[parahydrogen & orthohydrogen] The scattering cross sections of parahydrogen and orthohydrogen

In {§3.6:113} the differential cross section for a system of N identical nuclei located at fixed positions $\{\vec{\mathbf{r}}_1, \vec{\mathbf{r}}_2, ...\vec{\mathbf{r}}_i, ...\vec{\mathbf{r}}_N\}$ with assumed uncorrelated nuclear spins, $\{\vec{\mathbf{I}}_i, M_{I,i}\}$, is written as the sum of coherent- and incoherent-scattering contributions:

$$\frac{d\sigma(Q)}{d\Omega} = b_{coh}^2 \sum_{i=1}^{N} \left| \left\langle \exp\left[-i\vec{\mathbf{Q}} \cdot \vec{\mathbf{r}}_i \right] \right\rangle \right|^2 + N b_{inc}^2 . \qquad (3.108)$$

However, for molecules containing identical nuclei, the requirement for an antisymmetric overall wavefunction imposes a definite spin correlation so that (3.108) no longer holds. Solid hydrogen is an important example. The addition of the two proton spins $(I = 1/2)$ in H_2 results in $(\text{singlet}, J = 0;\ \text{antisymmetric})$ parahydrogen and $(\text{triplet}, J = 1;\ \text{symmetric})$ orthohydrogen. The overall wavefunction of the molecule is made up as the product of electronic, vibrational, rotational, and spin parts. Because the electronic and vibrational wavefunctions are symmetric, the rotational wavefunctions for parahydrogen and orthohydrogen must be symmetric and antisymmetric, respectively. At the lowest temperature the system condenses to the ground state which is parahydrogen with zero rotational angular momentum. For solid hydrogen at low temperatures, (3.108) is replaced by a more general form:

$$\frac{d\sigma(Q)}{d\Omega} = \frac{16}{9} \left\langle \chi(J) \left| \left\langle \left| \sum_{i=1}^{2} \exp\left(-i\vec{\mathbf{Q}} \cdot \vec{\mathbf{r}}_i \right) \left[b_{coh} + \frac{\vec{\sigma} \cdot \vec{\mathbf{I}}_i}{2I+1} (b_+ - b_-) \right] \right|^2 \right\rangle \right| \chi(J) \right\rangle . \qquad (1)$$

In the above equation, $\frac{16}{9} = \left(\frac{A_n A_H}{A_n + A_H} \right)^{-1} \left(\frac{A_n A_{H_2}}{A_n + A_{H_2}} \right)$, where the first factor is the inverse of the reduced mass for n-^{1}H scattering necessary that is needed to convert the scattering length for free H atom to that for bound H atom, see (3.55), and the second factor accounts for the scattering of a neutron from the nucleus bound in an H_2 molecule. (Note that this factor becomes unity if the molecule is infinitely heavy.) The matrix element is the same as that in (3.95), and finally, the $\langle ... \rangle$ denotes the average over the spin states of the unpolarized neutrons.

To evaluate the matrix element of (1) for unpolarized neutrons, we make use of the relations:

$$\left\langle \vec{\sigma} \cdot \vec{\mathbf{I}}_i \right\rangle = 0, \quad \left\langle \left(\vec{\sigma} \cdot \vec{\mathbf{I}}_i \right)^2 \right\rangle = I(I+1), \quad \text{and}$$

$$\left\langle \left[\vec{\sigma} \cdot \left(\vec{\mathbf{I}}_1 + \vec{\mathbf{I}}_2 \right) \right]^2 \right\rangle = \left\langle \left(\vec{\sigma} \cdot \vec{\mathbf{J}} \right)^2 \right\rangle = J(J+1) = 2I(I+1) + 2\left\langle \vec{\sigma} \cdot \vec{\mathbf{I}}_1 \right\rangle \left\langle \vec{\sigma} \cdot \vec{\mathbf{I}}_2 \right\rangle \text{ to obtain}$$

$$\frac{d\sigma(Q)}{d\Omega} = \frac{16}{9} b_{coh}^2 \left| \sum_{i=1}^{2} \exp\left(-i\vec{\mathbf{Q}} \cdot \vec{\mathbf{r}}_i \right) \right|^2 + \frac{32}{9} b_{inc}^2 \left\{ 1 + \left[\frac{J(J+1)}{2I(I+1)} - 1 \right] \cos \vec{\mathbf{Q}} \cdot \left(\vec{\mathbf{r}}_2 - \vec{\mathbf{r}}_1 \right) \right\} . \qquad (2)$$

Compared to (3.108) we note that the spin correlation in parahydrogen and orthohydrogen manifests itself in the *J*-dependent multipliable factor of incoherent scattering. The differential cross sections of parahydrogen (J = 0) and orthohydrogen (J = 1) for low-energy unpolarized neutrons are obtained from (2) by integrating over the solid angles with $I = 1/2$:

$$\sigma_{para} = \frac{16\pi}{9}\left(b_{H,-} + 3b_{H,+}\right)^2, \tag{3}$$

and

$$\sigma_{ortho} = \frac{16\pi}{9}\left[\left(b_{H,-} + 3b_{H,+}\right)^2 + 2\left(b_{H,+} - b_{H,-}\right)^2\right]. \tag{4}$$

In real systems such as a solid-hydrogen neutron moderator maintained at a temperature between 10 to 20 K, the hydrogen molecules cannot achieve 100% conversion to parahydrogen (even with the application of a catalyst), and neutrons may loss/gain energy by de-excitation/excitation between the para- and ortho-states. Therefore, accurate measurements of the cross sections of parahydrogen and orthohydrogen are of practical importance, e.g., for characterization of the moderator performance. For more details see [hydrogenous moderators].

References:

Schwinger, J. and E. Teller (1937), "The scattering of neutron by ortho- and parahydrogen", *Phys. Rev*. **52**, 286-295.

Squires, G. L. and A. T. Stewart (1955), "The scattering of slow neutrons by ortho- and para-hydrogen", *Proc. Royal Soc. London*, **A230**, 19-32.