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# Computational challenges to the development of modern theories of nuclear reactions

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**Abstract**

Detailed theories of nuclear reactions now lead to and require extensive computations. Only then can their results be used to make verifiable predictions and to contribute to the development of nuclear physics. I focus on low-energy reactions of nucleons and light clusters on heavier nuclei, and discuss the computational challenges in the evaluation of coupled-channel theories of those reactions.

Keywords: reaction theory, coupled channels, computational challenges

(Some figures may appear in colour only in the online journal)

## 1. Roles of reaction theories

Reaction theories have been developed for a variety of reasons. One reason concerns the use of reaction theory in analyzing experiments in order to learning something about the structure of the participating nuclei. Reaction theories are necessary here because they are an essential interface between structure and experiments. This connection is possible because the predictions of reaction calculations depend on the structure information used as input. This enables the physical accuracy of that structure information to be discerned by examining how well the results of the calculations fit the cross sections that have been measured in experiments. A second reason, no less important for nuclear physics, is to explore the novel dynamical processes that occur when two nucleons or nuclei react together. We often need, for example, to explore the interplay of elastic scattering, transfer reactions and breakup process if a satisfactory account is to be given of any of these individually.

It used to be that reaction predictions were simpler, and depended linearly on structure information such as spectroscopic factors, and that gave rise to the belief that 'experimental

  

spectroscopic factors' could be determined by observations. Now, however, we have more detailed reaction theories that necessarily depend on *multiple* aspects of the structure models in such a way that there is no longer any linear dependence on specific structure aspects. In this case—much more frequently found in recent years—the proper analysis of experiments requires the construction of *multiple* structure models, preferably in some kind of family or else from opposing assumptions. The role of reaction theories in this case is the make accurate predictions from *each* of those structure models in turn, and test them by comparison with the experimental measurements[1]. The ideal role of reaction theories, therefore, is in a sense to be 'invisible', so that the structure aspects are faithfully reflected in the predicted cross sections. In that way, we hope, structure models can be properly tested experimentally. The need for comprehensive structure models to start reaction calculations is now particularly great, since new accelerators are producing varies species of nuclides for the first time. In such cases there are no previous empirical scattering data to help in setting up the effective interaction or optical potentials. In such case, the best quality *structure* theories of one or both of the participating nuclei are essential.

For a reaction theory to be 'invisible', it should take into account all possible mechanisms in given reaction. Strictly speaking, that is impossible. So reaction theory for now concentrates mostly on including the *relevant* mechanisms following from the structure and substructure of *one* of the participating nuclei. We call such theory a *semi-microscopic* reaction theory. It will use, for one of the interacting nuclei, an extensive structure model of its ground state and excited states, and of the transition mechanisms that couple them together. The name 'semi' indicates that the *other* participating nucleus is treated still as one body[2]. The challenges described in this paper all come from the reaction theory trying to include more and more complicated participating nuclei, and more and more complicated structures of those nuclei.

## 2. Types of reaction theory and their computational complexities

The simplest theory for the reaction of two nuclei consists of using an effective interaction or optical potential between the two bodies. It will predict elastic scattering, polarization observables if it has spin-dependent components, and absorption cross sections if it has an imaginary component. Weak secondary channels may be calculated as perturbations from elastic scattering, using what is called the distorted wave Born approximation.

### *2.1. Adiabatic approximations*

To go beyond perturbation theory for the non-elastic channels, we have to consider further degrees of freedom of the participating nuclei. If these other degrees of freedom are *much faster* than elastic scattering, or either *much slower* than elastic scattering, then a variety of *adiabatic approximations* become useful. The validity of these approximations may also be phrased in terms of the ratio of excitation energies to the elastic energy. When the inelastic energies are small compared with the beam energy, an adiabatic approximation can be used which calculates the scattering from each inelastic configuration, and then averages the scatterings between the initial and final configurations to predict the cross sections [1–4]. When, conversely, the beam

[1] Ideally, there should be as little 'post-processing' of those experimental results as possible, to avoid possible contamination from model dependence. For example, two-body cross sections can be unambiguously transformed from laboratory to center-of-mass frames of references, but three-body (or more) final states can only be so transformed if kinematically complete measurements have been recorded.

[2] A theory which treated *both* nuclei as consisting of nucleons with defined interactions, would be called a *fully*-microscopic reaction theory.

energy is *low* compared with the excitations, then a kind of Born–Oppenheimer method can be used which calculates a series of perturbed stationary states are various distances. These states are then combined to make an 'energy surface' for generating the scattering cross sections [5].

### *2.2. Coupled-channel calculations*

Because, however, all these semi-microscopic theories describe reactions at high, low and middle energies, with *many* types of couplings, each with a range of strengths, it is difficult or impossible to decide in advance which couplings can safely be treated as perturbations, which are fast or slow, and which need treatment to all orders. Moreover, there may be intermediate channels which combine coherently, so the smallness of a certain exit channel does not always imply that it is needed only to first order[3]. Most often, therefore, the theories to be here described use a *coupled-channels* framework, in which all couplings are included to all orders. In particular, it becomes straightforward to include the couplings *between* non-elastic channels which are treated (approximately), in the adiabatic models. The above adiabatic cases can be considered as approximations to the full coupled-channels treatment when specific simplifications are made concerning either the relative motion energy operator, or else the energy of the internal degrees of freedom of the nuclei.

The challenges described below concern the generation of the couplings between all pairs of elastic and non-elastic channels, and then how to solve accurately the resulting set of coupled equations. Radial wave functions $\psi_\alpha(R)$ for $\alpha = 1 \cdots M$ are needed, where each partial-wave channel $\alpha$ consists of specific states of the interacting nuclei and their parts, of orbital partial waves between those parts, and of specific intermediate quantum numbers. These $\psi_\alpha(R)$ are constrained by satisfying at large distances (outside $R_m$) their matching boundary conditions

$$\psi_\alpha(R) \rightarrow_{R \geqslant R_m} \frac{\mathrm{i}}{2}\left[H_\alpha^{(-)}(k_\alpha R) - S^{J\pi}_{\alpha:\alpha_0} H_\alpha^{(+)}(k_\alpha R)\right], \tag{1}$$

where $\alpha_0$ is the incoming channel, and $H_\alpha^{(\pm)}$ are the Coulomb wave functions. The $S^{J\pi}_{\alpha:\alpha_0}$ are the elements of the scattering $S$ matrix, and are used to calculate the cross section angular distributions. A coupled-channel calculation consists of selecting in turn each total spin $J$ and parity $\pi$, and then solving as a complete set of all the $M$ partial-wave channels that couple up to $J^\pi$.

When solving the coupled set of equations, there is a large difference in complexity between having only *local* couplings, and having at least some *non-local* couplings. A local coupling can be represented by a potential $V(R)$ such that the result of its action on a wave function $\psi(R)$ is simply the product $V(R)\psi(R)$. A non-local coupling, by contrast, must be represented by a two-dimensional kernel function $V(R, R')$ such that the result at $R$ of its action on the wave function is the integral $\int V(R, R')\psi(R')\mathrm{d}R$. Local potentials may be stored numerically as a vector, but non-local potentials need to be represented by a matrix.

When there are only local couplings, such as result from most optical potentials and from inelastic excitation mechanisms, the coupled equations are a set of ordinary differential equations, and regular solutions can be found by progressive or 'shooting' methods. These integrate out from the origin a set of linearly-independent solutions, and then take a superposition of those to satisfy the boundary conditions of equation (1).

When there are non-local couplings, such progressive methods cannot be used as we have a set of integro-differential equations. The equations can either be solved iteratively (if the non-local couplings are not too strong), or else basis-function methods must be used which expand the channel wave functions as linear combinations of those basis functions.

[3] Such a rule fails obviously for *closed* intermediate channels, as they have zero exit cross sections.

These expansion methods are generally more time consuming, not least from the time for the solving an $NM$-square set of linear equations if there are $N$ basis functions used to expand each channel. The basis functions methods do facilitate a fully antisymmetrized treatment of reactions, which turns out to be practical for reactions of light nuclei [6].

### *2.3. Parallelism in coupled-channel calculations*

As the size $M$ of coupled-channels sets become larger, it becomes advantageous to speed up the overall duration of the calculations by means of parallel computation. It is a general rule in quantum mechanics, in fact, that the calculations for any conserved quantum number may be generated in parallel. The results for any uncoupled quantities may be calculated at the same time.

The most obvious parallelism for coupled-channels calculations is to solve the channel sets simultaneously for each combination $J^\pi$ of total spin and parity. These are the principal conserved quantum numbers in such calculations. In the adiabatic models there are many more uncoupled quantities (the internal configurations in the first adiabatic method, or the energy surface at each point in the second method) and so more parallelism may be employed in these cases.

Within each of the above concurrent calculations, more parallelism is possible. The couplings between all the different channel pairs may well be computed in parallel. The calculations of the $M$ linearly-independent solutions in the progressive method are logically independent and therefore available for parallel generation. The solution of the linear equations to satisfy the boundary conditions of equation (1) is not naturally parallel in the same sense, but parallel libraries exist already to accelerate the method of Gaussian elimination to solve linear systems. Finally, the calculation of cross sections for each exit channel can be performed concurrently. All of these methods can be used in the standard coupled-channels code FRESCO [7].

Of these proposed parallel schemes, only those of the $J^\pi$ sets and of the cross sections are particularly effective. That is because the generation of all the pairwise couplings usually requires many elements in common such as potentials and form factors of structure states. If these common elements are too numerous then the time spent in calculating these locally, or else calculating them once and distributing the results, is too large compared with the time saved by the parallelism. This problem is even more acute for the $M$ linearly-independent solutions, as they all require exactly the same diagonal and off-diagonal coupling factors. Generating the independent solutions, therefore, is best done with 'local' parallelism such as that offered by OPENMP. This is efficient provided computational threads are available that are not already used for the 'global' parallelism given by the MPI framework.

## 3. Nucleon–nucleus reactions

The most recent comprehensive calculations of reactions of neutrons or protons at low and medium energies have focused either on the excitation of rotational bands, or on the excitation of single-particle degrees of freedom. First we look at challenges in the calculation of rotational bands, then of particle excitations.

### *3.1. Excitation of rotational bands*

Coupled-channels calculations for neutron scattering on actinide nuclei found to need more excited states for convergence than was previously believed [4]. The poor convergence shows

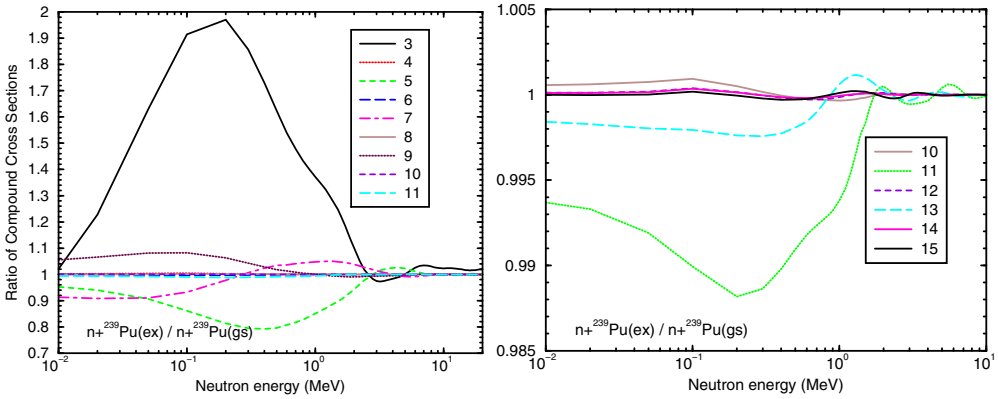


**Figure 1.** Ratio of compound-nucleus production cross sections for initial excited to initial ground states, with neutrons incident on $^{239}$Pu. The lines are for different sizes of coupled-channels sets. The right figure is an enlargement for 10–15 coupled levels.

up especially when calculating the total and the compound-nucleus production cross sections below 1 or 2 MeV incident neutron energy. This was first discovered [4] when trying to predict the compound nucleus (fusion or absorption) cross sections for neutrons incident on excited states in $^{239}$Pu, following the earlier results of [8]. We found the ratios of excited-state to ground-state cross sections shown in figure 1, and were astonished by the large fluctuations of the results with increasing the number s of levels in the coupled channels sets. We define $s$ by $s = 3$ for the ground state and two excited states, for example. Calculations with $s = 3$ (as has been commonly used in applications such as [9]) give this ratio nearly to 2.0 (figure 1, left side), whereas converged results (figure 1, right side) differ from unity only by 0.03%. We conclude in general that even–even nuclei (in their $K = 0$ bands) need coupled-channels sets of $s = 6$ levels, whereas even–odd nuclei (with half-integer $K$ bands) require up to 12 levels for accuracy. Since the number of partial-wave channels is 156 for a $K = 1/2$ band with $s = 12$, but only 66 for a $K = 0$ band with $s = 6$, and the computational time rises as the cube of the number of such channels. The accuracy is particularly critical in the fast-neutron energy range between 0.1 and 1 MeV incident energy.

### *3.2. One-particle–one-hole mean-field excitations of heavy nuclei*

For spherical closed-shell nuclei, a successful account of elastic nucleon–nucleus scattering has to include the effects from the excitation of non-elastic degrees of freedom, such as vibrational and particle–hole (p–h) excitations, along with transfer reactions to intermediate deuteron states. Nobre *et al* [10, 11] included in coupled-channels calculations (using FRESCO [7]) all the open channels that can be reached in one step from elastic scattering. An initial HFB calculation gave the particle and hole levels of a given nucleus and fixed the p–h basis states for generating excited states within the framework of (Q)RPA, thus accounting for correlations caused by the residual interactions within the target. To generate sets of excited states, they used RPA and quasi-particle RPA (QRPA) structure models for finite nuclei, which start from HFB structure models based on energy-density functionals. For each excited state, they calculated the one-body transition density and corresponding transition potential by the methods of [12, 13], in addition to which couplings to all pickup channels were included.

The primary purpose of these calculations was to predict the reaction cross section, by employing the *doorway approximation*, which takes the total flux leaving the elastic channel to

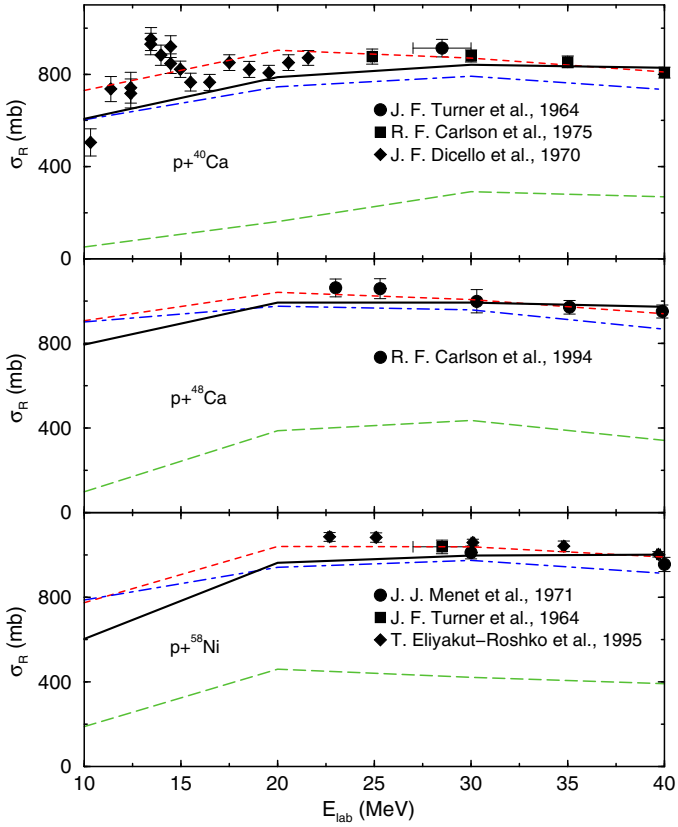


**Figure 2.** Total reaction cross section as a function of the incident energy for p + $^{40}$Ca, p + $^{48}$Ca and p + $^{58}$Ni. The results are shown for couplings to the inelastic states lying below 30 MeV (dashed lines), to the inelastic and transfer channels (dash–dotted lines) and to the inelastic and transfer channels with non-orthogonality corrections (solid lines). The Koning–Delaroche [14] optical model calculations are shown as short–dashed lines. The lines serve as guidance to the eye as calculations were performed only for $E_{\rm lab}$ = 10, 20, 30 and 40 MeV. Data from [15–20]. Reproduced with permission from Nobre *et al* [10], copyright (2010) by the American Physical Society.

all possible first-order channels to be independent of what happens afterwards: a nucleon later might escape as a free nucleon, the flux might equilibriate to compound-nuclear resonances, etc. A summary of the results for protons on $^{40,48}$Ca and $^{58}$Ni is given in figure 2, where the best predictions were the solid lines. The largest of these calculations included 1420 natural-parity excited states of the target up to spin 10, and this required 7234 partial-wave coupled channels.

These calculations were simplified by the observation that the couplings *between* inelastic states where found to be insignificant above about 10 MeV incident beam energy. This implies that the same results for elastic scattering can be obtained by calculating separately each second-order non-local operator $V_{0e}G_eV_{e0}$ for excitation to state $e$. The local $V_{e0} = V_{0e}$ are the inelastic transition densities, and the non-local $G_e$ is the Green's function propagator in the $e$th inelastic state. That enables the effect of *all* inelastic states to be summed to a full Feshbach operator $V_{\rm Fesh}(R, R', E, L)$ that is non-local, energy-dependent and angular-momentum dependent. Compared with a full coupled-channels calculation, nevertheless, its evaluation is relatively simple. Now up to 21 000 excited states have been included, requiring a second-order summation over 261 000 partial waves.

One procedure used in [11] was to evaluate the effect of all the *inelastic* states by means of such a $V_{\rm Fesh}$ operator, and include that operator in a multi-step basis-function calculation that furthermore included all the transfer channels. Such an combined approach yielded the final results shown in figure 2.

### 3.3. Combining collective and single-particle modes

As yet, no systematic treatment exists that combines collective and single-particle modes during reactions. A first attempt by Dupuis *et al* [21] begins this modeling, but so far only in the multi-step Born approximation without yet the collective couplings in the entrance and exit channels. There is not yet a comprehensive model of nucleon–nucleus collisions on deformed nuclei: one which will couple both collective and single-particle degrees of freedom, not to mention the rotational bands that are built on each separate single-particle intrinsic configuration. The availability of deformed-QRPA structural models will provide reaction theory with an important tool for such developments.

## 4. Two-body projectiles

When one of the interacting nuclei is a two-body cluster nucleus, then a great many excited states of that nucleus may be easily calculated by solving one-channel scattering equations, and used as a basis set for the reactions of such nuclei. The deuteron is the prime candidate for such a treatment, and, because of the widespread use of (d,p) transfer reactions to probe the neutron structure of heavy nuclei, such a treatment of deuteron excited states has become standard. Since all the excited states of a deuteron are in the continuum, such modeling has furthermore become a widely-used test bench for the treatment of breakup states during from or during nuclear reactions. The same techniques can be applied to $^6{\rm Li} = \alpha + {\rm d}$ or $^7{\rm Li} = \alpha + {\rm t}$, not to mention all the weakly-bound and one-nucleon halo nuclei such as $^8$B, $^{11}$Be, and $^{17,19}$C.

Some technique is need to regularize the continuum, since standard mono-energetic scattering states extend out to infinity, and are not square integrable. This lack of integrability does not show up in transitions to or from bound states, but only when transitions *between* scattering states need to be calculated. This need was spectacularly shown by Nunes and Thompson [22] for $^8{\rm B} \rightarrow {}^7{\rm Be} + {\rm p}$ breakup at low energies.

### 4.1. Continuum-discretized coupled channels (CDCC)

In order to have square integrable basis states, the most common treatment is to used *continuum bins*, which are integrals $\tilde{u}_p(r)$ of the true scattering wave function $u_k(r)$ over some section $[k_{p-1}, k_p]$ of the continuum (with some weight function $g_p(k)$):

$$\tilde{u}_p(r) = \sqrt{\frac{2}{\pi N_p}} \int_{k_{p-1}}^{k_p} g_p(k) u_k(r)\, {\rm d}k. \tag{2}$$

The normalization constant is $N_p = \int_{k_{p-1}}^{k_p} |g_p(k)|^2\, {\rm d}k$ to make the $\tilde{u}_p(r)$ form an orthonormal set when all the $(k_{p-1}, k_p)$ are non-overlapping continuum intervals, and so are suitable as a basis for breakup calculations. The resulting *bin* wave functions $\{\tilde{u}_p(r)\}$ from their construction have a simple form of overlap with the physical scattering states. Coupled channels calculations that use these bins are called coupled discretized continuum channels (CDCC). The need for breakup was shown by Johnson and Soper [23], and later developments by Rawitscher [24] and Austern [25–27] helped to introduce the more realistic CDCC representation of the continuum.

The method has been generalized [28, 29] (XCDCC) to include possible excitations of one of the clusters.

Alternative methods have used sets of Gaussians (often shifted or deformed in various ways), and also the 'pseudo-states' which come from a diagonalization of the two-body potential within some finite basis set [30, 31]. In principle all these methods should yield the same results when fully converged. The pseudo-state methods have fewer input specifications since the $\{k_p\}$ do not all need to chosen in advance. If the basis determined by the pseudo-state method are sufficient for convergence (as in [32, 33], for example), then all is well. Otherwise, it is an advantage of the CDCC that we can choose the bin widths for modeling (say) breakup to specific energy regions. The breakup to low relative energies is often needed, for example, to estimate the reverse process of low-energy capture to the ground state of a two-cluster system.

The computation challenges in CDCC calculations are of two kinds. First we note that the storage requirements are mitigated in many applications where only breakup needs to be predicted, since in that case the channels wave functions for the cluster-target scattering do not need to be stored: only the $S$ matrix calculated at the matching point by solving equation (1). The parallel computation of different $J^\pi$ combinations is the principal and most useful speedup available, in [7] for example.

If, on the other hand, the breakup channels are the intermediate channels before a transfer reaction, then the channel wave functions *do* need to be stored even if the transfer is calculated just to first order in a coupled-channels Born approximation scheme. That is because the transfer operator is necessarily non-local, and thus requires, in (d,p) reactions, the deuteron channel wave functions at all radii before any transfer source term can be completely generated. This requirement considerably pushes up the storage demands on each node.

If the transfer couplings are to be included to all orders, then a serious challenge remains that is as yet unsolved. The physics side of this all-order-transfer case is *also* problematic, since there is a significant non-orthogonality between even a single transfer state and the cumulative set of all the breakup states. This physics problem requires ideally a full three-body model expressed by means of the Faddeev equations. Bound states in multiple rearrangement partitions may then be handled as standard. Such models are well established for few-nucleon problems. The presence of Coulomb forces, however, leads to difficulties for transfer reactions on heavier nuclei. The most successful method to date is that of [34], where the Coulomb potentials are cut off after some screening radius so that the nuclear contribution may be calculated as the difference between the results for screened-Coulomb and screened-Coulomb + nuclear interactions. For light nuclei this difference converges as the screening radius increases, giving confidence in the results there, but convergence is difficult for nuclei heavier than $A \sim 40$. Mukhamedzhanov [35], however, formulates a three-body model in a momentum space constructed not from plane waves but from Coulomb-distorted waves. Recent work [36] shows how to regularize the needed overlap integrals of nuclear form factors with the Coulomb-momentum-space wave functions with their singularities.

## 5. Three-body projectiles

There has been less work on the scattering of three-body projectiles. Most of the results come from the groups of Rodríguez-Gallardo [37] and of Kamimura [38]. These both used the pseudo-state methods, this time for three-body systems, to define the ground and excited states of $^6$He in a model space using either hyper-spherical [37] or Gaussian [38]. expansions. Both groups calculated all the transition densities between pairs of states, and solved [39–41] the coupled-channels set with all these couplings. At the low energies around the Coulomb

barrier, the actual solution of the coupled equations took less time overall than the coordinate transformations and folding of all the three-body pseudo-states with the effective interaction for the target.

## 6. Conclusions

We see that there has been substantial progress in recent years in formulating and solving reaction theory problems that take into account a largest possible set of degrees of freedom that are excited in nuclear reactions. These models have been developed by solving various computational challenges, but many more challenges remain for the future. We need in the near future work toward a comprehensive model even of nucleon–nucleus collisions on deformed nuclei: one which will couple both collective and single-particle degrees of freedom, not to mention the various rotational bands. Another idea is to use the energy-density-functional methods that have been very successful for nuclear bound states across most of the periodic table. A recent proposal [42] is to extend those methods to the very lightest projectiles, so that basis states for projectile-on-target scattering can be generated by the mean field, and we might thus begin to have a unified nuclear theory of both bound and scattering states.

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