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DEUTERON-INDUCED FUSION IN VARIOUS ENVIRONMENTS

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Abstract

The theory of deuteron-induced fusion will be discussed, first in free space, then in muonic molecules where the Coulomb repulsion is highly screened. It will be shown how a consistent description of the d+t reactions can be obtained in these environments using *R*-matrix theory. We compare fusion rates obtained from time-dependent scattering theory with those implied by the partial widths of the resonance associated with muon-catalyzed d-t fusion. Finally, some speculative comments are made about how the d+d reactions might proceed in other media, such as metallic lattices. The unusual properties of states associated with "shadow" poles might account for some of the strange results seen in cold fusion experiments. We emphasize that the same methods can, and should, be used to describe this situation as well as the other two well-established phenomena.

R-Matrix Properties

Wigner's *R*-matrix [1] is an exceptionally useful tool for describing nuclear reactions in free space. If the data are good enough, it can be used to parametrize the behavior of all the reactions of a multichannel system in minute detail and with great precision. At the same time, *R*-matrix theory automatically builds in all known analytic properties of the multichannel *S*-matrix (*e.g.*, causality, generalized unitarity, cut structure, *etc.*), which have a particularly strong influence on the structure of its poles in the complex plane. As we shall see later, these complex-energy *S*-matrix poles play a central role in the expansion of the time-dependent wave function. Finally, and perhaps most importantly, the theory is easily modified to describe nuclear reactions in media other than free space, as will be illustrated by the application to nuclear fusion in muonic molecules (μCF).

The *R*-matrix as Wigner defined it can be expressed as

$$R^{B}_{c'c} = (c'|[H + \mathcal{L}_B - E]^{-1}|c) = \sum_{\lambda} \frac{(c'|\lambda)(\lambda|c)}{E_\lambda - E} \tag{1}$$

in which the channel-surface projections of the Green's operator for the total system hamiltonian H become simple pole terms due to the spectral expansion of the resolvent operator in terms of the eigenfunctions $|\lambda)$ and eigenvalues E_λ of the operator $H + \mathcal{L}_B$. The addition of $\mathcal{L}_B$, the so-called "Bloch operator",[2] to H restores its hermiticity on the finite region enclosed by the channel surface (*i.e.*, the "nuclear" region), thereby allowing the spectral expansion to be made, and makes its spectrum discrete by imposing fixed boundary conditions (B) on the logarithmic derivatives of the solutions of H at the channel surface.

Wigner's *R*-matrix can be transformed to one associated with the outgoing-wave Green's operator that is a central quantity in scattering theory,

$$R^L_{c'c} = (c'|[H + \mathcal{L}_L - E]^{-1}|c) = -(c'|G^+(E)|c) \tag{2}$$

in which the boundary values in the Bloch operator are taken to be the elements of L, the diagonal matrix of logarithmic derivatives of the outgoing-wave solutions for the long-ranged external potentials that act between fragments in the channel region. In free space, these are just the repulsive Coulomb potentials between the charged nuclear ions. In a muonic molecule, the electrostatic attraction of the μ^- to the positive ions must also be included. However, the form of the R^L-matrix and of the scattering matrix,

$$S = 2iO^{-1}R^LO^{-1} + O^{-1}I \ , \tag{3}$$

remains the same in both cases. It is simply a matter of using the incoming- (I) and outgoing- (O) wave solutions associated with the appropriate external potential. In this way, the nuclear information contained in an R-matrix determined by analyzing data for reactions in free space can be transformed to one that describes the nuclear reaction at short distances in a muonic molecule. This idea can be generalized to any environment in which the interaction between the nuclear particles outside the range of nuclear forces can be represented by an effective two-body potential, forming a system that we will describe as being "composite".

Resonance Poles

The poles of the composite-system S-matrix (which are identical with the poles of R^L) contain the effects of both the long-ranged external hamiltonian and the short-ranged internal hamiltonian. Near one of its poles, the S-matrix has the form

$$S_{c'c} = i\frac{\Gamma^{\frac{1}{2}}_{c'\mu}\Gamma^{\frac{1}{2}T}_{\mu c}}{E_\mu - E}, \tag{4}$$

with

$$\Gamma^{\frac{1}{2}}_{c\mu} = \sqrt{2}O_c^{-1}(c|\mu\rangle \tag{5}$$

the partial-width amplitude in channel c. The solutions $|\mu\rangle$ for the complex energies E_μ, together with their adjoints $|\tilde{\mu}\rangle$, form a normalizable, bi-orthogonal set in all space. The pole energy

$$E_\mu = E_r - \tfrac{1}{2}i\Gamma_\mu \tag{6}$$

occurs on an unphysical sheet of the many-channel Riemann energy surface in the case of a resonance or virtual state, and on the real axis of the physical sheet in the case of a bound state.

We shall see in a later section that the complex-energy (momentum) poles of the S-matrix make important contributions to the time-dependent wave function. These are "quasi-stationary" terms whose time dependence is given by $\exp[-iE_\mu t]$. Only the poles having $\Gamma_\mu > 0$, associated with decaying states, contribute to the wave function for $t > 0$. In terms of momenta (essentially the square root of the energy), this means that the real and imaginary parts must have opposite sign. Therefore, all channel momenta $k_{c\mu}$ associated with a decaying-state pole must lie in quadrants (Q) II or IV.

The complex-momentum states, including their exponential time factors, actually correspond to traveling waves in the channel regions. The type of traveling wave depends on the location of the pole in the complex k_c plane, as is shown in Fig. 1. If the channel momentum $k_{c\mu}$ associated with the pole is in Q II, it corresponds to a confined, ingoing-wave solution. In Q IV, it corresponds to an unconfined, outgoing-wave solution. Most visible resonances are caused by poles that have

outgoing waves in all open channels (*i.e.*, above the second bisector in Q IV) and ingoing waves in all closed channels (above the second bisector in Q II). These "conventional" poles are the only kind discussed in many articles and textbooks on resonance phenomena, giving the impression that there are no other possibilities for *S*-matrix singularities.

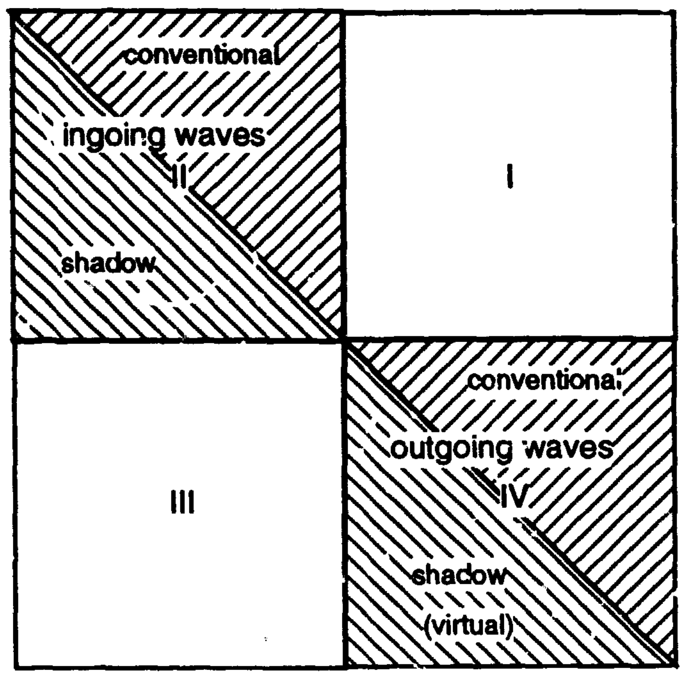

Fig. 1. Allowed regions for decaying-state poles in the complex momentum plane, and their characteristics as traveling waves.

However, it is possible for a pole to have outgoing waves in closed channels, or ingoing waves in open channels, as long as it has outgoing waves in at least one channel so that Γ is greater than zero. Such poles were discussed a number of years ago by Eden and Taylor,[3] who named them "shadow" poles. A shadow pole of the first type can occur in single-channel scattering, in which case it is called "virtual", or "antibound". A shadow pole of the second type can occur only in multichannel systems because of the restriction that it be outgoing in at least one channel. Perhaps for that reason, the existence of states with confined, ingoing waves in open channels is not yet widely recognized. The experimental evidence[4-6] for them has come to light only in recent years, and the physical consequences of such singularities in scattering theory are only beginning to be explored. The first example of such a pole in a nuclear reaction[6] was found in the ^{5}He system, which is the subject of the next section.

The ^{5}He System

This system contains one of the most famous resonances in nuclear physics: the $J^{\pi}=3/2^+$ resonance responsible for the large ^{3}H(d,n)^{4}He reaction cross section that peaks at E_d=108 keV. Values of the cross section at energies below the resonance are useful in a variety of fusion applications, and at higher energies, the differential cross section is of interest as a neutron source reaction.

The channels and data included in our analysis of the ^{5}He system for excitation energies up to 21.5 MeV are summarized in Table 1. In addition to the physical two-body channels d+t and n+α, an effective n+^{4}He*(0$^+$) channel was added to represent the effects of deuteron breakup (n+p+t). More than 2600 data points from 23 different types of measurements (cross sections, polarizations, *etc.*) were described in terms of 108 free *R*-matrix parameters that give a minimum in chi-square space for which χ^2 per degree of freedom is 1.48. We note that a generalized phase-shift fit would require 89 real parameters to achieve the same sort of description at a single energy.

Table 1. Channel configuration and data summary for the ^{5}He system analysis.

Channel	l_{max}	a_c (fm)
d+t	4	5.1
n+^{4}He	4	3.0
n+^{4}He*	1	5.0

Reaction	Energy Range	# Observable Types	# Data Points	χ^2
^{3}H(d,d)^{3}H	E_d=0-8 MeV	6	704	1164
^{3}H(d,n)^{4}He	E_d=0-8 MeV	14	1121	1379
^{3}H(d,n)^{4}He*	E_d=4.8-8 MeV	1	10	26
^{4}He(n,n)^{4}He	E_n=0-28 MeV	2	793	1150
Totals:		23	2628	3719

Examples of fits to some of the integrated cross-section data are shown in Fig. 2. At the left side of the figure are shown the fits to the reaction cross section (top) and neutron total cross section (bottom) over the whole energy range of the analysis. The right side of the figure shows essentially the same data enlarged over the region of the resonance. One sees that the calculations generally represent the data within their error bars, which, particularly in the case of the LEFCS measurements,[7] are reasonably small.

The energy dependence of the calculated *S*-matrix elements for J^{Π}=3/2$^+$ that are related directly to the reaction (σ_R) and total (σ_T) cross sections are shown over the resonance in Fig. 3. Unlike the behavior that would be expected for an isolated conventional resonance, the squared amplitudes corresponding to σ_R and σ_T do not peak at the same energy, and have a different energy dependence for the high-energy tail. Our analysis[6] shows that this behavior results from a two-pole structure of the resonance. One of the poles is a conventional pole that occurs on the (-,-)* Riemann sheet, and the other is a shadow pole on the (+,-) sheet. The total cross section is affected more by the conventional pole, shown as a circled "x" at the bottom left of Fig. 3, while the reaction cross section is influenced more by the shadow pole, shown by the same symbol near the real axis at 80 keV.

The resonance parameters for the poles are given in Table 2. The real and imaginary parts of the pole positions give the resonance energies E_r and total widths Γ, respectively, while the partial widths are defined in terms of the residues.[6] Note that for the conventional pole, the partial widths sum approximately to the total width, while for the shadow pole, the sum of the partials greatly exceeds the total. That is another manifestation of the unconventional character of a shadow pole,

*The Riemann sheets are labeled by the signs of the imaginary parts of the momenta in the d+t and n+α channels, respectively.

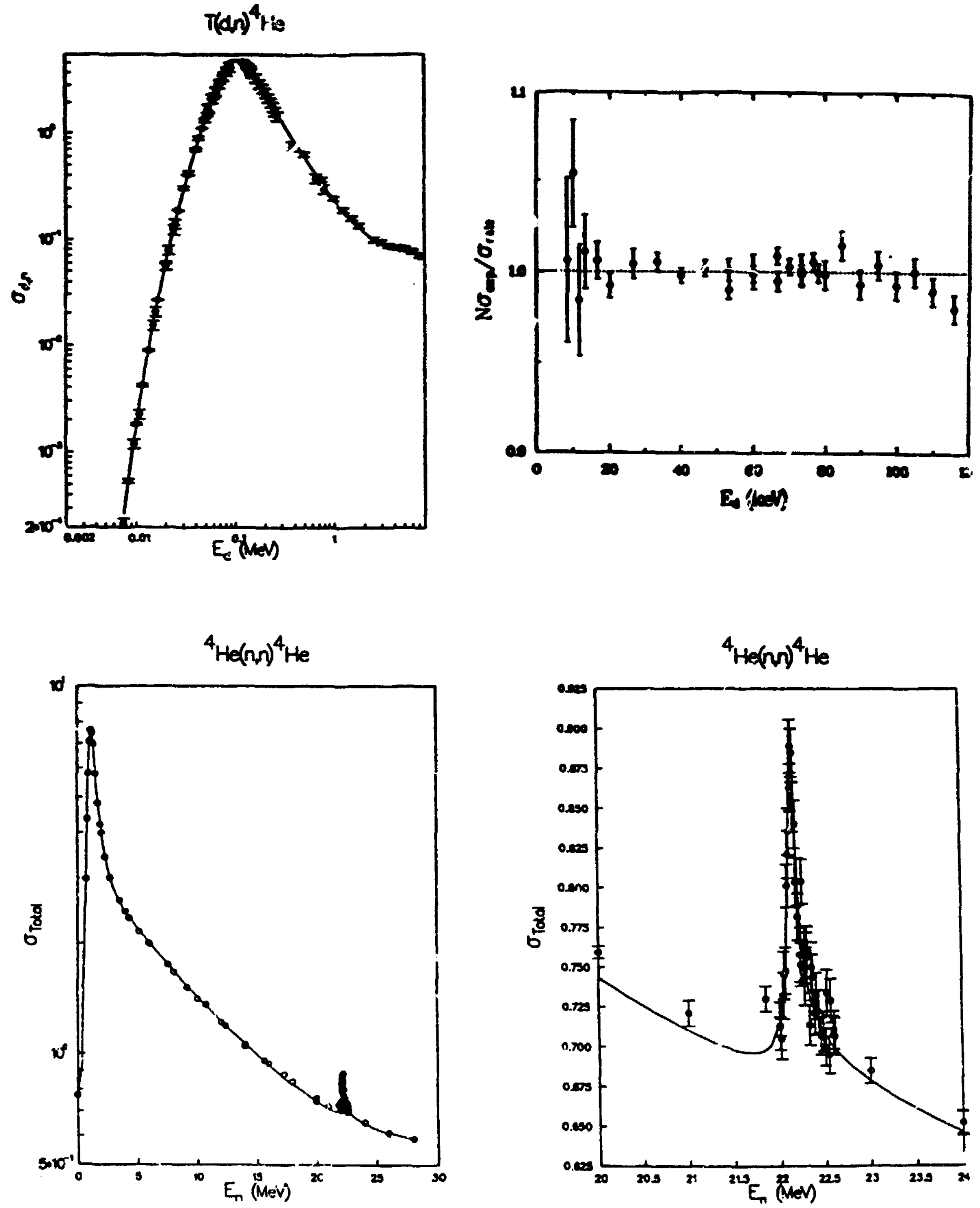

Fig. 2. Data for reaction (top) and neutron total (bottom) cross sections in the ^{5}He system compared with the R-matrix calculations. At the left of the figure, data are shown over the full range of the analysis; at the right they are shown in the region of the $J^{\Pi} = 3/2^{+}$ resonance, the upper part being the ratio of measured[7] to calculated values of the reaction cross section over the resonance.

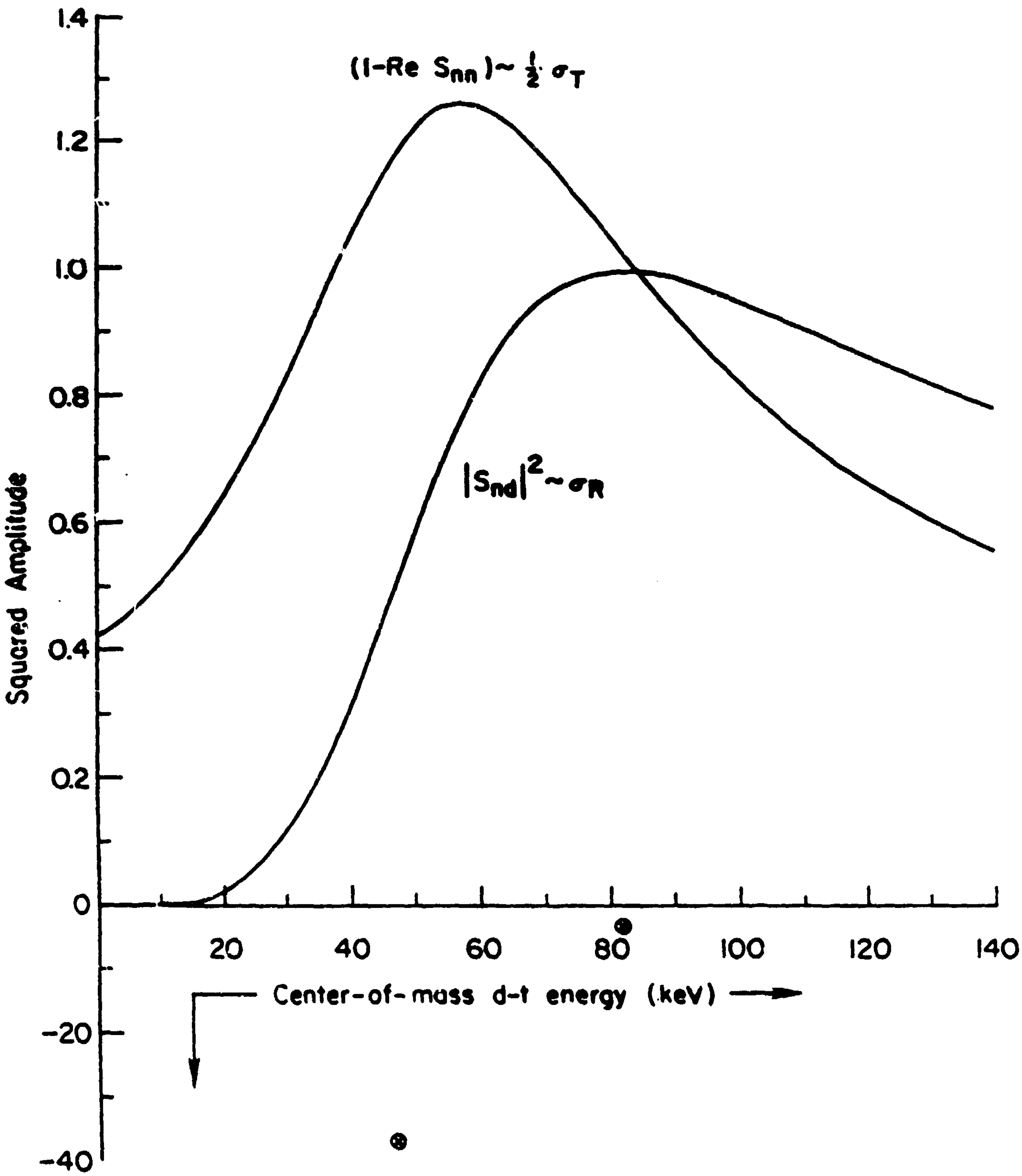

Fig. 3. S-matrix amplitudes for the $J^{\Pi}=3/2^{+}$ states of ^{5}He. The upper curve is proportional to the n+α total cross section, and the lower one is proportional to the $^{2}H(d,n)^{4}He$ reaction cross section. The conventional pole is marked by the circled "x" at the lower left of the figure, and the shadow pole by the one at the upper right.

and indicates that its small value of Γ does not produce any narrow structure in the cross sections. This scattering state has the unusual asymptotic behavior of confined, ingoing waves in the open d+t channel, acting in some respects as if it were bound in that channel. Indeed, the partial width Γ_d has in that case the significance of a bound-state asymptotic normalization constant, rather than that of a "decay" width.

Table 2. Pole parameters for the J^π=3/2+ ^{5}He resonance.

Sheet: (d,n)	(+,+)	(+,-)	(-,-)	(-,+)
E_r (keV)		81.57	46.97	
Γ (keV)		7.28	74.20	
Γ_d (keV)		2861.6	25.10	
Γ_n (keV)		68.77	39.83	

Time-Dependent Theory

In principle, the time-dependent description of a scattering process is the only valid one. Even for a steady-state process, the rates can only be properly derived starting from a time-dependent description. The time-dependent wave function is given in terms of the retarded Green's function at time $t \geq 0$,

$$G^+(t) = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} dE e^{-iEt} G^+(E) \quad [=0 \text{ for } t < 0], \tag{7}$$

and the initial wave function $\psi(0)$ by

$$\psi^+(t) = G^+(t)\psi(0)\,. \tag{8}$$

We have developed a somewhat different approach to evaluating the inverse Fourier transform in Eq. (7), which can be illustrated by considering a 2-channel system in which channel 1 has the lowest threshold. First of all, the integration path is taken in momentum (k), rather than energy (E), variables. By choosing a contour that encloses the poles in the lower half of the k_1 plane, one obtains the expansion

$$G^+(t) = \sum_\mu e^{-iE_\mu t}|\mu\rangle\langle\tilde{\mu}| + \int_{-\infty}^{0} dE_1 e^{-iE_1 t}|\psi_1^+\rangle\langle\tilde{\psi}_1^+| + \int_0^{\infty} dE_2 e^{-iE_2 t}|\psi_2^+\rangle\langle\tilde{\psi}_2^+|, \tag{9}$$

that is equivalent to the usual expansion in terms of the physical bound and scattering states of the system. Although the first two terms of the expansion above involve states that are "unphysical" because they diverge at large distances in channel 1, the sum of these terms always leads to a time-dependent wave function in which the divergences cancel, so that it is properly regular in all space. The advantage of using this expansion instead of the usual one is that it makes explicit the contribution of some of the resonances in the time-dependent wave function. The poles enclosed are outgoing in channel 1 and ingoing in channel 2, so that those below the channel-2 threshold are conventional, but those above it are the lesser-known type of shadow pole described in the second section, of which the ^{5}He shadow pole is an example.

If the initial state $\psi(0)$ has no appreciable overlap with the positive-energy channel-2 scattering states, then the time-dependent wave function in the channel-1 region ($r_1 > a_1$) is given in the case of S-waves with no Coulomb by

$$\psi_1(t) = \frac{1}{2}\sum_\mu \alpha_\mu e^{-iE_\mu t}|\mu,1)\,\mathrm{erfc}(z_{\mu 1}), \tag{10}$$

with

$$z_{\mu 1} = \left(\frac{m_1}{2it}\right)^{\frac{1}{2}}\left(r_1 - a_1 - \frac{k_{1\mu}t}{m_1}\right),$$

$$(r_1|\mu,1\rangle = \left(\frac{m_1\Gamma_{1\mu}}{4\pi k_{1\mu}}\right)^{\frac{1}{2}}\frac{O_{1\mu}(r_1)}{r_1},$$

and

$$\alpha_\mu = \langle\tilde{\mu}|\psi(0)\rangle.$$

In these equations, m_1 is the reduced mass of the two particles in channel 1. The *rate* at which normalization builds up in the channel-1 region can be calculated from the equation of continuity,

$$\frac{\partial}{\partial t}|\psi(t)|^2 = \nabla\cdot\frac{1}{m_1}\Im[\psi_1^*(t)\nabla\psi_1(t)], \tag{11}$$

giving an expression

$$\dot{N}_1(t) = \frac{\partial}{\partial t}\int_{a_1}^{\infty} r_1^2 dr_1|\psi_1(t)|^2 = \frac{4\pi a_1^2}{m_1}\Im\left[\psi_1^*(r_1,t)\frac{\partial}{\partial r_1}\psi_1(r_1,t)\right]_{r_1=a_1}, \tag{12}$$

that involves the wave function of Eq. (10) only at the channel surface, since it vanishes asymptotically.

We show in Fig. 4 examples of rates calculated from Eq. (12) for a single resonance in the cases that it has either ingoing or outgoing waves in channel 1. For the outgoing wave case, the rate starts near t=0 at the value expected from the width (Γ= 0.4) of the resonance, and shows approximately exponential decay with time. For the ingoing-wave case, however, the rate is negative at almost all times, meaning that the particles of channel 1 from the reaction would never be observed asymptotically for this type of state.

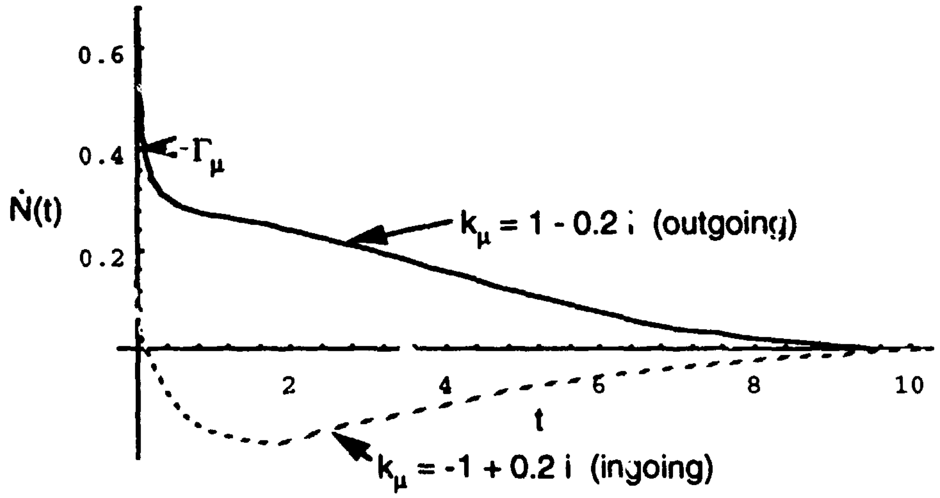

Fig. 4. Time-dependent rates calculated from Eq. (12) for: (a) an outgoing-wave pole (solid line) and (b) an ingoing-wave pole of the same energy (dashed line).

Muon-Catalyzed d-t fusion

In order to apply this sort of approach in the case of muon-catalyzed d-t fusion, one can use the R-matrix parameters for the nuclear ^{5}He system from the analysis described in the third section, but transformed to the outgoing-wave R-matrix of Eq. (2) using the outgoing-wave solutions for the (screened) dtμ potential, rather than those for a purely repulsive Coulomb potential, in the d+t channel. This has been done by Struensee *et al.*[8] for various types of adiabatic dtμ potentials. The most realistic of these is the so-called "improved adiabatic" (IA) potential shown in Fig. 5. The d-t Coulomb repulsion is screened so effectively by the muon that the potential has an attractive well at about 2 muonic atomic units (m.a.u.), or approximately 500 fm, which supports two bound states. The ground-state radial wave function, having rotational-vibrational quantum numbers $L = 0$ and $v = 0$, and its energy, about 317 eV below the mass of d+tμ, are also shown in the figure, but the wave function and energy for the first $L = 0$ excited state, having vibrational quantum number $v = 1$, are not shown.

From the poles and residues of the composite-system S-matrix in Eq. (4) can be determined the resonance parameters of the system. These are given in Table 3 for resonances on the (+,-) sheet, which are the ones that appear in the sum over μ for the time-dependent wave function in Eq. (10). The ro-vibrational bound states of the muonic molecule have been turned into narrow resonances with non-zero widths (Γ_n) for decay into the n+α channel by the nuclear forces at short distances, while the nuclear shadow pole has acquired a substantially different value of asymptotic normalization constant (Γ_d) due to the screened potential in the d+t channel. (Differences in E_r between Tables 2 and 3 for this resonance result mainly from differences in the reference energy, which in Table 3 is the mass of d+tμ, but in Table 2 is the mass of d+t.)

Also given in the table are the neutron rates, $\lambda_n = \Gamma_n/\hbar$, associated with each partial neutron width, and the magnitude of the overlap α_μ of each resonant state with the initial dtμ ground state in the time-dependent wave function. Because these coefficients are so small for all except the (L,v) = (0,0) resonance, the time-dependent neutron rate calculated from Eq. (12) falls off exponentially from the expected value $\lambda_n = 1.29 \times 10^{12}$ s^{-1} at all but the shortest times, where the effect of the shadow pole appears, but probably could never be measured. One sees from the table, however, that a different initial state having strong overlap with the shadow-pole state could produce a neutron rate as much as eight orders of magnitude larger than that initiated from the molecular ground state.

Table 3. ^{5}Heμ Resonances on the (+,-) Sheet in the IA Approximation

(L,v)	(0,0)	(0,1)	shadow pole
E_r (meV)	-317192.6	-31194.1	73281×10^3
Γ (meV)	0.8504	0.7100	7.338×10^6
Γ_d (meV)	1.156×10^9	2.480×10^6	6.172×10^7
Γ_n (meV)	0.8504	0.7100	6.876×10^7
λ_n (s^{-1})	1.29×10^{12}	1.08×10^{12}	1.04×10^{20}
$\lvert\alpha_\mu\rvert$	0.999···	2.9×10^{-6}	1.08×10^{-4}

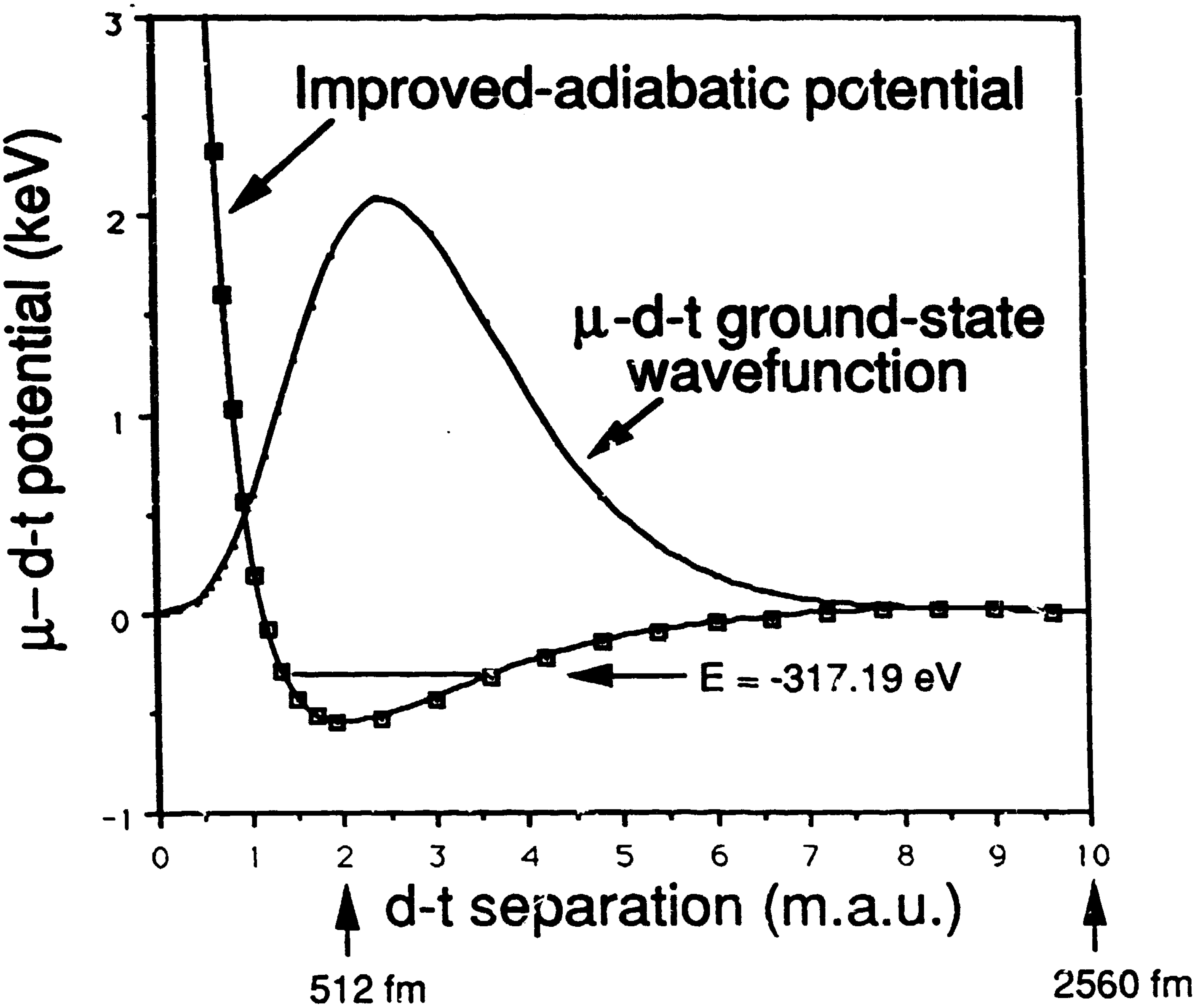

Fig. 5. Improved adiabatic dtμ potential (squares) and ground-state radial wave function (solid line) as functions of d-t separation in muonic atomic units. The ground-state energy of the molecule is also shown relative to the mass of d+tμ.

Summary and Conclusions

We have seen that R-matrix theory can give an excellent parametric representation of multichannel nuclear reactions on the real energy axis of the physical sheet, as was illustrated by the reactions in the ^{5}He system. The application to the dtμ system showed how the description can be generalized to a composite system that includes the effects of particles or media other than free space at large distances on the nuclear reactions at small distances. The theory has well-defined continuations into the complex plane that reveal the existence of "shadow" poles in many composite systems. Some of these poles correspond to confined, ingoing-wave states in open channels.

A proper formulation of the composite-system problem involves using time-dependent scattering theory, in which the time-dependent Green's operator gives the possibilities for how the reaction might proceed. For multichannel systems, the shadow poles with ingoing waves in open channels make important contributions to this operator because they are naturally enclosed by the only sensible integration contour that makes resonant effects explicit. Rates based on partial widths have no meaning for ingoing-wave states. In these cases, the time-dependent theory gives mostly negative rates (*i.e.*, particle flux leaving the channel region), and the partial width has the significance of a bound-state asymptotic normalization constant. Therefore, if the initial conditions just prior to the nuclear reaction select such a state in the time-dependent Green's operator, no particles will come out in the ingoing-wave channel, even though that channel is open. This is a situation in which the time-dependent solution is qualitatively different from the stationary (definite-energy) solutions from which it was constructed, allowing the branching ratios for various reaction channels to deviate substantially from the values they have when measured in beam-target scattering experiments.

Now, we turn to some speculative comments directed more specifically at cold fusion phenomena. Although there was no time to discuss it, we have an R-matrix description of reactions in the ^{4}He system[9] similar to that for the ^{5}He system, containing the channels p+t, n+^{3}He, and d+d. States exist in the nuclear ^{4}He system for several values of J^π that are outgoing only in the p+t channel, the closest to the d+d threshold being a shadow pole to the (first) excited 0^+ state of the alpha-particle. Perhaps such states also exist in ^{4}He + lattice systems, just as the ^{5}He nuclear shadow-pole state exists in the dtμ molecule. If any of these states has sufficient overlap with the initial d+d confined state in the lattice, the resulting p+t rate could be much larger than the standard rate formulas predict, and there would be no detectable neutron emission, in qualitative agreement with the anomalously low neutron/tritium branching ratios observed in some cold fusion experiments. Furthermore, if the overlap occurs primarily for $J^\pi=0^+$, no gamma-producing transitions are allowed from this state to the ^{4}He ground state, since this would be an electric monopole (E0) transition.

In order to get fusion without any type of particle or γ emission, it is necessary to postulate the existence of 0^+ states that are outgoing only in the E0 channel. No such states have yet been sought or found in the ^{4}He system. However, the search for some type of photon emission should continue, because the amount of energy released in radiationless fusion would be sufficient to excite highly energetic phonon modes in the lattice, with X-rays and possibly high-energy (conversion) electrons accompanying the eventual de-excitation processes.

It is important to realize that the qualitative, speculative statements made above can be made quantitative, using the theoretical framework outlined in this paper. The first requirement is to know the effective d+d potential in a metal lattice, in analogy with the IA potential in muonic molecules. This is a much more difficult question, however, involving which lattice sites are occupied at high deuterium loading, how the electrons and deuterons participate in screening, periodic and coherence effects, *etc.* The second requirement is to know the initial state of the d+d system in the lattice just prior to fusion. In our view (perhaps not surprising for nuclear physicists), there is now more uncertainty in these quantities than in the properties of the ^{4}He nuclear system near the d+d threshold. Once these quantities are determined, however, the calculation of rates for various outgoing particles can be performed using the expressions developed here. Achieving sufficient accuracy in a multichannel calculation would be a challenging numerical task, but it is likely the only way to answer, once and for all, the theoretical questions about cold fusion to the satisfaction of the scientific "mainstream".

References

1. E. P. Wigner and L. Eisenbud, *Phys. Rev.* **72,** 29 (1947); A. M. Lane and R. G. Thomas *Rev. Mod. Phys.* **30,** 257 (1958).

2. C. Bloch, *Nucl. Phys.* **4,** 503 (1957); A. M. Lane and D. Robson, *Phys. Rev.* **151,** 774 (1966).

3. R. J. Eden and J. R. Taylor, *Phys. Rev.* **133,** B1575 (1964).

4. A. Herzenberg and D. Ton-That, *J. Phys. B* **8,** 426 (1975).

5. K. L. Au, D. Morgan, and M. R. Pennington, *Phys. Rev. D* **35,** 1633 (1987).

6. G. M. Hale, R. E. Brown, and N. Jarmie, *Phys. Rev. Lett.* **59,** 763 (1987).

7. N. Jarmie, R. E. Brown, and R. A. Hardekopf, *Phys. Rev. C* **29,** 2031 (1984); R. E. Brown, N. Jarmie, and G. M. Hale, *Phys. Rev. C* **35,** 1999 (1987).

8. M. C. Struensee, G. M. Hale, R. T Pack , and J. S. Cohen, *Phys. Rev. A* **37,** 340 (1988).

9. See: D. R. Tilley, H. R. Weller, and G. M. Hale, "Energy Levels of Light Nuclei A=4," *Nucl. Phys.* **A541,** 1 (1992).