K_{i}^{(+)}(\mathbf{x}_{0} - \mathbf{x}_{1}, 0 - t_{1})$$

$$\cdots K_{i}^{(+)}(\mathbf{x}_{n-1}' - \mathbf{x}_{n}, t_{n-1} - t_{n}) G'(\mathbf{x}'_{m}, t'_{m}; \mathbf{x}'_{m-1}, t'_{m-1}; \dots; \mathbf{x}'_{0}, 0 \mid \mathbf{x}_{0}, t; \mathbf{x}_{1}, t + t_{1}; \cdots; \mathbf{x}_{n}, t + t_{n}),$$
where the $(m + n + 2)$ -particle space-time correlation function G is defined by
$$G(\mathbf{x}'_{mi}; t'_{m}; \mathbf{x}'_{m-1}, t'_{m-1}; \cdots; \mathbf{x}'_{0}, t' \mid \mathbf{x}_{0}, t, ; \mathbf{x}_{1}, t + t_{1}; \cdots; \mathbf{x}_{n}, t + t_{n})$$

$$= \sum_{n'} \cdots \sum_{\nu' \neq \mu'} \sum_{n'} \cdots \sum_{\nu' \neq \mu} \ll \hat{\vartheta} (\mathbf{x}'_{m} - \mathbf{r}_{\nu}, (t'_{m})) \hat{\vartheta}(\mathbf{x}'_{m-1} - \mathbf{r}_{n'}(t'_{m-1})) \cdots \hat{\vartheta}(\mathbf{x}'_{1} - \mathbf{r}_{n'}(t_{1}'))$$
and the propagation functions $K_{0}^{i}(\pm)(\mathbf{r}, t)$ are given by

(4)

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Evaluation of Thermal	Neutron	Scattering	Cross	Sections	for	Reactor Mode	erators	JAERI 1181

(8)

$$K_{i}^{(\pm)}(\mathbf{r},t) = \pm \frac{i}{\hbar} \theta_{\pm}(t) K_{i}(\mathbf{r},t), \qquad (7)$$

and

$$K_{i}(\mathbf{r},t) = \frac{2\pi\hbar^{2}}{m} a \int \frac{d\mathbf{k}}{(2\pi)^{3}} e^{i(\varepsilon_{i}-\varepsilon_{k})t/\hbar} e^{i\mathbf{k}\mathbf{r}},$$

$$\theta_{\pm}(t) = \begin{cases} e^{-\varepsilon_{i}t/\hbar} & \text{for } t \ge 0\\ 0 & \text{for } c t \le 0 \end{cases}.$$

The time-dependence of $K_{i\pm}(\mathbf{r}, t)$ is caused by the recoil effect of the neutron. The first term in the right-hand side of (5) is the contribution from the single scattering and coincides with the Van Hove formula. The other terms describe the effect of the multiple scattering. A method obtaining a classical approximation for this multiple scattering cross section is studied along the line of reasoning of the previous paper³⁾. \mathbb{R}^{2}

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Research Works

JAERI 11

Quasi-classical Theory of Slow Neutron Scattering

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Several years ago, VINEYARD¹¹ proposed a prescription of a classical approximation to the Van Hove formula²⁾ for the scattering of a slow neutron. The Vinevard's classical formula for the cross section, however, does not satisfy the condition of detailed balance, because of the obvious defect that the recoil effect of the scattered neutron is completely discarded. In order to correct this defect, great efforts have been made-by many authors, 31, 41 but these results still have some unsatisfactory features. In the previous paper, 51 a new method for obtaining a classical approximation of the scattering cross section is proposed. In this treatment, the recoil effect of the scattered neutron is fully taken into consideration. The condition of detailed balance, however, is not satisfied rigorously, since the effect of the quantum mechanical thermal average is discarded. The aim of the present note is to remedy this defect and to obtain a well-defined classical formula which satisfies the condition of detailed balance rigorously.

For this purpose, we reformulate the quantum-mechanical formula for the scattering cross section so as to be quite adequate to get the classical formula. By making use of the generalized cumulant expansion method⁶⁾, and with the aid of the fluctuation-dissipation theorem for the cumulant function $K_{\alpha\beta}(p,t)$ defined below, we can transform the scattering cross section into the following form

$$\frac{d^2\sigma}{d\Omega d\varepsilon_f} = \left(\frac{m}{2\pi/j^2}\right)^2 |\langle p_f | t(\varepsilon_i) | p_i \rangle|^2 \frac{p_f}{p_i} c^{-\tilde{\rho}\varepsilon/2} \sum_{\alpha_i,\beta} \int_{-\infty}^{\infty} \frac{dt}{2\pi/i} c^{i\varepsilon t/\hbar} \Lambda_{\alpha\beta}(p,t), \qquad (1)$$

where the scattering function $A_{\alpha\beta}$ is defined by

$$\mathcal{H}_{a\beta}(\boldsymbol{p},t) = \exp\left[-\left\{\left(\operatorname{cosec}\frac{\beta h}{2} \frac{d}{dt}\right) \operatorname{Im} K_{a\beta}(\boldsymbol{p},t) + C(\boldsymbol{p})\right\}\right]$$

and m, p_i and p_f are the mass, the initial momentum and the final one of the neutron, respectively. The momentum transfer p and the energy transfer ε are denoted by $p = p_f - p_i$, and $\varepsilon = \varepsilon_f - \varepsilon_i$. The cumulant function $K_{af}(p, t)$ (2) is defined by

$$K_{a\beta}(p,t) = \langle \exp_{s} \left[\frac{i}{\hbar} \left(pA_{1}(t) + p^{2}A_{2}(t) + p^{3}A_{3}(t) + \cdots \right) \right] - \frac{1}{\sqrt{2}} \sum_{cum} (3)$$

where?

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$$A_{1}(t) = r_{ab}(0) - r_{\beta b}(t),$$

$$A_{2}(t) = \frac{1}{2if_{i}} [r_{ab}(0), r_{\beta b}(t)]^{-},$$

$$A_{3}(t) = \frac{1}{12} \left(\frac{1}{if_{i}}\right)^{2} \left(\left[(r_{ab}(0), r_{\beta b}(t)], r_{\beta b}(t)\right]^{-} - \left[(r_{\beta b}(t), r_{ab}(0)], r_{ab}(0)\right],$$

$$(4)$$

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and a second 3 The bracket $\langle \cdots \rangle_{cum}$ designates a cumulant average and exp, indicates the symmetrized exponential. The operator r_{ap} in (4) refers to the component of r_a in the direction of p. The constant of integration C(p) in (2) is determined by the initial condition

$$\int_{0}^{0} C(\boldsymbol{p}) = \operatorname{Re} K_{\alpha\beta}(\boldsymbol{p}, 0) + \left[\left(\operatorname{cot} \frac{\beta h}{2} \frac{d}{dt} \right) \operatorname{Im} K_{\alpha\beta}(\boldsymbol{p}, t) \right]_{t=0}^{0}$$

The condition of detailed balance is of course satisfied in the quantum mechanical formula (1) owing to the extra factor $\exp(-\beta \varepsilon/2)$ and to the following property of the scattering function $\Lambda_{\alpha\beta}$: $\Lambda_{\alpha\beta}(p,t) = \Lambda_{\alpha\beta}(-p',-t),$ (6)

which is valid under the condition that the Hamiltonian of the target system is invariant under space reflection

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(2)

(5)

and time-reversal operation. Since the scattering function $J_{\alpha\beta}$ is written in terms of the commutators A_n ,

- the formula (1) involves the recoil effect of the neutron explicitly, and it will be quite convenient to obtain a well-defined classical formula.
- As already mentioned in the previous paper⁵, all terms in the exponent of the right-hand side of (3) should be retained in the classical limit by replacing the commutators by the classical Poisson brackets $\{\cdots\}_{c}$. Thus the classical limit of (1) is given by

$$\frac{d^2 \sigma^c}{d\Omega d\varepsilon_f} = \left(\frac{m}{2:\hbar^2}\right)^2 |\langle p_f| t(\varepsilon_i)|^2 p_i \rangle e^{-i\delta t/2} \frac{h_f}{p_i} \sum_{\alpha,\beta} \int_{-\infty}^{\infty} \frac{dt}{2\pi\hbar} e^{i\delta t/\hbar} A_{\alpha\beta}^{c}(p,t), \qquad (7)$$

where

$$I_{a\beta}^{c}(\boldsymbol{p},t) = \exp\left[-\left\{\left(\operatorname{coscc}\frac{\beta h}{2}\frac{d}{dt}\right)\left[\operatorname{Im} K_{a,i}(\boldsymbol{p},t)\right]_{\text{classical}} + C^{c}(\boldsymbol{p})\right\}\right], \qquad (8)$$

$$\left[\operatorname{Im} K_{a\beta}(\boldsymbol{p},t)\right]_{\text{classical}} = \operatorname{Im} \ll \exp\left[\frac{i}{E}\left(pA_{1}^{c}(t) + p^{2}A_{2}^{c}(t) + p^{3}A_{3}^{c}(t)\cdots\right)\right] - 1 \gg_{cum}, \qquad (9)$$

(10)

(15)

(16)

and

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where

$$C^{c}(\boldsymbol{p}) = [\operatorname{Re} K_{\alpha\beta}(\boldsymbol{p}, \boldsymbol{\theta})]_{\text{classical}} + \left[\left(\operatorname{cot} \frac{\beta \hbar}{2} \frac{d}{dt} \right)^{\Box} [\operatorname{Im} K_{\alpha\beta}(\boldsymbol{p}, t)]_{\text{classical}} \right]_{t=0}.$$

The bracket $\ll \cdots \gg_{c_{NM}}$ indicates the classical cumulant average, and $A_1^c(t), A_2^c(t) \dots$ are defined by $A_1^c(t) = r_{ab}^c(c) - r_{ab}^c(t),$

$$\begin{aligned} H_{2^{c}}(t) &= \frac{1}{2} \left\{ r_{ab}^{c}(0), r_{bb}^{c}(t) \right\}_{c}, \\ H_{3^{c}}(t) &= \frac{1}{12} \left\{ \left\{ \tilde{r}_{ab}^{c}(0), r_{bb}^{c}(t) \right\}_{c}, r_{bb}^{c}(t) \right\}_{c}, -\left\{ \left\{ r_{bb}^{c}(t), r_{ab}^{c}(0) \right\}_{c}, r_{ab}^{c}(0) \right\}_{c} \right\}_{c} \end{aligned}$$

The function $r_{\alpha\beta}(t)$ is a solution of the classical equation of motion of the target atom. On the basis of the condition that the Hamiltonian is invariant under space reflection and time-reversal operation, we can show classically that $\Lambda_{\alpha\beta}\epsilon$ has the symmetric property : $\Lambda_{\alpha\beta}\epsilon(\mathbf{p}, t) = \Lambda_{\alpha\beta}\epsilon(-\mathbf{p}, -t),$ (12)

The classical expression of the scattering cross section (7), therefore, does satisfy the condition of detailed balance, and furthermore the recoil effect is taken into consideration. When the motions of the atoms are described by linear equations, the Poisson bracket $A_2(t)$ becomes

independent of the statistical average, and the Poisson brackets $A_{s}(t)$, $A_{4}(t)$,... vanish. In this case, the selfpart of the scattering function A_{s} has the simple Gaussian form:

$$A_{s}^{c}(\boldsymbol{p},t) = \exp\left\{-p^{2}\left\{\left(\operatorname{cosec}^{\beta \underline{h}}_{2} \frac{d}{dt}\right)\left[\operatorname{Im} \lambda_{2}^{s}(t)\right]_{\operatorname{classical}}^{n} - \left(\operatorname{cot} \frac{\beta \underline{h}}{2} \frac{d}{dt}\right)\left[\operatorname{Im} \lambda_{2}^{s}(t)\right]_{\operatorname{classical}}\right]_{t=0}\right\}\right], \quad (13)$$
where \circ

$$\left[\operatorname{Im} \lambda_{2}^{s}(t)\right]_{\operatorname{classical}} = \frac{1}{2h}\left\{r_{a}f_{2}^{*}(o), r_{\beta}p^{c}(t)\right\}_{c}.$$

Finally, we shall apply the new classical formula to a simple illustrative example. Consider a system composed of independent isotropic harmonic oscillators with an identical frequency ω and a mass M. The dynamical motion of an atom α in this system is described by

$$\boldsymbol{r}_{\alpha}^{c}(t) = \boldsymbol{r}_{\alpha}^{c}(o) \cos \omega t_{\alpha} + \frac{\partial \boldsymbol{p}_{\alpha}^{c}(o)}{M\omega} \sin \omega t,$$

and then the scattering function $\overline{\neg} l_i^{c_i}$ has the Gaussian form. In (15), $r_a(o)$ and $p_a(o)$ are the initial position and momentum of the atom α , respectively. Substituting (15) into (14), (we have

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$$[\operatorname{Im} \lambda_{2}^{s}(t)]_{\text{classical}} = \frac{1}{2M\hbar\omega} \sin \omega t,$$

and obtain the classical incoherent scattering cross section

$$\frac{d^2\sigma_{inc}}{d\Omega d\varepsilon_f} = a^2_{inc} \frac{p_f}{p_i} e^{-\beta\varepsilon/2} c^{-f^2/M\beta'h^2\omega^2} \sum_{n=-\infty}^{\infty} I_n(z)\partial(\varepsilon+nf_i\omega),$$

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$\frac{1}{\beta} = \frac{\hbar\omega}{2} \operatorname{coth} \frac{\beta\hbar\omega}{2} ,$	 A second s		 A state of the sta	
$z = \frac{p^2}{M\beta' \hbar^2 \omega^2} \sqrt{1 - (\beta' \hbar \omega)}$	7 <u>2)</u> ² •	a a construction of the second s		
Since $[\operatorname{Im} \lambda_2^*(t)]_{\text{classical}}$ has the same form	as the quantum mechar	nical one, the result	(17) based on the	e present -
classical formula coincides precisely with	that obtained in quant	tum-mechanical wa	y.	en al d'an este est
The details of the present work will be	e published in the near	future.		
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Evaluation of Thermal Neutron Scattering Cross Sections for Reactor Moderators 90 Phonon Spectrum and Thermal Neutron Scattering in Light Water Ice Y. NAKAHARA (J. Nucl. Sci. Eng. 5, 31, 268) Japan Atomic Energy Research Institute Ice is a hexagonal crystal, belonging to D_{6k}^{4} , over the temperature range about $-100 \sim 0^{\circ}C^{\circ}$. The unit cell contains four H2O molecules. Each oxygen atom is arranged in the crystal ice as shown in Fig. 1 and is surrounded by four neighboring oxygen atoms in tetrahedral arrangement. We assume that point molecules with mass of H₂O molecules are arranged at the positions of oxygen atoms. In other words, we consider that the lattice vibrations are not affected by molecular rotations and vibrations. We calculated the phonon/spectrum of light water ice at 0°C by means of the root sampling method for a sampling of 1,050 points in an irreducible sampling region of the first Brillouin zone. The force model used in our computation is a non-central force model formulated by FORSLIND, in which interactions with only the nearest neighbors are taken into consideration²). The number of the atomic force constants introduced as model parameters is seven. The values of force constants have been determined by ForsLIND from the experimental values of the elastic constants obtained by JONA and SCHERRER: a' = 2830 $\alpha = 379$ B = 4445 $\epsilon = 1616$ $\kappa = 21549$ r = 3600in dyne/cm $\delta = 2830$ The cell dimensions at 0°C are a=4.5226 Å, c=7.3670 Å. The phonon spectrum of ice at 0°C and dispersion relations in the crystallographic a- and c- axis are n e en strenet per general en ser en en en ser en ser en ser en de service de la service de la service de la s nome l'antide la della de secondation matrix se facturalisation de la service de la service de la service service de la shown in Fig. 2. So far we have neglected the effects of intramolecular motions. The complete frequency distribution for ice can be given approximately by superimposing frequency distributions of hindered molecular rotations and intramolecular vibrations upon the phonon spectrum obtained above by the root sampling method. We approximate frequency distributions of molecular rotations and vibrations by descrete ô-type levels (Fig. 3). The characteristic frequencies for molecular rotations and vibrations of H2O molecules in ice are known from the infrared and Raman spectrocopic investigations1) :- $\omega_r = 0.0756 \text{ eV},$ Ţ, rotation $\omega_{v}^{1} = 0.2033 \text{ eV},$ $\omega_{\nu}^2 = 0.3896 \text{ eV}, \text{ o}$ ^B vibrations $\omega_{\nu}^{3} = 0.4030 \text{ eV}.$ Although intensities of these discrete modes will be somewhat different from the values for liquid water, use the same values as those obtained by NELKIN for liquid water3). The effective masses for molecular ro-02.0 tations and vibrations are m, = 2.32σ mo = 1.95.

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We used the GASKET code written by KOPPEL et al.4) to evaluate the scattering law for ice. The double differential scattering cross section and the scattering law for thermal neutron scattering in light, water ice at 268°K have been measured by HARLING⁵⁾. The calculated values of the scattering law for ice at 0°C are shown in Figs. 4~10, together with the experimental values at -5°C by HARLING. Our calculations resulted in good agreement with the neutron scattering measurements.

The author is indebted to Dr. H. Takahashi for the initial suggestion of this problem and for the most $\mathbf{V}_{\mathcal{B}}$.





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Fig. 4 Scattering law (per H) for light water ice: $\beta = 0.5$ The solid curve is the ų: calculated value at 0°C. Experimental values are from Harling: • for upscattering, o for down-scattering. ÷. \mathcal{O} ιųλ., - Å ÷ ...



Fig. 5 Scattering law (per H) for ice: $\beta = 1.0$. The dotted curve is the calculated scattering law for liquid water at room temperature (based on the Haywood model). Experimental values are from Harling. Also in Figs. 6—10.





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	ffusive or Brownian motion, Mode 3Harmonic
	isotropic vibrations with continuous frequency spect-
	rum, Mode 4 Harmonic anisotropic vibrations with
	continuous frequency spectrum, Mode 5 Harmonic
	isotropic vibrations with discrete frequency spectrum.
	W1-W5 means the weight of each mode. The fre-
	quency (RHO) of mode 3 and the values (OPHON)
	which is deduced multiplying the frequency by the
	factor of $e^{\frac{\pi}{2T}/2}\omega$ sinh $\frac{\omega}{2T}$ are tabulated as a func-
	• tion of OMEGA (w, eV). The frequencies of disc-
	rete oscillators are given in eV with weights and
	maximum number of phonon terms calculated for the
	corresponding oscillators.g



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Frequency Distribution of Graphite and States and
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a ine numerical values of the frequency distribution
of graphite, which must be supplied as input to the
UNCLE code, are given below, The physical mean-
ings of the symbols are as follows.
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$\mathbf{A}(\mathbf{J},\mathbf{I}) = \lim_{\omega^* \to 0} \left[\rho_j^*(\omega) / \omega^2 \right]$
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Frequency Distributions of Be and BeO The numerical values of the frequency distributions of Be and BeO, which must be supplied as input to the UNCLE code, are given below. In the case of an isotropic crystal, or when lattice vibrations are assumed to be isotropic, the $J = 1^{1}$ set is eliminated and RHO21 gives the isotropic frequency distribution.

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