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Re-evaluating low-energy neutron-deuteron elastic scattering using three-nucleon theory.

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Abstract. Using a well-established nucleon-nucleon interaction that fits the NN scattering data (Bonn potential), and the AGS form of three-body theory, we perform precise calculations of low-energy neutron-deuteron scattering. There appear to be problems for this system in the ENDF/B-VI.8 (ENDF/B-VI.5 through VI.8) data library, which persist in the newest version, ENDF/B-VII.0. Supporting experimental data in this energy region are rather old (> 25 years), sparse and often inconsistent. Our three-body results at low energies, 50 keV to 10.0 MeV are compared to the ENDF/B-VII.0 and JENDL-3.3 evaluated angular distributions. The impact of these results on calculated reactivity for various critical systems involving heavy water is shown.

1 Introduction

The theory of nuclear structure and reactions is now accurate enough in many regions of the periodic table that information derived from theory should be adopted, wherever possible, in the evaluated nuclear data libraries used in practical applications. One such region is the very light nuclei ($A < 6$), where few-body theory applies. The specific problem dealt with here is the scattering of low-energy (< 3 MeV) neutrons from deuterium. Not only is this a fundamental problem of nuclear physics, since it is the next-most complex system of nucleons beyond the nucleon-nucleon (NN) interaction, but it is also a problem of practical importance in heavy-water (D_2O) moderated and/or reflected nuclear power systems. In this paper, we outline the variations between the current data libraries and experimental data for low-energy $n+d$ scattering, and propose using modern three-nucleon theory to provide additional information on this system. The implications of these results on reactor physics calculations will be outlined.

2 The neutron-deuteron database

One might have assumed that such a simple and fundamental system as $n + d$ would have been extensively studied experimentally, and that the evaluated nuclear data libraries (DLs) would be complete and consistent. In fact, that is not so. Most of the experimental data are quite old and there are significant gaps in the data coverage. Also, there are inconsistencies among experimental data sets and between the measured data and the evaluated nuclear DLs. We have looked at the deuterium data in DLs ENDF/B-VI.4, ENDF/B-VI.8, JENDL 3.3, and JEFF 3.1 in the range from 220 keV to 3.2 MeV. Some examples from the second and third of these are shown here. The $n+d$ scattering data of interest in this work are the same for the ENDF/B-VI.5 through VI.8, ENDF/B-VII.0 and JEFF-3.1 DLs.

In fig. 1 are shown the differential cross section for elastic neutron-deuteron scattering at 220 keV taken from two DLs and the experimental data from Adair *et al* [1]. Here and in other figures, the cross section is plotted against the parameter $\mu = cos(\theta)$, where θ is the centre-of-mass scattering angle. Clearly, these data from 55 years ago favour a more isotropic

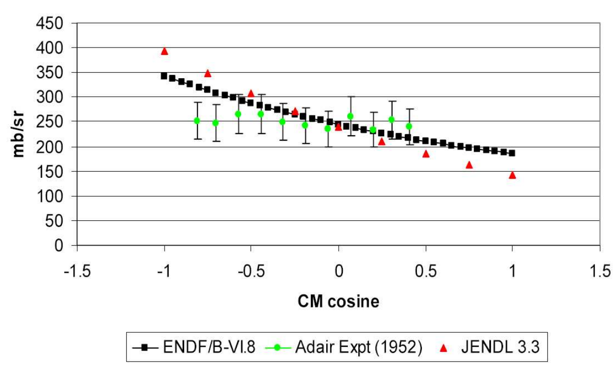

Fig. 1. Differential cross section (mb/sr) for scattering of 220 keV neutrons from deuterium, taken from data [1] and two nuclear DLs.

distribution than do the DLs. But there is also a significant difference in slope of the two curves from ENDF/B-VI.8 and JENDL-3.3. A similar comparison at 1.0 MeV (fig. 2) shows less dramatic differences, but there is still a substantial discrepancy between data [2] and both DLs at back angles, as well as small differences through the entire angular range. Yet, newer data from Vendrenne [3] at an energy 0.2 MeV higher (fig. 3) shows much greater discrepancies with both DLs,

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which, however, agree quite well with each other except at back angles. Such differences between what data are available and the DLs persist up to 3.2 MeV, though the disagreement among DLs gets less at the higher energies. There is a need for new experiments, and for a re-evaluation of the evaluated DLs, in this energy regime.

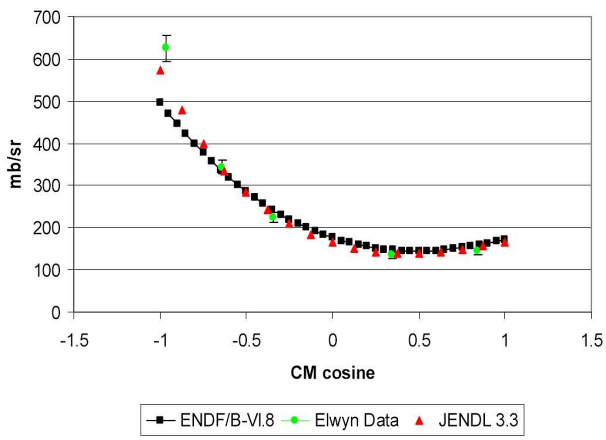

Fig. 2. As in fig. 1 for 1.0 MeV neutrons. Data from Elwyn *et al* [2].

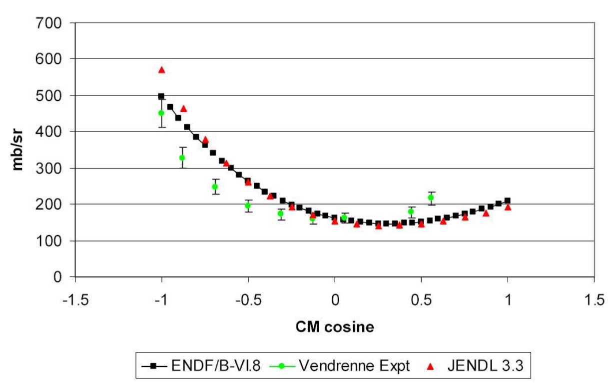

Fig. 3. As in fig. 1 for 1.2 MeV neutrons. Data from Vendrenne [3].

In these DLs, essentially no nuclear theory was used in obtaining the evaluated data. ENDF/B-VI.8 uses an R-matrix model to interpolate and extrapolate from known experimental data to obtain scattering angular distributions. JENDL 3.3 uses, in a similar way, results of very old Faddeev-type calculations [4] using a single separable s-wave Yamaguchi NN interaction.

3 Three-body theory

In the absence of more consistent experimental data for low-energy $n + d$ scattering, we turn to the few-body theory. Faddeev in 1961 published the complete quantum theory of the three-body system, which was later extended to a larger number of particles. That, coupled with accurate understanding of nucleon-nucleon interactions that fit well the NN scattering data (at least up to the pion-production threshold at 290 MeV, lab.), as well as advances in computer technology, have made it possible to perform precise calculations of bound states and scattering of three-nucleon systems.

Using the AGS re-formulation [5] of the Faddeev three-body equations, Canton *et al* [6] carried out calculations, between 3 and 19 MeV, of cross sections and various spin observables in the $n + d$ system using various nucleon-nucleon interactions. Here we extend these calculations, using the Bonn-B NN interaction, to lower energy down to 50 keV, for comparison to available data and the nuclear DLs. The AGS equation is written

$$U_{\beta\alpha} = \bar{\delta}_{\beta\alpha} G_0^{-1} + \Sigma_\gamma \bar{\delta}_{\beta\gamma} T_\gamma G_0 U_{\gamma\alpha}. \quad (1)$$

The AGS equation has the advantage over Faddeev's original formulation of the three-body problem in that the 'unknowns', $U_{\beta\alpha}$, relate directly to observables. Matrix elements of the U-s taken between suitable incoming and outgoing states give, directly, the transition matrix (T-matrix), from which all manner of experimental observables can be extracted. The subscripts in eq. (1) are the three-body 'channel' labels using the odd-man-out convention. That is; for example, $\alpha = 1$ is particles 2 and 3 interacting, particle 1 free. In eq. (1), T_γ is the two-body T-matrix in channel γ (i.e., if $\gamma = 1$, it describes the scattering between nucleons 2 and 3, with nucleon 1 as spectator): $T_\gamma = V_\gamma + V_\gamma G_0 T_\gamma$, where V_γ is the NN interaction in channel γ. G_0 is the free resolvent operator, $G_0(E) = (H_0 - E)^{-1}$, where H_0 is the Hamiltonian for three free particles. Finally, $\bar{\delta}_{\beta\alpha} = 0$ if $\beta = \alpha$ and $\bar{\delta}_{\beta\alpha} = 1$, otherwise.

The AGS equation is a set of coupled integral equations in two vector variables. However, with angular-momentum reduction it reduces to a set of integral equations in two radial variables. A further, and substantial, simplification comes about if the NN potentials are expressed as sums of separable terms. The AGS equation then becomes a set of integral equations in one radial variable. Therefore, in our work, we use the Graz separable representations of the realistic NN interactions. In particular, for the Bonn-B potential used here, we have used the BBEST potential [7]. In fig. 4 we show the energy dependence of the differential cross sections at zero, 90 and 180 degrees obtained from our AGS calculations (Bonn-B) and DL ENDF/B-VII.0 [8]. The figure shows one of the problems with DL ENDF/B-VII.0 (and ENDF/B-VI.8): the discontinuity and gap in the data between 3.2 MeV and 5.7 MeV. Also, there is considerable disagreement between that and the Bonn-B results, especially at back angles (180°).

In figs 5 and 6 we show calculated results for differential cross section as function of μ, together with those from the same two DLs [8] and at the same energies as in figs 1 and 2, respectively. It is clear that the theoretical result favours the JENDL-3.3 DL. This persists at other energies up to 3.2 MeV, where there is little difference between the theory and the two DLs, as shown in fig. 7 The strongest differences between theory and the ENDF data occur at the most extreme backward angles. But small differences are also seen at different angular ranges. It should be noted that the AGS calculations are highly accurate given the particular choice of NN potential. However, in these theoretical results,

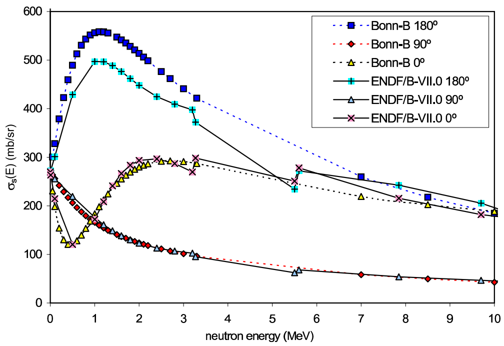

Fig. 4. Differential cross section (mb/sr) for scattering of neutrons from deuterium, at 0°, 90° and 180°. AGS calculations with the Bonn-B NN interaction, compared to the ENDF/B-VII.0 library.

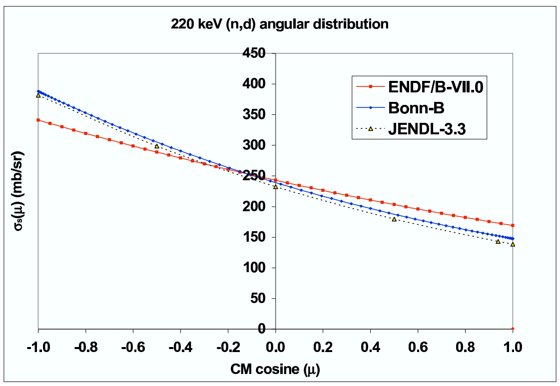

Fig. 5. Differential cross section (mb/sr) for scattering of 220 keV neutrons from deuterium. AGS calculations with the Bonn-B NN interaction, compared to two nuclear DLs.

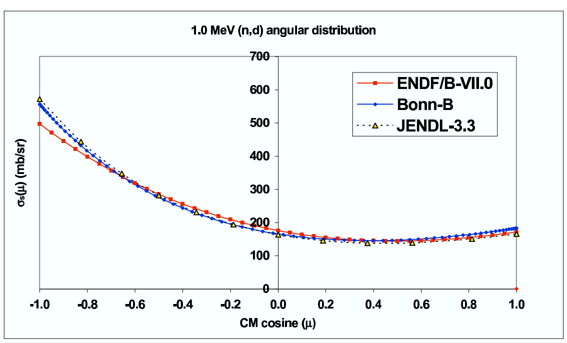

Fig. 6. As in fig. 5 for 1.0 MeV neutrons.

two effects have not been included. One is the consequence of an irreducible three-nucleon interaction. This is discussed in ref. [6] and affects mainly spin observables, though it may also affect cross sections. In addition, at low energies and especially at small angles, an electromagnetic effect, due to the interaction of the magnetic moments of the neutron and

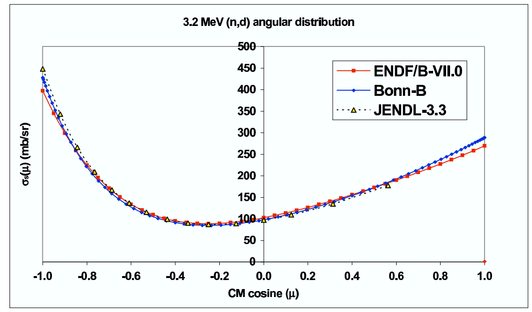

Fig. 7. As in fig. 5 for 3.2 MeV neutrons.

deuteron, should also be taken into account. This has not been evaluated, as yet.

4 Implications for critical systems containing heavy-water

Shortly after the release of ENDF/B-VI.8 in 2001, it was noticed at Los Alamos National Laboratory (LANL) that the calculated eigenvalues for a set of heavy-water solution benchmarks involving highly enriched uranium (HEU; 93.7 atom %) had decreased significantly relative to earlier versions of ENDF/B-VI. Such changes resulted from modifications to the angular probability distributions for elastic scattering at $E < 3.2$ MeV. We now show the results of calculated reactivity impact for various critical systems involving heavy water based on the AGS results compared to those from DLs ENDF/B-VII.0, ENDF/B-VI.4 and JENDL-3.3.

The critical experiments that have been simulated with the MCNP5 (Monte Carlo N-Particle) neutron transport code are:

1. Two sets of LANL HEU; D_2O Solution (uranyl fluoride in D_2O) Thermal critical experiments (1950s), involving simple geometries with a high degree of neutron leakage:
(a) HEU-SOL-THERM-004 (HST-004): This set includes six experiments involving spheres at various ^{2}H-to-^{235}U concentrations, reflected by an outer spherical annulus containing pure D_2O. The benchmark k_{eff} values for this set are 1.0 and the estimated experimental uncertainties range from ±3.3 to ±5.9 mk (1 mk is a change in k_{eff} of 0.001).
(b) HEU-SOL-THERM-020 HST-020: This set includes five experiments of unreflected cylinders at various ^{2}H-to-^{235}U concentrations. Because there is no surrounding neutron reflector, correction for "room return" of neutrons from the surroundings is made, leading to the benchmark k_{eff} values being < 1.0, with larger estimated experimental uncertainties, ranging from ±7.7 to ±11.9 mk.

The main problem with the HST critical experiments is that they are too imprecise to be used to select between the various ^{2}H data files. For reasons of space, we do not show these results are here, but we note that the Bonn-B k_{eff} value lies in the middle, being on average about 7.4 mk higher than ENDF/B-VII.0 values, 1.8 mk lower than ENDF/B-VI.4 values, and 3.4 mk less that JENDL-3.3 values, respectively.

2. AECL Chalk River Laboratory (CRL) ZED-2 (Zero Energy Deuterium) Coolant Void Reactivity (CVR) critical experiments. These involve low neutron leakage, heterogeneous arrangements of lattices of natural-uranium (NU; 0.71 atom % ^{235}U) fuel rods. The geometry is much more complex than the HST series. There exist dozens of such experiments with various fuel types, coolants, lattice pitches and arrangements. The experiments are modern and ongoing. The experimental uncertainty in any k_{eff} determination is estimated to be ±0.2 mk, dominated by measurement uncertainty of the D_2O purity. Also, the MCNP model of ZED-2 is quite detailed and extends outward to include the surrounding concrete shielding.

Two representative pairs of experiments involving D_2O cooled and air cooled (voided) experiments were chosen. Both sets involve 55 fuel channels of 28-element NU UO_2 fuel bundles similar to those used in the Pickering CANDU power reactors. Each fuel channel contains a vertical stack of five fuel bundles contained inside concentric aluminium tubes that mimic the zirconium-alloy pressure tube and calandria tube of a real CANDU fuel channel. The lattice arrangement is a regular triangular/hexagonal lattice array with a pitch of 31.0 cm. For more details on the ZED-2 experiments, we refer to the paper by Kozier [9] elsewhere in these proceedings.

The ZED-2 k_{eff} results show a rising trend with calculated neutron leakage. Since the leakage increases when air is substituted for D_2O coolant, the k_{eff} bias (i.e., the difference between the calculated k_{eff} and 1.0) also increases. This gives rise in turn to a small positive coolant void reactivity (CVR) bias – defined here as the difference between the k_{eff} bias for the air-cooled and D_2O-cooled cases. The smaller the magnitude of the CVR bias, the better job MCNP5 does of calculating the reactivity perturbation associated with D_2O coolant voiding when using a particular nuclear DL.

The MCNP5 simulations were performed using the ENDF/B-VII.0 nuclear DL that was released officially in December, 2006. The corresponding ACE (A Compact ENDF)-format files needed to execute MCNP5 were prepared by the U.S. National Nuclear Data Center and distributed by the Radiation Safety Information Computational Center (RSICC). Four calculations were performed (fig. 8), changing just the ACE file for ^{2}H:

1. ENDF/B-VII.0: this is the reference case. It is based on an R-matrix analysis and, hence, also incorporates information from experiments using positive ion beams.
2. Bonn-B: this uses a modified ENDF/B-VII.0 file for ^{2}H in which was implanted the Bonn-B results for both the total elastic scattering cross section and the energy/angle scattering probability distribution over energy range from 50 keV to 10 MeV. A corresponding ACE file was then generated using the NJOY99.0 cross section data processing code.
3. ENDF/B-VI.4: this uses an ACE file for ^{2}H that was produced by LANL. The $(n + d)$ data are the same as for ENDF/B-VI.0 through VI.4.
4. JENDL-3.3: this uses an ACE file from RSICC for ^{2}H corresponding to the current Japanese DL. It is based on the old Faddeev model calculations.

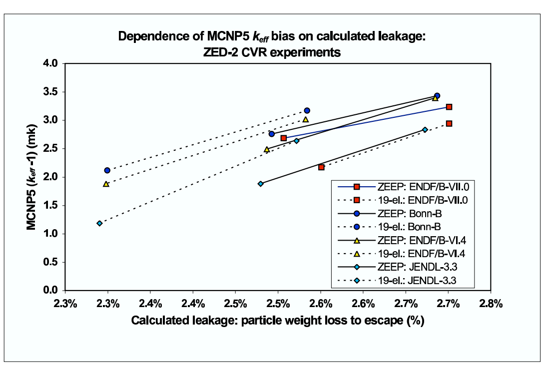

Fig. 8. MCNP5 ZED-2 CVR k_{eff} bias results for selected CVR experiments: dependence on calculated neutron leakage.

For the ZED-2 results in fig. 8: (i) The k_{eff} bias is highest with Bonn-B (2.87 mk), slightly lower with ENDF/B-VII.0 (2.76 mk) and VI.4 (2.70 mk) and lowest with JENDL-3.3 (2.14 mk). (ii) The CVR bias with Bonn-B (0.86 mk) is only slightly higher than ENDF/B-VII.0 (0.66 mk), slightly smaller than ENDF/B-VI.4 (1.02 mk) and quite a bit better than JENDL-3.3 (1.20 mk).

5 Conclusions

We conclude that, if the ENDF/B-VII.0 data for ^{2}H are flawed, our next preference, based on the lower CVR bias value, are theoretical results from AGS calculations using the Bonn-B NN interaction. Our other main conclusion is that modern nuclear model calculations produce results for practical applications that are noticeably different, and likely better, than those based on older Faddeev calculations with a simple Yamaguchi potential. This leads to a more general conclusion, relevant to this conference: Future nuclear data evaluations should pay more attention to the availability of modern theoretical approaches to nuclear structure and reaction information, and make use of such results to improve the quality of Evaluated Nuclear Data Libraries.

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