Scattering cross sections and transport properties of H_2 and D_2 as obtained from a synthetic model

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ABSTRACT: In the frame of a synthetic scattering function, the interaction of slow neutrons with H_2 and D_2 is described in a simple way. The main advantage of the synthetic model is contained in the analytical expressions it produces for the total cross section and the isotropic and anisotropic energy-transfer kernels. They allow a very fast evaluation of neutron scattering and transport properties in liquid hydrogen and deuterium, including variation of the concentration in the ortho and para forms. The calculations are compared with available experimental data, showing very good agreement. The results presented here are relevant to cold neutron source design.

Introduction

As examples of simple molecular systems, liquid hydrogen and deuterium have attracted considerable interest from a theoretical point of view, whereas their unique neutronic properties have made them a natural choice as moderating materials for the production of cold neutrons.

After the early total cross-section measurements performed by Squires and Steward[1] on liquid H_2 and the theoretical work of Sarma[2], many calculational techniques were developed, most of them based on the gas model of Young and Koppel[3]. As a consequence, the differentiating feature of those bound atom models has been in the treatment of the translational motion of the molecular unit, some of them[4,5] following the lines of the Egelstaff-Schofield prescription for liquid systems[6], while others have adopted a continuous frequency spectrum for this mode[7,8]. However, there is still a lack of experimental information on the neutron field behavior in those systems[9].

The transformation properties of the total wavefunction in a homonuclear diatomic molecule causes the total nuclear spin I and the total angular momentum J to be correlated, thus producing a well-defined "selection rule" that governs the transitions between states corresponding to those quantum numbers[10]. Those correlations are especially important in the case of H_2 and D_2 at low temperatures, where not many rotational levels are excited and, consequently significant interference effects show up in the neutron cross sections for the ortho and para forms.

A knowledge of the full molecular dynamics is generally required to compute the cross sections for the neutron-molecule interaction. However, many neutron

properties can be evaluated through the use of a simplified scheme to represent the actual frequency spectrum, and this is the basic idea behind the development of the Synthetic Scattering Law[11]. The latter has been successfully applied to the description of neutron scattering and transport properties in several hydrogenous materials[12]. We present here some results of the synthetic model for H_2 and D_2 and compare them with available information.

The model for H_2 and D_2

The basic hypotheses borne into the synthetic scattering function have already been described[11,12], so that only its main characteristics will be briefly commented upon here. The actual frequency spectrum of the system is lumped into discrete harmonic oscillator modes, each of these having an occupation number for the excited levels controlled by the system's temperature and an associated effective mass, which is a measure of its relative weight. Furthermore, collision-induced transitions between those levels are allowed in the neutron-molecule interaction, which in turn depends on the incident neutron energy E_0. In this way, a synthetic scattering function $T(Q, w, E_0)$ is obtained, where the effects of the molecular dynamics on the cross sections is represented through the variation of an effective mass, temperature and vibrational factor.

Our model for H_2 and D_2 is built on the basis of the Young-Koppel[3] formalism to describe the rotational elastic and one-phonon inelastic cross sections, together with the prescriptions of the general synthetic model for the vibrational and translational forms of the molecular scattering function. Concerning this latter mode, an additional Einstein oscillator was introduced to represent the low-energy collective excitations, as it is well known that a simple gas model is not adequate to predict some scattering properties at low neutron energies[4,5,13]. The complete set of input parameters for our model calculations has been given elsewhere[14].

Intermolecular interference effects show up in the measured total cross section of liquid H_2 and D_2 at low energies (~0.003 eV)[15], where they partially cancel the intramolecular interference contribution for neutron wavelengths longer than the average distance between molecular centers. We have taken this behavior into account in a crude manner by imposing a complete cancellation of the coherent elastic scattering, whereas a more rigorous treatment of these effects should be based on the consideration of the static structure factor of the liquid system[16].

By virtue of its simple form, the synthetic model produces analytical expressions for several magnitudes of interest in neutron thermalization problems, and consequently evaluations involving changes of parameters (ortho:para concentration, density, temperature, weighting spectrum) can be easily performed in a fast and accurate manner.

Results

We show in Fig. 1 the results of our model, together with the experimental data of Seiffert[15] for the total cross section of para- and normal-hydrogen. The discrepancies observed at the low energy side are due to the crudeness in the treatment of the

translational motion in the case of n-H_2 and the forced neutralization of scattering components in the other case (p-H_2). Besides those differences, the overall agreement is reasonably good.

The total cross-section data of Seiffert for liquid D_2 are compared in Fig. 2 with the synthetic model results for ortho- and normal deuterium. The agreement between experiment and calculation in this case is not as good as for H_2, but still quite satisfactory.

Figure 3 shows the evaluated energy-transfer kernel for liquid H_2 at an incident neutron energy $E_0 = 0.018$ eV. It is observed that o-H_2 presents an almost gas-like behavior at this energy, while p-H_2 shows the effect of the $J = 0 \geq 1$ flipping transition through a pronounced down-scattering contribution.

We used the analytically generated scattering kernels to evaluate some other integral properties. The slowing down power $\xi\sigma$ (per atom) of ortho- and para-hydrogen is shown in Fig. 4, while the results corresponding to deuterium are presented in Fig. 5. In the case of o-H_2 (Fig.4), the large negative values of $\xi\sigma$ even at energies above 0.001 eV, reflect the importance of upscattering processes through the transition $J = 1 \geq 0$.

Besides the macroscopic density, neutron transport parameters are strongly dependent on the ortho:para ratio as well as on the neutron spectrum. We have adopted a Maxwellian distribution as a first order approximation to the actual spectrum, with different characteristic temperatures T_M to simulate the spectrum hardening due to leakage in large buckling geometries. The results of our model for the neutron-transport-mean-free path λ_{tr} in liquid hydrogen and deuterium are shown in Figs. 6 and 7, respectively, over temperature ranges centered around the accepted equivalent Maxwellian temperature[17].

The dependence of λ_{tr} on the ortho:para concentration in H_2 is shown in Fig. 8, where our results ($T_M = 37$ K[17]) are compared with Würz's calculations. A satisfactory agreement between both evaluations is observed over most of the range, except in the high para- concentration limit where our model gives larger values.

Finally, Fig. 9 shows calculated scalar fluxes for two concentrations of parahydrogen in liquid H_2 at 20 K, together with Maxwellian distributions corresponding to T = 37 K.

Conclusions

We have applied the synthetic scattering formalism to produce a simple model to describe neutron scattering and transport in liquid H_2 and D_2. Based on the analytical expressions derived from the model, we evaluated several magnitudes of interest in cold neutron source design. From the comparison of its predictions with the available information and its ability to produce in a fast way the scattering matrices for any desired physical condition, we believe that this model could be a useful tool for the above mentioned design and optimization work.

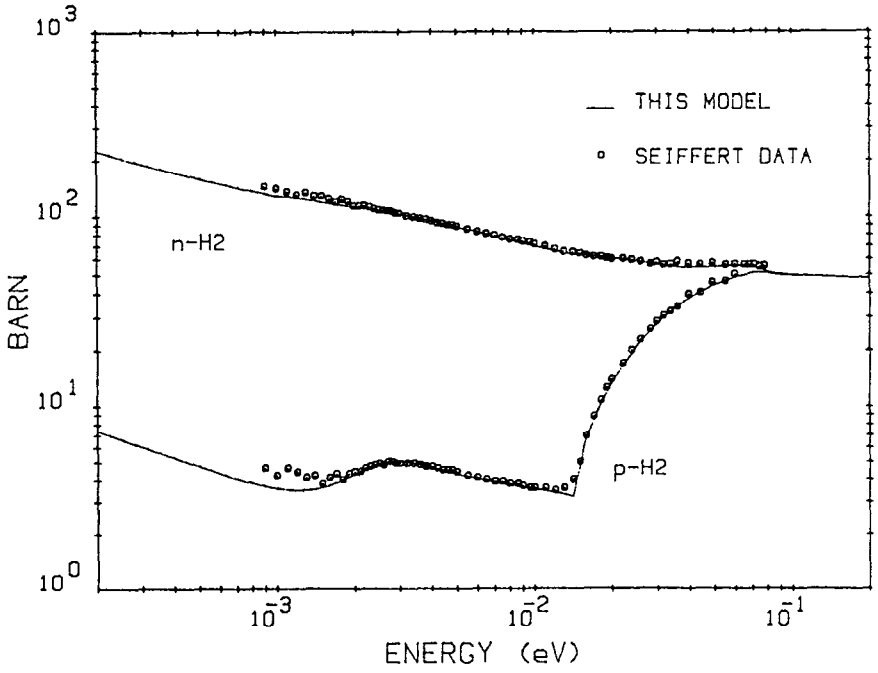

Fig. 1 Total cross section of normal and para hydrogen.

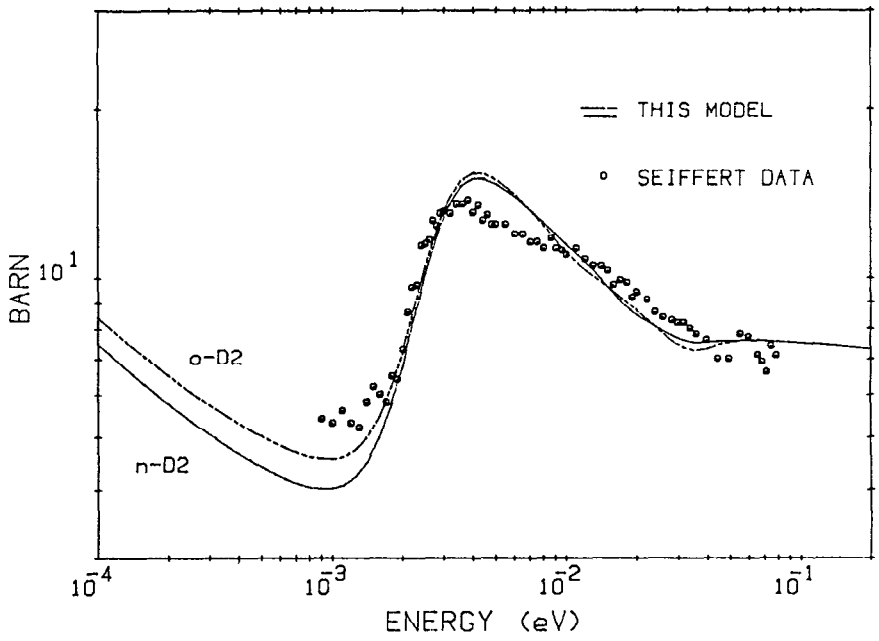

Fig. 2 Total cross section of normal and ortho deuterium.

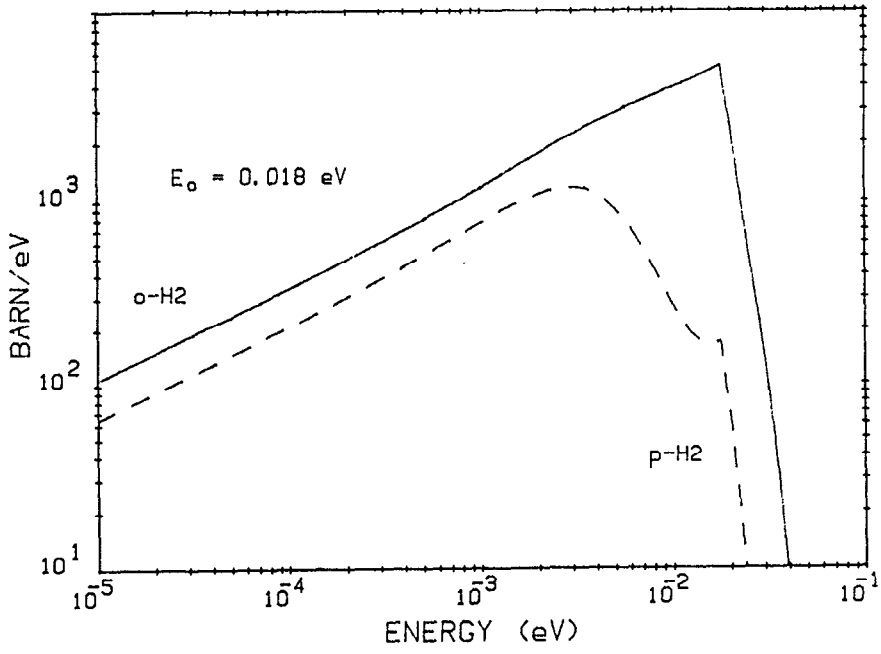

Fig. 3 Energy-transfer kernels for H_2 at E_0 = 0.018 eV.

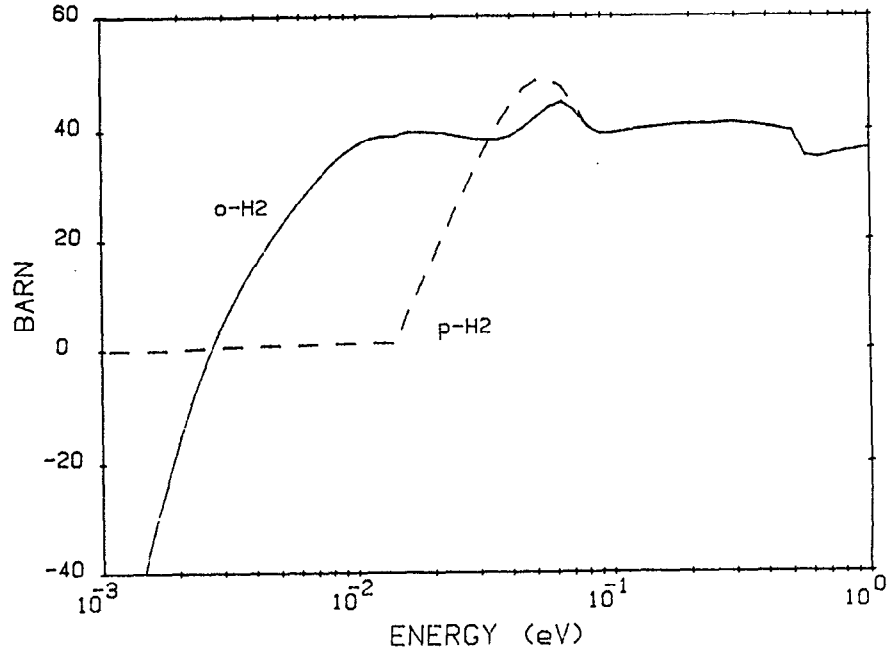

Fig. 4 Slowing down power of liquid H_2.

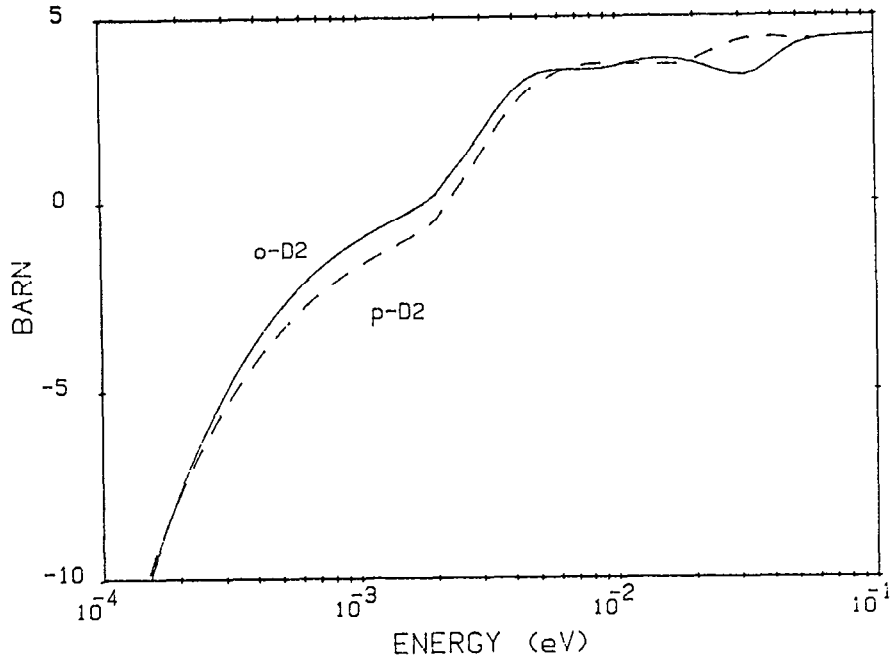

Fig. 5 Slowing down power of liquid D_2.

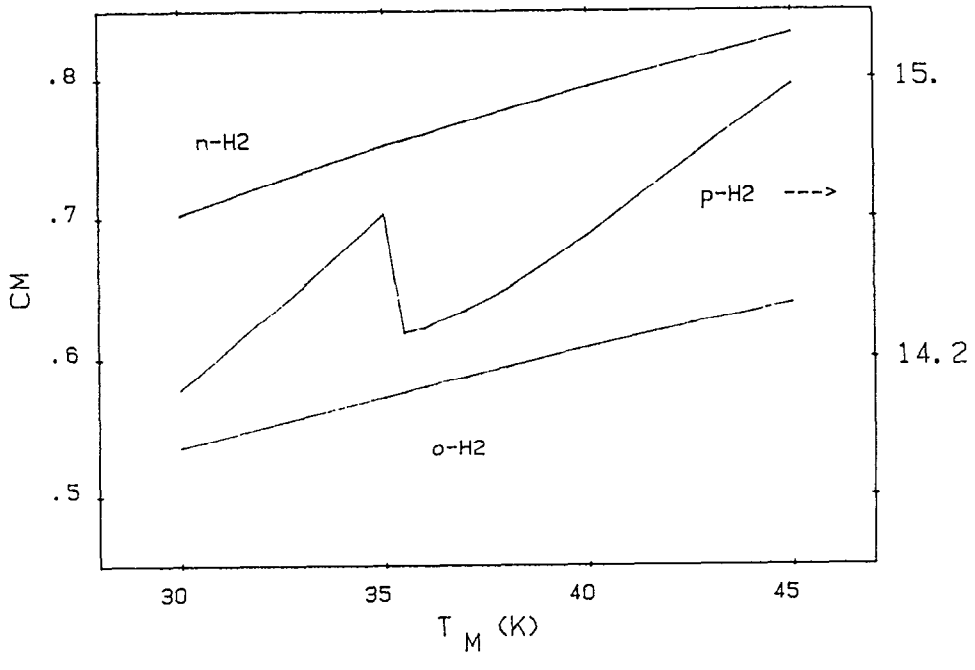

Fig. 6 Mean free path in H_2 vs. spectrum "temperature" (see test for details).

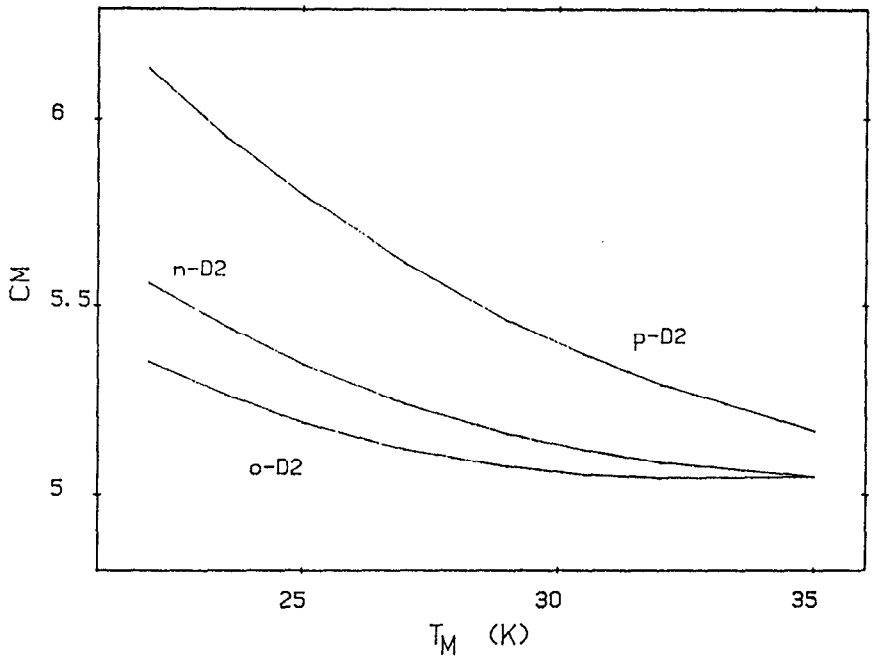

Fig. 7 Same as Fig. 6, but for D_2.

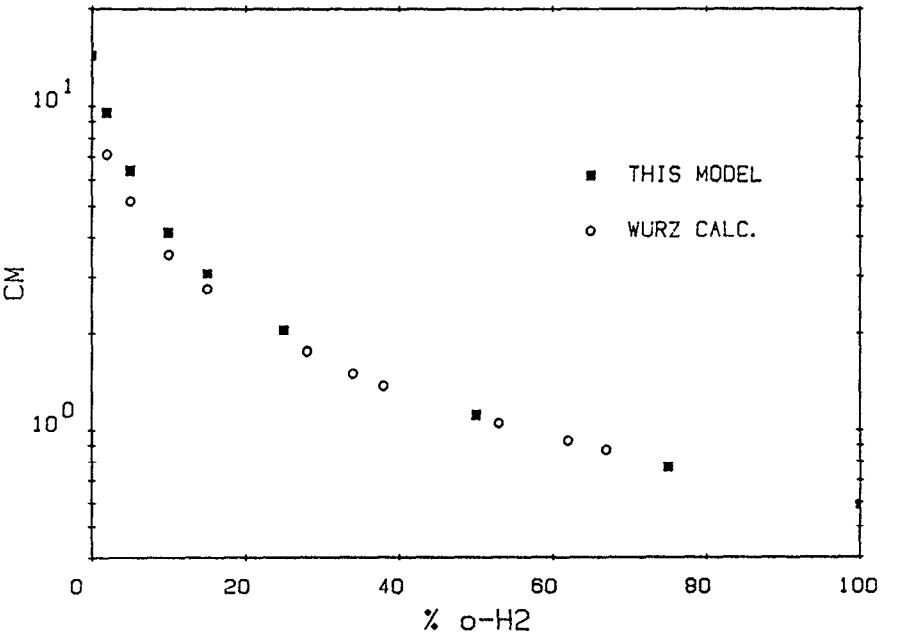

Fig. 8 Mean free path in H_2 vs. ortho:para concentration.

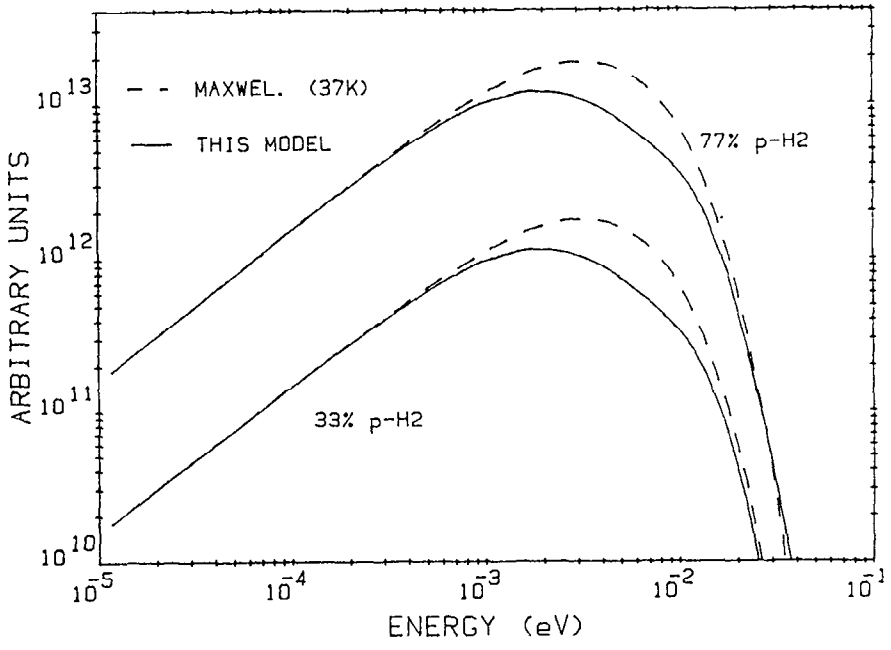

Fig. 9 Calculated scalar flux in liquid hydrogen at 20 K.

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