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p-d CAPTURE REACTIONS IN MUONIC MOLECULES

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ABSTRACT

Capture reactions for very low-energy n-d and p-d systems are calculated and compared with experiment, as are low-energy n-d and p-d scattering. We find excellent agreement for the n-d scattering lengths, but poor agreement for the p-d case, which we believe is a problem with the experimental extrapolation. The n-d radiative capture is sensitive to details of the meson-exchange currents, but reasonable models agree with the data. The latter models are in good agreement with experiment when extended to the p-d case. Our large quartet capture rate resolves a long-standing anomaly. The E0 capture matrix element recently obtained from a reanalysis of internal conversion in muonic molecules is in excellent agreement with our predictions. This matrix element is very clean theoretically and provides the best test of the calculations.

1. Introduction

1.1 Overview

Complete or "exact" solutions of the Schrödinger equation with realistic potentials have been obtained during the previous six years for a variety of problems: the ground states of ^3He and ^3H [1] (including a three-nucleon force, and a Coulomb interaction in the former case), the ground state of ^4He [2] and low-lying continuum of ^5He [3], above-breakup n-d scattering[4], and, more recently, zero-energy n-d and p-d scattering[5] (including three-nucleon forces, and a Coulomb interaction for the latter case). The purpose of these calculations is to probe the limits of our understanding of the binding and interactions of the few-nucleon systems. The goal is to establish whether our current level of experimental and theoretical sophistication can unambiguously detect the presence of three-nucleon forces in these systems.

In pursuing this goal, a wide variety of few-nucleon scattering, breakup, and capture reactions have been calculated, as well as the properties of the ground states. To date, most calculated properties agree well with experiment, if models are adjusted in some way to produce the correct ground-state binding energies. Typically, models containing only two-nucleon forces will underbind the triton by 0.6-1.0 MeV and the alpha particle by roughly four times that amount. While this binding defect is only a few percent of

the total potential energy, the binding energy sets the size scale, and an underbound model will be too large in size. Consequently, size-dependent properties such as the charge radius and the Coulomb energy will be too large and too small, respectively.

Adding a "realistic" three-nucleon force based on two-pion exchange provides additional binding in roughly the correct amount. There is typically a severe short-range sensitivity to these forces, which cannot be well-constrained theoretically, and which precludes an *ab initio* prediction of binding energies. Nevertheless, the addition of a reasonable three-nucleon force to the Hamiltonian can produce proper binding for the three- and four-nucleon systems, and this allows us to extrapolate calculated observables to the correct binding energy (or size scale). We will see the importance of this later. To date, the primary effect of three-nucleon forces has been to set this size scale, and, unfortunately, not to change observables in a way that is incommensurate with a modified two-body force.

1.2 Low-energy Reactions

In this talk we report on calculations of low-energy scattering and reactions involving three nucleons, which utilize complete or "exact" solutions of the Schrödinger equation. Our goal is to describe μ -catalyzed p-d fusion reactions at (essentially) zero energy, but in order to benchmark this process we must also examine the n-d capture, as well as n-d and p-d scattering, which are two of our building blocks.

The quantity that characterizes very low-energy scattering is the scattering length, a . Neutron scattering lengths can be obtained by measuring (or calculating) scattering at thermal energies, which are effectively zero on the nuclear scale. They can also be obtained by calculating the usual effective-range function, $k \cot(\delta)$, at finite energy, and extrapolating this quantity to zero energy: $-1/a$. Capture reactions at thermal energies can be directly measured. Reactions involving positively charged particles at zero energy are much more difficult to obtain. Direct laboratory measurement is inhibited by a dominating Coulomb barrier which keeps the particles apart, and dramatically suppresses reaction rates and, even worse, the amount of nuclear scattering compared to pure Coulomb scattering. Laboratory scattering measurements are typically performed at fairly high energies, and the Coulomb-modified effective-range function obtained from them is subsequently extrapolated to zero energy. This methodology presupposes that the nuclear amplitudes are rather smooth functions of energy.

1.3 Muonic Molecules

The one exception to this extrapolation scheme is provided by fusion in muonic molecules. If negative muons are captured by two positively charged ions, they can form a molecule, which eliminates the problems described above. The molecular binding keeps the particles together, and the (negative) muon charge between the ions decreases the Coulomb barrier, which greatly increases transition rates. If these rates are faster than the normal muon β -decay rate, charged-particle reactions in the molecules can be directly measured. Moreover, the size scale of these molecules is roughly a muonic Bohr radius (~ 250 fm), and the relative kinetic energy of the ions can be estimated using the uncertainty principle to be several hundred electron volts, which is negligible on the nuclear scale. Thus, muonic molecules are potentially an ideal laboratory for low-energy charged-particle reactions, analogous to that provided by thermal neutrons.

There are possible difficulties with this scenario. The familiar product of beam current with target thickness, which occurs in laboratory beam-target experimental rates, is replaced by the probability of molecular coalescence, determined by the square of the molecular (i.e., non-nuclear) wave function, which must be accurately calculated. In addition, a wide variety of competing processes must be disentangled, and this

requires a sophisticated understanding of the atomic and molecular physics involved. Fortunately, both of these problems have been largely resolved in recent years[6].

2. n-d and p-d Scattering Lengths

Calculating the n-d and p-d scattering lengths is relatively straightforward. The Los Alamos/Iowa collaboration prefers to solve the Faddeev partial differential equation at zero energy, subject to the appropriate boundary conditions for elastic scattering (breakup being energetically impossible)[5]. The only difficulty in principle is the set of weak, long-range, Coulomb-induced (multipole) polarization potentials, which will modify the usual Coulomb boundary conditions for p-d scattering, or even the long-range magnetic force in the n-d case, which has a similar effect. These long-range forces are important in principle, but negligible in practice[7], if one follows customary procedures. A similar situation would result if the usual Coulomb interaction were a factor of 10^6 smaller: implementing non-Coulomb boundary conditions in the usual way, although wrong in principle, would introduce negligible error.

Fig. 1. n-d and p-d doublet scattering lengths plotted vs corresponding trinucleon binding energy.

The results of the Los Alamos/Iowa collaboration for s-wave doublet scattering are shown in Fig. 1, where the doublet scattering lengths for a variety of potential models are plotted against the ^3H (for n-d) or ^3He (for p-d) binding energy of that model. That is, with the exception of two experimental points with error bars, every point on the plot represents a theoretical calculation. This type of presentation is called a Phillips plot[8]. The filled squares and circles correspond to complete (34-channel) calculations. The circles represent models containing the Reid Soft Core N-N potential[9], while the squares represent models based on the Argonne V_{14} potential[10]. Approximately half of the points contain either the Tucson-Melbourne[11] or Brazilian[12] three-nucleon force. Almost invisible is the n-d experimental datum[13], which falls on the solid curve. The latter is a simple fit to the various theoretical points. On the other hand, the p-d datum[14-16] is far from the dashed curve, which is a fit to the p-d (Coulomb-modified) scattering-length points.

The quartet results have a similar disposition. The latter channel is insensitive to everything but the 3S_1 - 3D_1 N-N force, and does not require any extrapolation. The average for the models we solved is 6.34(4) fm, while the experimental value is 6.35(2) fm; excellent agreement is obtained. In this example and later ones, we will quote a subjective "theoretical error bar", which merely reflects the spread in the theoretical values. The calculated p-d scattering length, on the other hand, is 13.6(1) fm, while the experimental value is about 11.5 fm [16]. This disagreement reflects the same problem we saw in the doublet case.

The experimental n-d scattering lengths can be directly obtained from low-energy neutron scattering, while the p-d scattering lengths must be obtained by extrapolating the Coulomb-modified effective-range function to zero energy. Unfortunately, the latter must be done from rather large energies. In order to check the extrapolation we calculated [17] the s-wave phase shifts as a function of energy. The calculations agree with the experimental values, and also extrapolate to the result one gets by solving for a directly at zero energy. For CM energies above 200 keV the doublet effective-range function is rather flat. Unfortunately, for energies below that value (and well below the data) there is enormous curvature in that effective-range function, which is equivalent to a huge effective range, r_0 . This curvature is consistent with a sub-threshold pole. Although ref. [16] was well aware of the possibility of such a pole, the data gave no such indication, because the lowest datum was nevertheless too high in energy. We believe that the problem is an experimental one and will not be resolved until experiments can be performed at lower energies. We emphasize that there is no disagreement with actual measured quantities, but only with extrapolated values.

3. n-d Capture

3.1 Overview

Given ^3H and (zero-energy) n-d wave functions, one can calculate capture reactions accurately, provided one has an accurate model for the transition interaction. A well-studied process is thermal n-d radiative capture, which is almost entirely magnetic dipole (M1) in nature. The average of the experimental cross sections [18] is 0.518(8) mb, which is more than a factor of 600 smaller than for the corresponding n-p capture. The reason for this suppression is found in the spin-flip nature of the M1 operator in impulse approximation. The dominant part ($\sim 90\%$) of the ^3H ground state (the S-state) is an eigenfunction of this operator and, after enforcing orthogonality of initial and final wave functions, this large component does not contribute to the transition, as shown originally by Schiff [19].

Meson-exchange currents (MEC) will play a much larger role when the impulse approximation is suppressed. Although only a 10 percent correction to the n-p rate, such currents change the n-d rate by a factor of two. Thus, the latter case is sensitive to details of the MEC. We emphasize that constructing a model of the MEC requires information not contained in the potential model. Indeed, a completely specified current requires a theory of the photon-meson-nucleon system, which exists only in part. The dominant part, fortunately, is the long-range one-pion-exchange (OPE) part, for which a reasonable model can be constructed, just as it can for the N-N force. Unfortunately, the short-range parts are much more problematic. Consequently, we restricted ourselves in these calculations to a MEC model consisting only of the OPE part, modified by a short-range cutoff (a standard monopole form factor with a mass Λm_π). Typically one finds that the shorter-range contributions (i.e., other than OPE) are comparable to the

3.2 Results of Calculations

We can summarize our results[20] as follows. For models which are extrapolated to the physical ^3H binding energy (as we did for the doublet scattering length) we find:

1. In impulse approximation the quartet capture is larger than the doublet capture;
2. The impulse and MEC parts of the doublet matrix element are comparable and constructive;
3. The quartet MEC matrix element is only about 10 percent of the impulse approximation and is destructive;
4. Without MEC the capture cross section is a factor of two too low;
5. With MEC the doublet capture dominates the quartet by roughly 3:1;
6. With MEC the experimental capture cross section is reproduced within a ± 20 percent uncertainty due to reasonable variations in Λ ;
7. The variation in Λ causes a variation of 25 percent in the MEC matrix elements, which greatly affects the total doublet matrix elements, but hardly changes the quartet ones;
8. Values of Λ which give a reasonable total cross section also reproduce the results of the recent experiment[21] on the circular (photon) polarization in polarized thermal neutron capture, which is sensitive to the quartet/doublet matrix element ratio.

The strong sensitivity of the total capture rate to the short-range behavior of the MEC can be used to test and refine models of the latter[22], although this is not our motivation. In order to calculate p-d capture with as little uncertainty as possible, we adjust the value of Λ to produce reasonable agreement with the n-d total capture cross section, which reproduces the polarized capture experiment as well. This gives us a reasonable (although semi-phenomenological) MEC model which can then be used with no free parameters to test our understanding of the former (p-d) reaction. We will display our sensitivity to Λ in that reaction, which is very similar to the n-d case, although slightly less so because of the Coulomb repulsion.

4. p-d Capture

4.1 Laboratory Measurements

Laboratory measurements of p-d radiative capture have been performed in the past and extrapolated (with some assumptions) to zero energy in order to obtain the astrophysical S-factor (which is proportional to the total cross section) for the s-wave reaction: S_0 . The best available experimental value[23] from this source is $S_0 = 0.12(3)$ keV mb. The large uncertainty reflects the difficulty in performing these experiments at the very low laboratory energies necessary for the extrapolation. The Los Alamos/Iowa prediction[24] for this quantity is $0.108(4)$ keV mb, and is based on the MEC models which were adjusted to the n-d capture and then extrapolated to the physical ^3He binding energy.

4.2 Fusion in Muonic Molecules

Fusion of protons with deuterons was discovered more than thirty years ago in muonic molecules formed in a hydrogen bubble chamber[25]. The reaction which was

first seen was internal conversion: $\mu^- + p + d \rightarrow {}^3\text{He} + \mu^- + (5.5 \text{ MeV})$. This reaction competes with the more common radiative-capture process, $\mu^- + p + d \rightarrow ({}^3\text{He} + \mu^-) + \gamma$, where the final muon almost always resides in the 1S Bohr orbit of the residual He atom[26]. In the former reaction the muon reappears and can reinitiate the complex molecular capture process and generate more fusions; hence the name: μ -catalyzed fusion.

Because the molecular energies are very small compared to nuclear energies, these nuclear reactions are s-wave in nature, as we discussed in the introduction. This restricts the possible electromagnetic matrix elements to four: E0, E2, M1(3/2), M1(1/2). The E2 matrix element, which is interesting because of its sensitivity to the tensor force, is not believed to play a significant role, while the E0 matrix element dominates the internal conversion process (and cannot occur for radiative capture). Magnetic dipole capture from the quartet and doublet states contributes only negligibly to internal conversion because the muon is very heavy and consequently generates a small current. It dominates the radiative capture, however.

Early theoretical work focussed primarily on the atomic and molecular aspects of the fusion process, although estimates of the nuclear rates were made using the relatively primitive (and largely phenomenological) methods which were available. A very influential paper[27] argued that the quartet capture should be very small, because the spins of any two nucleons would have to be aligned ($J=1$), which is Pauli-forbidden for two s-wave protons. Although the very small molecular energies force the p-d system into a relative s-wave, this does not mean that the p-p system resides in a relative s-wave, because of the large zero-point motion of the neutron and proton in the deuteron. Indeed, this mechanism leads to the S' -state (mixed-symmetry s-wave component of the wave function), which can produce non-negligible quartet capture.

4.3 Wolfenstein-Gerstein Effect

During the molecular formation process in a low-temperature mixture of normal hydrogen with a weak concentration of deuterium, the muon is preferentially captured by protons, and subsequently during collisions transfers from the ground state of that atom to the deuterium, which atom has a lower ground-state energy because of its larger mass. The resulting μ^- -d atom has a significant hyperfine splitting in its ground state, which exceeds the value of kT in liquid hydrogen. At sufficiently high deuterium concentrations, collisions between the μ^- -d atom and deuterium nuclei can lead to transitions between the atomic hyperfine states, which will eventually equilibrate into the lowest state. Thus, although the deuterium spin is randomly distributed in the liquid, the complex set of atomic processes during the formation of the molecule can lead to a non-statistical distribution of spins which depends on the deuterium concentration. After the final molecule is formed, the quartet and doublet spin states of the p-d system will also have a non-statistical spin weighting (which favors the doublet). Because doublet fusion dominates, the fusion rate will increase as the deuterium concentration increases. This is the Wolfenstein-Gerstein (WG) effect[28], which allows the experimentalist to "dial" varying amounts of quartet and doublet spin into the initial nuclear state prior to fusion, and permits these competing M1 processes to be disentangled. This interesting and valuable phenomenon accomplishes the same thing as polarized beams or targets in the more usual beam-target experiments.

Tests of the WG effect were initially successful. Subsequent tests[29-30] using improved calculations of the atomic physics were in poorer agreement, if the no-quartet conjecture was also used. This anomaly (the WG anomaly) has persisted until recently, and led to speculation about exotic atomic hyperfine mechanisms for restoring

agreement; the latter have never survived quantitative calculations[6].

4.4 Molecular Wave Functions

An important simplification in calculating the reaction rates occurs when one realizes that the fusion occurs for small nuclear (*i.e.*, p-d) separations, $R < 10$ fm, while the average separation in the molecule is very much greater. Indeed, the p-d- μ reaction is a four-body problem which would be beyond our current calculational abilities to do exactly. Approximating the nuclear separation in the molecule by zero, the transition rate factorizes[31] into a nuclear part and a molecular part: the molecular coalescence probability. The latter is different for the two different reactions. For the internal conversion it is given by the square of the molecular wave function evaluated at the point where all three charged particles overlap. For the radiative capture, it is given by an integral with respect to the muon's coordinate over the square of the wave function. Highly accurate calculations by the Florida group[32] exist for the latter probability. In order to obtain the former probability we performed our own calculation of the molecular wave function using Faddeev techniques, and later compared this result to one obtained from the Florida wave function. Good agreement at the one percent level was obtained.

4.5 Internal Conversion

Fig. 2. E0 p-d internal conversion matrix elements plotted vs corresponding ^3He binding energy.

The internal conversion process is determined by the square of the E0 matrix element, which is just the mean-square radius of the charge distribution in the transition region, if one neglects retardation (*i.e.*, the muon's momentum) in the multipole operator. This operator is very clean theoretically and contains none of the usual exchange currents which complicate calculations of the magnetic multipoles. Our results[24] are shown in Fig. 2, after the fashion of Fig. 1. The matrix element scales roughly as E_B^{-2} . This illustrates clearly how sensitive some observables are to the binding. Our numerical results are 963(10) $\text{fm}^{7/2}$ for the unretarded matrix element and 888(10) $\text{fm}^{7/2}$ for the retarded (*i.e.*, physical) one, while the experimental matrix element extracted from the measured rate using our wave function is 844(45) $\text{fm}^{7/2}$. The experimental rate was

recently obtained by reanalyzing old bubble chamber data[33]. The agreement is very good.

4.6 Radiative Capture

Fig. 3. p-d doublet and quartet M1 transition matrix elements plotted *vs* corresponding ^3He binding energy.

In addition to sensitivity to the model binding energy, the M1 matrix element is sensitive to the short-range behavior of the MEC. For purposes of display, we restrict ourselves to only two potential models, based on the RSC and AV_{14} potential models with a three-nucleon force added to produce the correct ^3He binding energy. For these two models we calculate[24] the quartet and doublet (reduced) matrix elements, which are displayed in Fig. 3, together with the experimental data extracted from the experimental rates[30]. As before, the circles correspond to RSC model calculations, while the squares correspond to AV_{14} results. The various values of Λ (i.e., the short-range cutoff mass) for the RSC model are [5.8, 7.5, 8.6, 17.0, 99.0] from left to right, while for the AV_{14} case they are [5.8, 8.6, RS, 17.0, 99.0]. The Riska-Schiavilla[22] prescription is denoted RS. The values of Λ fitted to n-d capture are 7.5 for the RSC case and 8.6 for the AV_{14} case. Note the sensitivity of the doublet matrix element to Λ , and the insensitivity of the quartet one. The values of Λ fitted to the n-d capture process work well for p-d. Overall, these M1 results are very satisfactory.

Table 1. Results of Ref. [24] (theory) compared to experiment. References a, b, c are Ref. [33], [30], and [23], respectively.

<u>Process</u>	<u>Theory</u>	<u>Experiment</u>
$\lambda_{1/2}^{\mu}[\cdot 10^6 \text{sec}^{-1}]$	0.062(2)	0.056(6) ^a
$\lambda_{3/2}^{\gamma}[\cdot 10^6 \text{sec}^{-1}]$	0.107(6)	0.11(1) ^b
$\lambda_{1/2}^{\gamma}[\cdot 10^6 \text{sec}^{-1}]$	0.37(1)	0.35(2) ^b
$S_s[\text{keV}\cdot\text{mb}]$	0.108(4)	0.12(3) ^c

The calculated and experimental fusion rates are given in Table 1. The four processes are internal conversion, quartet radiative capture, doublet radiative capture, and astrophysical S-factor, respectively. The substantial quartet fusion rate confirms our previous argument that the no-quartet conjecture of ref.[27] is inadequate, and this, in fact, resolves the anomaly in the Wolfenstein-Gerstein effect.

5. Summary

We have calculated the nuclear reactions in μ -catalyzed p-d fusion. Accurate wave functions have been generated for the AV₁₄ and RSC models for the first time, and these have been used to compute matrix elements. A pion-exchange-current model which reproduces thermal n-d radiative capture has been used with these wave functions to calculate radiative-capture matrix elements and rates. The latter are in good agreement with experiment. Our internal conversion rates are in very good agreement with a recent reanalysis of old bubble-chamber data. Our substantial value of the quartet capture rate resolves the anomaly in the Wolfenstein-Gerstein effect, which was based on an erroneous no-quartet conjecture.

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