THE SCATTERING OF SLOW NEUTRONS BY ORTHOHYDROGEN

by

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Joint Nuclear Research Center
Ispra Establishment - Italy
Reactor Physics Department
Experimental Neutron Physics
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The result shows that the cross sections depend on the direction of quantization as it is expected.

A numerical calculation for application has been performed in some typical cases and the result is shown in the graphs.
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ABSTRACT

The differential and total slow neutron cross sections by ortho-hydrogen have been derived by taking into account the removal of the degeneracy of the rotational states of the molecule.

The result shows that the cross sections depend on the direction of quantization as it is expected.

A numerical calculation for application has been performed in some typical cases and the result is shown in the graphs.

KEYWORDS
EPITHERMAL NEUTRONS
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QUANTUM MECHANICS
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1. Introduction *)

Solid hydrogen shows a $\lambda$- anomaly in the specific heat at temperatures below 1.6 °K, which is caused by the ortho-H$_2$ molecules $[^{7}1]$. The attempts to explain this anomaly assume that the degeneracy of the rotational ground state of the ortho-H$_2$ molecule is removed by a crystalline field. Consequently, the ortho-H$_2$ molecules are split up in two groups which have a different z component of the rotational momentum, namely $m_J = 0$ and $m_J = \pm 1$. Furthermore, a cooperative ordering process leads to the creation of an ordered state between these two groups $[^{7}2, 3, 4]$. 

The differential scattering and the total cross section of an ortho-H$_2$ molecule have been derived for these two groups of molecules in order to evaluate the possibility of obtaining information about the structure of solid ortho-hydrogen below the $\lambda$ temperature by neutron scattering experiments. The result of this evaluation and the proposal for such an experiment have been published elsewhere $[^{5}]$. 

The theory given by Schwinger and Teller for the scattering of slow neutrons by para- and ortho-H$_2$ molecules in their ground state $[^{6}]$ has been modified in order to obtain for the two groups of ortho molecules separate expressions of the total cross section, of the elastic differential cross section and of the differential cross section with deexcitation of the first rotational state. For the derivation of these expressions it is necessary to introduce as additional variable the angle between quantization axis and momentum transfer vector and to evaluate separately the transition probabilities from the initial states, $m_J = 0$ and $m_J = \pm 1$ for the elastic and inelastic scattering of a neutron by an ortho molecule. The obtained expressions have been evaluated numerically and some typical results are given in the graphs of this report.

*) Manuscript received on 23 April 1970
2. Derivation of the Cross Sections

A. Basic relationships

A scattering process, in which a slow neutron with initial momentum $p^0$ is scattered through an angle $\theta$ into the solid angle $\Omega$ by a $\text{H}_2$ molecule in the center of mass system is considered. The $\text{H}_2$ molecule is initially in a state with the vibrational quantum number $\nu$, the resultant spins $s$ of the two protons, the rotational momentum $J$ and the magnetic quantum number $m_J$. This state is described by the wave function $\phi_{\nu, J, m_J}(\mathbf{r})$, where $\mathbf{r}$ is the distance between the two protons.

The neutron will change the momentum from $p^0$ to $p$ by exciting the molecule into the state defined by the quantum numbers $\nu'$, $s'$, $J'$, $m_J'$, and described by the wave function $\phi_{\nu', J', m_J'}(\mathbf{r})$.

In the chosen system of coordinates the z-axis coincides with the direction of $p^0$ (fig. 1). The direction of quantization $\mathbf{q}$ of the molecule is defined by the angular coordinates and the direction of the momentum $p$ by the scattering angle $\theta$ and $\phi$. (fig. 1).

The scattering cross sections will be derived for all possible transitions for the initial states with the quantum numbers $m_J = 0$, and $m_J = \pm 1$ separately.

The neutron differential cross section is therefore obtained by summing the final states over all possible $m_J$ values. According to previous derivation [6]: the differential cross sections are:
for the transition without spin change and:

(2) \[
\frac{d\sigma_{\nu',J',J',m',m'}}{d\Omega} = \frac{4}{9} \frac{p}{p} (3-2s)(a_o-a_f)^2 \sum_{m_y} \left| \sum_{m_y} \left( \frac{r_{\nu'} r'_{J',J'} m_y}{r_{\nu}} \right) \alpha \beta \gamma \right|^2 \]

for the transitions with spin change; \( a_0 \) and \( a_f \) are the singlet and triplet state scattering lengths for the free proton \((*)\). Both (1) and (2) obey the condition \((-1)^J = (-1)^S\) imposed by the Pauli exclusion principle; as a consequence the transition selection rule \((-1)^{J+S} = (-1)^{J'+S'}\) has to be observed.

In the temperature range of interest here the vibrational quantum number \( \nu \) is always zero. In addition the considered neutron energies are too low to excite vibrations. For these reasons the eigenfunction of the molecule is given by the expression:

(3) \[
\Phi_{J,m} (r, \theta, \chi) = \frac{1}{r_e} \left[ \delta (r-r_e) \right] \frac{1}{2} Y_{J,m} (\theta, \chi)
\]

where \( r, \theta, \chi \) are the molecule coordinates with respect to a system, where \( z \)-axis coincides with the direction of quantization \( q \); \( r_e \) is the equilibrium nuclear separation; \( Y_{J,m} (\theta, \chi) \) is the spherical harmonic of \( J \)th degree and \( m \)th order, normalized to 1 \((**))

\( (*) \) \( a_o = -2.373 \times 10^{-12} \) cm

\( a_f = 0.537 \times 10^{-12} \) cm

\( (**)) \)

For the notations used in the following, see J.M Blatt and V.F. Weisskopf, Theoretical Nuclear Physics 1960, 781, 793, and M.E. Rose, Elementary Theory of Angular Momentum, 1957.
If we write \( E \) and \( E' \), for the internal energy of the molecule in the state belonging to the quantum numbers \( J \) and \( J' \) with \( v = v' = 0 \), the conservation of energy provides:

\[
\alpha = \alpha^2 \frac{4}{3} \frac{M^2}{\hbar^2} (E - E')
\]

with

\[
\alpha = \frac{1}{\hbar} \mu^2 \quad \alpha' = \frac{1}{\hbar} \mu' \mu^2
\]

\( M \) is the neutron mass.

After expanding the functions \( \cos \left[ \frac{1}{2} \left( \mathbf{r} - \mathbf{r}' \right) \cdot \mathbf{r} \right] \) and \( \sin \left[ \frac{1}{2} \left( \mathbf{r} - \mathbf{r}' \right) \cdot \mathbf{r} \right] \) of the expressions (1) and (2) in spherical harmonics and integrating over \( r \), we obtain:

\[
(4) \quad \frac{d \sigma_{s', s; j, s, m_j}}{d \omega} = \frac{\alpha}{\alpha^*} \mathcal{C}_{s, s'} \sum_{m'' = -J'}^{J'} 2 \pi \frac{k^2}{\hbar} \left| \frac{1}{I_{s', s; (1)}} \int \psi_{l, m, m'} \left( \Theta, \varphi \right) \varpi \left( \Theta, \varphi \right) \right|^2
\]

with

\[
\mathcal{C}_{s, s'} = \frac{4}{9} \left( (s + 1)(s + 2) \right)^2 \left[ (s + 1) (1 - 2s) \right]
\]

\( \varpi = \frac{k \tau}{2} ; \quad \kappa = \frac{1}{\hbar} (\mathbf{r} - \mathbf{r}') \)

where \( \mathcal{J}_1 \) \( (\mathbf{r}) \) is the spherical Bessel function of fractional order of first kind of the argument \( \mathbf{r} \); \( \Theta \) and \( \varphi \) are the angular coordinates of the \( \mathbf{r} \) vector with respect to a system, where the \( z \)-axis coincides with the direction of quantization and:

\[
(5) \quad \left| \int_{\mathbb{S}^2} \psi_{l, m, m'} \left( \Theta, \varphi \right) \varpi \left( \Theta, \varphi \right) \right|^2 = \int_{\mathbb{S}^2} \chi_{l, m} \left( \Theta, \varphi \right) \chi_{l, m}^* \left( \Theta, \varphi \right) d \omega
\]

The expression (5) is developed, by using the Clebsch-Gordan expansion of \( \chi_{l, m} \left( \Theta, \varphi \right) \chi_{l, m}^* \left( \Theta, \varphi \right) \) and the property of orthogonality of the spherical harmonics; one gets:
with the conditions:
\[ m = m_l - m_j, \quad |j' - j| = l = j + j'. \]

By remembering that \( C_{j', j^*} (1, 0, 0, 0) = 0 \) unless \((-1)^{l+j+j'} = 1\), the relation (4) is rewritten as:

\[
\frac{d\sigma_{4j}^{(L, m, m_l, m_j, \alpha_{l', \alpha_j})}}{d\Omega} = \sum_{l', l''} \frac{1}{((2l+1)(2l'+1))^{1/2}} \left[ \sum_{m'} C_{j} (1, m; l') C_{j'} (l'', m'; l''') \right] x \left[ \sum_{m''} C_{j''} (l, m''; m_l, m_j) C_{j'} (l', m''; m_j, m_j') \right] C_{j''} (l', m''; m_j, m_j') \gamma_{l, m} (\theta, \varphi) \gamma_{l', m} (\theta, \varphi) \gamma_{l''} (\theta, \varphi) \gamma_{l'''} (\theta, \varphi)
\]

The following coefficients and functions are introduced:

\[
C_{\lambda, \mu}^{(L)} = \left[ \frac{(2l+1)(2L+1)^2}{2\lambda + 1} \right] C_{L, \mu} (\lambda, 0; 0, 0);
\]

\[
G_{m, m'}^{(L, m, m)} (L, L) = C_{L, \mu} (\mu', \mu; m, m') C_{L, \mu'} (\mu, \mu; m', m')
\]

\[
\psi_{m}^{(L, m, m)} (\theta, \varphi) = \gamma_{l, m} (\theta, \varphi) \gamma_{l', m} (\theta, \varphi) \gamma_{l''} (\theta, \varphi)
\]

which have the properties:

\[
C_{\lambda, \mu}^{(L)} = 0, \quad \text{unless } (-1)^{\lambda + L + \mu'} = 1
\]

\[
G_{m, m'}^{(L, m, m)} (L, L') = (-1)^{m' + m''} G_{m, m'}^{(L, m, m)} (L, L')
\]

\[
\psi_{m}^{(L, m, m)} (\theta, \varphi) = \psi_{m}^{(L, m, m)} (\theta, \varphi)
\]
The expression of the differential cross section for all the permitted transitions from the initial state belonging to $J$, $s$, $M$, into the final state belonging to $J'$, $s'$ is now given by:

\[
\frac{d\sigma}{d\Omega} = \sum_{\ell \geq |m'|} C_{\ell} \sum_{m, m'} \sum_{\ell' \geq |m'|} C_{\ell'} \sum_{m, m'} \left\{ C_{m, m'}^{(\ell)} C_{m', m}^{(\ell')} \right\} \sum_{m, m'} \left\{ C_{m, m'}^{(\ell)} C_{m', m}^{(\ell')} \right\} \left\{ Y_{m, m'}^{(\ell)} Y_{m', m}^{(\ell')} \right\}
\]

The cross section (8) depends on the direction $\mathbf{q}$, through the angles $\theta$ and $\phi$ and has the same form for the initial states $m_J$ and $-m_J$.

**B. The formula of the differential cross section for the ortho-H$_2$ molecule**

For the reasons explained in the introduction, the further derivation will be limited to the cross section of the ortho-H$_2$ molecule in the ground state, i.e. $J = 1$.

The condition $J = 1$ enables us to transform the expression (8) by writing the Clebsch-Gordan coefficients explicitly:

\[
\frac{d\sigma}{d\Omega} = \sum_{\ell \geq |m'|} C_{\ell} \sum_{m, m'} \sum_{\ell' \geq |m'|} C_{\ell'} \sum_{m, m'} \left\{ C_{m, m'}^{(\ell)} C_{m', m}^{(\ell')} \right\} \sum_{m, m'} \left\{ C_{m, m'}^{(\ell)} C_{m', m}^{(\ell')} \right\} \left\{ Y_{m, m'}^{(\ell)} Y_{m', m}^{(\ell')} \right\}
\]

We recall that $\mathcal{L} = \frac{3}{2}$

\[
8 \pi \sum_{m=-1}^{1} m^2 \left| \chi_{l, m} \right|^2 = l(l+1)(1-\cos^2\theta)
\]
By developing (9); taking into account (10), one gets:

\[
\frac{d\sigma_{\text{el},\text{O}} (\theta, \alpha_s)}{d\Omega} = \frac{\alpha_c}{\alpha_s} \sum_{l=1}^{\infty} \left\{ \frac{1}{4} \left( \frac{3}{2} (3 |m_j|-2)(3 \cos^2 \theta_j-1) \right) \delta_2 (\hat{\sigma}) \left[ \frac{2 \hat{\sigma}_1}{J_0 (\hat{\sigma})} - \frac{\hat{\sigma}_2}{J_0 (\hat{\sigma})} \right] \right\}
\]

The expression (11) is the differential slow neutron cross-section in the center of mass system for an ortho-hydrogen molecule in the ground state with the magnetic quantum number \( m_j \).

The most interesting transitions from the ground state \( J = 1 \) are into the states \( J' = 1 \), and \( \Gamma' = 0 \).

In the case of elastic scattering, i.e. \( J = J' = 1 \) the cross section is

\[
\frac{d\sigma_{\text{el},\text{O}} (\theta, \alpha_s)}{d\Omega} = \frac{\alpha_c}{\alpha_s} \sum_{l=1}^{\infty} \left\{ \frac{1}{4} \left( \frac{3}{2} (3 |m_j|-2)(3 \cos^2 \theta_j-1) \right) \delta_2 (\hat{\sigma}) \left[ \frac{2 \hat{\sigma}_1}{J_0 (\hat{\sigma})} - \frac{\hat{\sigma}_2}{J_0 (\hat{\sigma})} \right] \right\}
\]

and in the case of inelastic scattering, i.e. \( J = 1 \) and \( J' = 0 \)

\[
\frac{d\sigma_{\text{el},\text{O}} (\theta, \alpha_s)}{d\Omega} = \frac{\alpha_c}{\alpha_s} \sum_{l=1}^{\infty} \left\{ \frac{1}{4} \left( \frac{3}{2} (3 |m_j|-2)(3 \cos^2 \theta_j-1) \right) \delta_2 (\hat{\sigma}) \left[ \frac{2 \hat{\sigma}_1}{J_0 (\hat{\sigma})} - \frac{\hat{\sigma}_2}{J_0 (\hat{\sigma})} \right] \right\}
\]

in this process, the neutron gains an energy of 0.023 eV.

C. The formula of the total cross section for the ortho-H\(_2\) molecule

From the definition of \( \gamma \), \( \alpha_o \), and \( \alpha \) it follows (fig. 1)
\[ \cos \theta = \frac{1}{2 \alpha \omega} \left( \alpha \cos^2 \phi + \omega^2 \right); \quad \sin^2 \Phi = \frac{4 \omega}{\alpha \omega} \cos \phi \]

Since (fig. 1) \[ \sin(\Phi) = \frac{\alpha \cos \phi}{2 \omega} \]

it is easy to find:

\[ \cos \theta = \frac{1}{2 \frac{\alpha}{\sqrt{\omega}}} \left\{ \alpha \sin \phi \sin \Phi \cos (\phi - \phi) + (\alpha \cos \phi - \alpha) \cos \Phi \right\} \]

\[ \int_{\alpha}^{2 \pi} \left( \frac{3 \cos^2 \Phi - 1 \Phi}{4 \omega} \right) \left( \frac{3 \cos^2 \Phi - 1 \Phi}{4 \omega} \right)^2 \left( \alpha^2 - \alpha \right)^2 + 2 \left( \alpha^2 - 3 \alpha \right) \Phi + 12 \Phi^3 \]

Therefore the total cross section is obtained by the integration of (11) over the whole solid angle described by \( \Phi \) and \( \Phi \):

\[ \sigma_{\text{tot}}^{(m)}(\alpha, \omega) = \frac{\beta}{\sqrt{\omega}} \left\{ \frac{1}{4} \left( \alpha^2 - \alpha \right)^2 \right\} \]

\[ \left( \frac{3 \cos^2 \Phi - 1 \Phi}{4 \omega} \right)^2 \left( \alpha^2 - \alpha \right)^2 + 2 \left( \alpha^2 - 3 \alpha \right) \Phi + 12 \Phi^3 \right\} \]

The previous integral can be solved with the help of the recurrence formulae \( 8 \) for the Bessel functions. The final result is:

\[ \sigma_{\text{tot}}^{(m)}(\alpha, \omega) = \frac{\pi \beta}{\sqrt{\omega}} \left( \frac{2 \gamma}{\alpha} \right) \left\{ \frac{3 \cos^2 \Phi - 1 \Phi}{4 \omega} \right\} \left( \alpha^2 - \alpha \right)^2 + 2 \left( \alpha^2 - 3 \alpha \right) \Phi + 12 \Phi^3 \]

\[ + 6 \left( \frac{\alpha^2 - \alpha \omega}{2} \right) \left( \frac{3 \cos^2 \Phi - 1 \Phi}{4 \omega} \right) \left( \alpha^2 - \alpha \right)^2 + 2 \left( \alpha^2 - 3 \alpha \right) \Phi + 12 \Phi^3 \right\} \]

\[ \frac{\alpha + \omega}{2} \]

\[ \frac{\alpha - \omega}{2} \]
Where:

\[ C_l(2x) = \int_0^{2x} \frac{1 - \cos t}{t} \, dt; \]

\[ q_l(x) = \delta_l(x) - \frac{2l + 1}{2l + 1} \delta_{l+1}(x) - \frac{2l + 3}{2l + 1} \delta_{l-1}(x) + \frac{l(l+1)}{k(k+1)} \delta_k(x); \]

\[ u_l(x) = (l+1)^2 \delta_l(x) - (2l+1)^2 \delta_{l+1}(x) - (l+1) \delta_l(x) + 4l(l+1) \delta_{l-1}(x); \]

(16)

In the most interesting cases \( J' = 1 \) and \( J'' = 0 \) the total cross sections are:

\[ \sigma^{(m)}_{\text{tot}}(\alpha_e) = \frac{3\pi C_{\text{int}}}{\alpha_e^2} \left[ \sigma \{ \text{C}(2\alpha_e) - 2\alpha_e^2 \delta_l(\alpha_e)^2 + 2\alpha_e \delta_l(\alpha_e) \delta_l(\alpha_e) - 3\delta_l(\alpha_e)^2 \} + \right. \]

\[ \left. + \frac{(3\pi - 2)(1 - 3 \cos^2 \theta)}{2 \alpha_e^2} \left\{ 3 \alpha_e^2 \delta_l(\alpha_e)^2 + 2 \alpha_e \delta_l(\alpha_e) \delta_l(\alpha_e) + 2 \alpha_e^2 \delta_l(\alpha_e)^2 + \delta_l(\alpha_e)^2 \right\} \right] - \]

\[ - 2 (\alpha_e^2 + 3) \text{Cln}(2 \alpha_e); \]
and

\[
\sigma_{\rho, \rho'}(\alpha, \alpha') = \frac{e_{\rho \rho'}^2}{\alpha_s^2} \left[ \alpha \left[ \cos(2\beta) - \beta^2 \beta^2 \alpha_s^2 \right] + \beta^2 \beta^2 \alpha_s^2 \right] + \\
\frac{(3|m| - 2)(1 - 3 \cos^2 \theta)}{4 \alpha_s^2} \left[ 2\beta^2 (3\alpha_s^2 - 6) \beta^2 \beta^2 \alpha_s^2 \right] - \\
\frac{3}{8} \left[ (\alpha_s^2 - 6)^2 \beta^2 \beta^2 \alpha_s^2 \beta^2 \beta^2 \alpha_s^2 \right] + 12 \beta^2 \beta^2 \beta^2 \beta^2 \beta^2 \alpha_s^2 - 2(3\alpha_s^2 - 6) \beta^2 \beta^2 \alpha_s^2 \right]
\]

(D. Conclusions)

The differential and total cross section for the two types of molecule \( m = 0 \) and \( m = 1 \) have been numerically calculated and the most significant results are shown in the figures.

According to these results one may conclude that the most promising experiment is the measurement of the differential cross section for a single crystal, because one can analyse one of the two processes: \( \tau = 1, \tau' = 1; J = 1, J' = 0 \); for the total cross section the two processes overlap and no real difference is detectable.

According to these results it is possible to obtain information about the solid ortho-hydrogen below the \( \lambda \) -point by measuring the differential cross section of a single crystal of \( o-H_2 \) for temperatures above and below the \( \lambda \) -temperature. The implications and the possible results have been discussed elsewhere.

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Fig. 2- Ortho-$H_2$ differential elastic cross-section $J=1, J'=1$ as function of incoming neutron energy, for a scattering angle of $\theta_o = 0$ and $\frac{\pi}{2}$, and for the angle $\theta_o = \frac{\pi}{2}$.

- $m_J = 0$
- $m_J = \pm 1$
Fig. 3 - Ortho-H₂ differential inelastic cross-section \( J=1, J'=0 \) as function of incoming neutron energy, for a scattering angle of \( \frac{\pi}{2} \) and for the angle \( \theta_o=0 \) and \( \theta_o=\frac{\pi}{2} \).
Fig. 4 - Ortho-$^3$H$_2$ differential elastic cross-section $J=1, J'=1$ as function of the scattering angle $\Phi$ for a neutron of incoming energy $E=20$ meV, for the angle $\Theta_0 = 0$ and $\Theta_0 = \frac{\pi}{2}$

$O$ for $m_J = 0$

$\triangle$ for $m_J = \pm 1$
Fig. 5 - Ortho-$\text{H}_2$ differential inelastic cross-section $J=0$, $J'=0$ as function of the scattering angle $\phi$, for a neutron of incoming energy $E=20$ meV and for the angle $\Theta_0=0$ and $\Theta_0=\frac{\pi}{2}$.

- $m_J=0$ (open circles)
- $m_J=\pm1$ (open triangles)
Fig. 6—Ortho-$H_2$ elastic and inelastic total cross-section as function of incoming neutron energy, for an angle of the direction of quantization, with the incoming direction, $\xi = 0$

- $J = 1$, $J' = 1$, $m_J = 0$
- $J = 1$, $J' = 0$, $m_J = 0$
- $J = 1$, $J' = 1$, $m_J = \pm 1$
Fig. 7 - Ortho-$H_2$ elastic and inelastic total cross-section as function of incoming neutron energy, for an angle of the direction of quantization, with the incoming direction. $\xi = \frac{\pi}{2}$

- $J = 1, J' = 1, m_J = 0$
- $J = 1, J' = 0, m_J = 0$
- $J = 1, J' = 1, m_J = \pm 1$
- $J = 1, J' = 0, m_J = \pm 1$
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Alfred Nobel
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