Nuclear Transition Rates in μ-Catalyzed p-d Fusion

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Nuclear transition rates in μ-catalyzed p-d fusion have been calculated using numerically converged ^{3}He bound-state and p-d scattering wave functions for the first time. The transition rates for $M1$ radiative capture in both quartet and doublet initial states have been computed using a model of meson-exchange currents which reproduces the thermal n-d capture cross section, and are in excellent agreement with experiment. The muon internal-conversion rate is in very good agreement with a recent reanalysis of old bubble-chamber measurements. Furthermore, our nonvanishing quartet capture rate resolves the anomaly in the Wolfenstein-Gerstein effect.

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Muon-catalyzed nuclear reactions were accidentally discovered in an experiment by Alvarez *et al.*[1] more than thirty years ago. The possibility of such reactions had been discussed previously.[2] In the Berkeley experiment, secondary muons with an energy of 5.3 MeV were observed after the primary muon had been stopped in a hydrogen bubble chamber containing a tiny deuterium contamination. That reaction is now known[3] to proceed primarily via capture of the stopped muon by a hydrogen atom, transfer of the muon to a deuteron, formation of a μ-p-d molecule, and subsequent fusion via the nuclear reaction $\mu^- + p + d \to {}^3\mathrm{He} + \mu^- + (5.5\ \mathrm{MeV})$. This internal-conversion process competes with the more common radiative capture in the molecule: $\mu^- + p + d \to ({}^3\mathrm{He} + \mu^-) + \gamma$, where the final muon is most likely to reside in the $1S$ atomic level of the residual He atom.[4] These reactions, together with other atomic processes, compete with the normal β^- decay of the μ^-.

Early theoretical work was aimed both at the atomic and molecular reactions and at the nuclear-fusion mechanisms. For the nuclear-fusion process, the initial proton (spin $\frac{1}{2}$) and deuteron (spin 1) can reside in states with nuclear spin $J = \frac{3}{2}$ (quartet) or $J = \frac{1}{2}$ (doublet). However, Cohen, Judd, and Riddell[5] in an extremely influential paper conjectured that no capture occurred from the quartet state. It was argued that the nucleon spins in the quartet state are aligned and the Pauli principle forbids the protons from being in a relative s wave, and that the probability for a p wave to exist in a molecule where the kinetic energies are on a scale of electron-volts must be tiny. So influential was this work, despite claims to the contrary,[6] that most subsequent analyses[7] of experimental data neglected *a priori* any fusion from the initial quartet state to the final doublet ^{3}He ground state. (In fact, this "no-quartet theorem" is valid only if one neglects the mixed-symmetry components.)

Following a suggestion by Wolfenstein, Gerstein[8] showed that at low temperatures the hyperfine splitting in the μ-d atom could alter the final distribution of nuclear spins in the μ-p-d molecule, even though the initial distribution of spins was statistical. At sufficiently high deuterium concentrations and low temperatures, μ-d atom scattering from deuterium atoms freezes out the upper ($F = \frac{3}{2}$) μ-d atomic hyperfine state. This leads to a strong reduction in the amount of initial quartet nuclear spin in the μ-p-d molecule, which thereby enhances the amount of the doublet configuration. Because the doublet fusion rate is dominant, the fusion yield must increase with deuterium concentration. This is the Wolfenstein-Gerstein effect, which allows one to dial different amounts of $J = \frac{3}{2}$ and $J = \frac{1}{2}$ nuclear spin into the μ-p-d molecule prior to fusion, and therefore affords a method for separating experimentally the doublet and quartet fusion rates. Although the predicted increase in yield was corroborated experimentally,[7] the measurement is now in disagreement with predictions of accurate atomic calculations,[9] *if one accepts the no-quartet theorem*. This is the Wolfenstein-Gerstein anomaly. Alternatively, one can speculate[10] that other anomalously large atomic-scattering processes[3] might alter the nuclear-spin distributions and bring the predictions back in line with the measurements.

Since those earliest experiments, much of the subsequent (and recent) work[3] has focused on the possibility of muon-catalyzed fusion as a cost-effective source of energy, because the muon which is released in internal conversion can be reused to facilitate the nuclear reaction. Conversely, the muon in radiative capture "sticks" to the nucleus, and it is lost to the catalysis process. Unfortunately, the radiative process dominates in p-d fusion, and much of the recent theoretical and experimental work has focused on d-t fusion, where the sticking probability is small. Nevertheless, molecules such as μ-p-d present us with an unparalleled laboratory for studying nuclear reactions at extremely low energies, much lower than can be obtained in traditional scattering experiments. Some recent experiments at the Paul Scherrer Institute[10,11] (PSI) have focused on this aspect of the field, in general, and on the Wolfenstein-Gerstein anomaly, in particular.

Significant progress has been made in the study of three-nucleon systems. The Schrödinger equation (or the equivalent Faddeev equations) can now be solved for "realistic" potentials (those with a strong short-range repulsion and a tensor force) without the basis truncations which were necessary in the past. Such complete or converged calculations have been performed for the ^{3}H and ^{3}He ground states[12] (the latter includes a Coulomb interaction between protons), for n-d scattering above breakup threshold,[13] and for zero-energy n-d and p-d scattering[14] (including a Coulomb interaction). It is therefore possible to perform *ab initio* calculations for the first time with realistic N-N potentials for the low-energy p-d capture reactions, including Coulomb interactions between the charged particles and possibly three-nucleon potentials as well. In this Letter, we describe such a calculation and compare it with recent PSI experiments[11] on p-d fusion.

At the extremely low energies between the proton and deuteron in a μ-p-d molecule, only relative s waves are expected to be important. This restricts electromagnetic interactions to the $E0$, $M1$, and $E2$ multipoles, with only the latter two contributing to radiative capture (i.e., real photons) where $M1$ dominates. Internal conversion can involve all three, but only $E0$ is expected to be important. Because the muon's mass is large, its electromagnetic current is very small, which suppresses $M1$ internal conversion. Using ^{3}He ground-state and zero-energy p-d scattering wave functions, the multipole matrix elements can be calculated once the operators are specified. The doublet rate for muon internal conversion is given by[15]

$$\lambda^{\mu}_{1/2}=3\left[\frac{2\pi}{27}\alpha^2\mu q|\psi_{\rm mol}(0,0)|^2|\langle{}^3{\rm He}||\hat{E}0||pd\tfrac{1}{2}\rangle|^2\right] \quad (1)$$

and

$$\hat{E}0=\sum_i e_i\left[r_i'^2-\frac{q^2}{20}r_i'^4+\cdots\right], \quad (2)$$

where the factor 3 in Eq. (1) is a conventional statistical factor and the total rate is $\lambda^{\mu}=\lambda^{\mu}_{1/2}/3$. In addition, e_i is the charge of the ith nucleon, $\mathbf{r}_i'$ is its position relative to the nuclear center of mass (c.m.), q is the recoiling muon's momentum (33.45 MeV/c), μ is its reduced mass with respect to ^{3}He, α is the fine-structure constant, and $\psi_{\rm mol}(\mathbf{R},\mathbf{r})$ is the μ-p-d molecular wave function expressed in terms of the internuclear coordinate $\mathbf{R}$ and the muon's coordinates relative to the nuclear c.m., $\mathbf{r}$. The factor $|\psi_{\rm mol}(0,0)|^2$ gives the probability of nuclear coalescence in the molecule, replacing the usual beam flux and target density in laboratory experiments. We have recently solved the Faddeev equations for the μ-p-d molecular ground state and have obtained this quantity directly from the molecular wave function. Our value of 8.07×10^{-20} fm^{-6} is quite different from the estimate made in Ref. 15. We also define

$$\rho_0=\int d^3r|\psi_{\rm mol}(0,r)|^2\cong 8.67\times10^{-13}\ {\rm fm}^{-3}$$

for later use. Our values for these molecular constants differ by less than 1% from those calculated with the more accurate wave function of the University of Florida group.[16] These differences are tiny compared to the uncertainties associated with the model operators.

Our results for the reduced matrix element $E0 \equiv\langle||\hat{E}0||\rangle$ are shown in Fig. 1. Equation (2) shows that $E0$ is the mean-square radius of the transition region, if the retardation terms ($\sim q^2,\ldots$) are ignored, and this is sensitive to the model binding energy of ^{3}He. Realistic

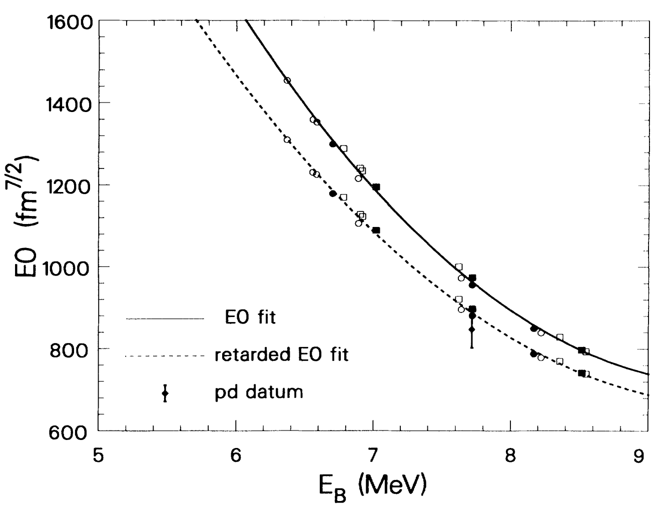

FIG. 1. $E0$ internal-conversion transition-matrix elements for $p+d+\mu^-\rightarrow{}^3{\rm He}+\mu^-$ for a variety of nuclear models plotted vs the model ^{3}He binding energy E_B. The strong sensitivity to the binding energy is similar to that of the ground-state mean-square charge radius (Ref. 17) ($\sim 1/E_B$). Circles correspond to the Reid soft-core N-N force model (Ref. 22), while squares correspond to the AV14 model (Ref. 23). Solid symbols correspond to 34-channel (complete) ^{3}He bound states and the corresponding p-d scattering states. Points with $E_B>7.2$ MeV contain a three-nucleon force. The datum is from Ref. 15.

N-N forces underbind ^{3}He by up to 1 MeV. Three-nucleon force models generate roughly the needed extra binding, but are quite sensitive to the short-range behavior, and the latter is not well determined. Consequently, we must resort to scaling plots,[17] where calculated observables are plotted as a function of the calculated binding energy of ^{3}He for a given model. This procedure only makes sense if the various values fall on a smooth curve, as they do in Fig. 1 and almost all other examples.[17] The solid circles and squares correspond to "complete" or converged calculations (34 three-body channels for ^{3}He); the other points represent a truncated force and are included for plotting purposes. Points with binding in excess of 7.2 MeV include a three-nucleon force. The points at the physical binding energy, 7.72 MeV, have had the latter force adjusted slightly to produce that binding.

Our results extrapolated to the ^{3}He binding energy are 963(10) fm$^{7/2}$ for the unretarded matrix element (i.e., $q=0$) and 888(10) fm$^{7/2}$ for the (physical) retarded one. The theoretical error bars are subjective and merely reflect the spread of our curves in Fig. 1. The 8% difference in retarded and unretarded matrix elements gives a scale for the effective nuclear interaction radius $(\langle r^4\rangle/\langle r^2\rangle)^{1/2}=7.7$ fm, since the overlap of initial and final doublet wave functions must vanish (by orthogonality) and consequently has no natural size scale. The rates are given in Table I. The $E0$ matrix-element calculation is straightforward, involves no meson-exchange currents, and is quite stable. The rate agrees well with a recent experimental value obtained[15] from old bubble-chamber measurements. Note again that this agreement requires a good calculation of the coalescence probability.

TABLE I. Results of this calculation (theory) compared to recent experiments or recent analyses of older experiments.

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

[a]Reference 15.
[b]Reference 11.
[c]Reference 18.

The radiative-capture process is complicated by the fact that the magnetic dipole transitions contain a large contribution from meson-exchange currents, in addition to the usual radiation from the individual nucleon dipole moments. Although the long-range one-pion-exchange process dominates these currents, the short-range behavior of the pion currents and detailed form of other intrinsically short-range currents are not well constrained. In order to deal with this problem for p-d capture, we first look at n-d capture, where the total cross section for the capture of thermal neutrons is known experimentally[19] to be 0.518(8) mb. We have previously studied this reaction[20] and have adjusted the π-nucleon range parameter (form factor) moderating the one-pion-exchange current's short-range behavior so that the total cross section is reproduced; this procedure leads to very reasonable values of the range parameter ($\sim$1200 MeV). Turning now to p-d capture, the $M1$ capture rates can be calculated with no further assumptions.

The doublet and quartet capture rates are given by

$$\lambda^{\gamma}_{J}=\left[\frac{6}{2J+1}\right]\frac{2\alpha}{9}\left(\frac{\omega_\gamma}{\hbar c}\right)^3\left[\frac{\hbar}{2mc}\right]^2\rho_0 c\,|\langle{}^3\mathrm{He}||\hat{\mu}||pdJ\rangle|^2\,, \tag{3}$$

where $\lambda^{\gamma}\equiv\frac{1}{3}\lambda^{\gamma}_{1/2}+\frac{2}{3}\lambda^{\gamma}_{3/2}$. We have defined the magnetic-moment operator in units of nuclear magnetons, the photon energy to be ω_γ, and the nucleon mass to be m. We have introduced the *conventional* statistical factors[3] in the square brackets (3 and $\frac{3}{2}$ for doublet and quartet). In addition, the (s-wave) astrophysical factor for p-d capture in laboratory experiments is given by

$$S_s=\frac{2\pi}{9}\alpha^2\mu c^2\left(\frac{\omega_\gamma}{\hbar c}\right)^3\left[\frac{\hbar}{2mc}\right]^2\left(|\langle{}^3\mathrm{He}||\hat{\mu}||pd\tfrac{1}{2}\rangle|^2+|\langle{}^3\mathrm{He}||\hat{\mu}||pd\tfrac{3}{2}\rangle|^2\right). \tag{4}$$

Numerical results are given in Table I. The individual doublet and quartet $M1$ capture rates are in good agreement with a recent PSI experiment.[11] The theoretical error bars are subjective and merely reflect the spread of our numbers, which have been extrapolated to the physical binding energy in a procedure analogous to that of Fig. 1. In addition, we agree well with the s-wave astrophysical S factor measured in a laboratory experiment.[18] The effect of the Coulomb interaction both on p-d scattering and on $M1$ capture rates is fairly substantial, although the basically isovector nature of the capture process would nominally make the n-d and p-d capture matrix elements the same. Overall, the quartet capture[21] is largely given by the impulse approximation, while the doublet capture has large exchange-current contributions. If the constraint of fitting n-d capture had not been used, then the estimated theoretical uncertainty in $\lambda_{3/2}$ would be (8) and that in $\lambda_{1/2}$ would be (7).

In summary, we have calculated the nuclear reactions in μ-catalyzed p-d fusion. Accurate wave functions have been generated for the AV14 and Reid soft-core 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 excellent agreement with experiment. Our internal-conversion rates are in very good agreement with a recent reanalysis of the 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 theorem.

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