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NEW APPROACHES FOR BOUND AND SCATTERING STATES

CONVENER'S REPORT

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1. Introduction

Since its inception, the field of few-nucleon physics has been driven by the desire to obtain accurate solutions of the Schrödinger equation for physically interesting problems. These problems include the bound and scattering states of Hamiltonians which contain "realistic" potentials. This quest has been considered so important and so difficult that a major component of our field has devoted itself as much to methods of solution as to the physics inherent in the problems. Lack of convergence of different methods in the past had many different causes, but the result was an inability to extract that physics.

This preoccupation with improving the quality of methods (both numerical and formal) has paid off. We have now achieved "exact" or complete solutions to a variety of important 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 in the latter case). Such solutions might be conveniently defined as those with fractional errors of less than one percent in relevant observables (or perhaps more restrictive in some cases). The realistic potentials referred to above are those containing OPEP (and thus a strong long-range tensor force), a strong short-range repulsion, and which provide at least a moderately good quantitative fit to two-nucleon scattering data. The qualitative importance of OPEP in the few-nucleon systems has only recently been recognized[6], although the importance of the tensor force has long been recognized. As much as 80 percent of the potential energy in the triton is due to OPEP[7] (in the variational sense: $\langle V \rangle$). Moreover, in the recent Nijmegen N-N phase shift solutions[8], where the pion masses are *fit* rather than input parameters, they find $m_{\pi^0} = 135.6(13)$ MeV and $m_{\pi^\pm} = 139.4(10)$ MeV. The very small error bars demonstrate the importance of OPEP in the scattering data. The concomitant tensor force has proven to be a formidable obstacle to numerical solution. Techniques which work well in the absence of a tensor force often work much less well in the presence of such a force.

From an historical perspective these diverse efforts to solve the Schrödinger equation have evolved in somewhat unexpected directions, as evolutionary and revolutionary improvements have been made. The result has been that we have achieved a rather good understanding of the three- and four-nucleon systems and are beginning to develop insight into "real" nuclei with five or more nucleons (where the Pauli principle can be expected to play a pivotal role).

Improvements in the future are not only expected, they are essential. Our problems of current interest are becoming progressively more difficult and their solution will require improved methods. Moreover, as techniques improve and solutions become easier to obtain, the latter will disseminate more rapidly into the nuclear physics community.

We present below a rather personal view (i.e., very incomplete and somewhat biased) of the development of the primary methods that have been used for solving the few-nucleon Schrödinger equation, all of which have achieved a significant measure of success when applied to realistic potentials, and which may be promising in the future. Much other work has contributed to this success and must necessarily go unmentioned. The new developments described in this discussion session by the various speakers have some connection with one or more of these methods.

One thing is virtually certain: the future holds surprises for us. It is not at all clear that the methods of choice today will be those at the turn of the century. Our future lies in new and improved methods.

2. Variational Techniques

The earliest technique used to solve the few-nucleon Schrödinger equation was the Rayleigh-Ritz variational principle. This method is employed because of two powerful properties:

1. The variational estimate $\langle H \rangle$ is an upper bound to the ground state energy;
2. An error of order ϵ in the wave function produces a contribution of order ϵ^2 to that upper bound.

In 1935 Thomas[9] used the first of these properties to demonstrate that nucleon-nucleon forces of zero-range would lead to the collapse of the triton ground state. Subsequently, Gerjuoy and Schwinger[10] undertook 50 years ago the first variational calculation of the triton binding energy for a Hamiltonian which includes a tensor force. The latter forces have proven significantly more difficult to treat than purely central forces. Much of the work before 1970 took the variational route[11].

Two different approaches have been followed in selecting the variational trial functions. One approach uses appropriately symmetrized products of Jastrow[12] pair (two-body) correlation functions, which are physically motivated and are currently rather sophisticated[7]. The other approach is a brute-force expansion in a complete set of functions which appropriately spans the space. The variational parameters of the latter are usually chosen to be linear in order to facilitate the numerical solution. The advantage of the first approach is that it can be used for a wide variety of nuclear systems ranging from the triton and ^4He to ^{16}O [13] and nuclear matter[14]. Its disadvantage is that it is not yet a fully converged approach and for realistic potentials produces errors on the order of several percent in the binding energies of few-nucleon systems. Converged calculations exist for ^3H and ^3He which use the other approach[15].

The latter calculations exploit the Faddeev decomposition[16,17] of the Schrödinger wave function, Ψ . Writing

$$\Psi(\mathbf{x}, \mathbf{y}) = \psi(\mathbf{x}_1, \mathbf{y}_1) + \psi(\mathbf{x}_2, \mathbf{y}_2) + \psi(\mathbf{x}_3, \mathbf{y}_3) \equiv \psi_1 + \psi_2 + \psi_3,$$

where the function ψ is the *same* function of *different* coordinate (and spin) variables for the case of identical particles. Thus, in that case only one of these functions needs to be modeled. This representation is the essence of the Faddeev method, since it decomposes the very complicated Schrödinger wave function into simpler functions, which represent the separate (physical) rearrangement channels. It is this device which allows the boundary conditions for scattering to be implemented in a tractable and transparent way[18].

Thus, although it is the oldest weapon in the few-nucleon arsenal, the variational approach is currently very successful and holds promise for the future. We also note that other techniques (discussed below) which produce a wave function can make effective use of variational bounds to check or improve their eigenvalues.

3. Faddeev Techniques

The Faddeev approach to solving the Schrödinger equation was developed in order to resolve a problem pointed out long ago by Foldy and Tobocman[19]. Traditional scattering theory converts the Schrödinger equation to the Lippmann-Schwinger equation, whose integral form facilitates the implementation of the usual outgoing-wave boundary conditions. Nevertheless, the latter equation has no unique solution for n-d scattering above breakup threshold, because there is no way to control the amount of “initial” plane wave for the *rearrangement* channels. Specifying this component of the boundary conditions requires two additional equations which, together with the original equation, comprise the triad equations[20]. Equivalently, one can solve the three Faddeev equations (which for identical nucleons are identical equations). This clever decomposition by Faddeev isolates the rearrangement channels into the permuted Faddeev wave function components (i.e., ψ_2 and ψ_3). Adding these permuted components to ψ_1 to form Ψ produces a more complex wave function with the correct rearrangement amplitudes. Although originally devised in order to satisfy the requirements of scattering theory, this scheme has proven highly effective for bound-state problems, as well. The cusps and ridges of the virtual “rearrangement channels” in the wave function are just as difficult to model numerically in the bound states as they are in the scattering states, although the boundary conditions for the former problem (finiteness) have never been in doubt.

The seminal calculations of Malfliet and Tjon[21] for realistic potentials decomposed to include only a few nucleon-nucleon partial waves (“channels”) were soon followed by the calculations of the Purdue[22] and Hannover[23] groups, which involved many more partial waves. Convergence requires roughly 34 channels[1] for the trinucleon ground states, and this has become the standard for such calculations. The original converged calculations treated only strong two-nucleon forces; they have since been extended to include the Coulomb force in ^3He and the three-nucleon force in ^3H and ^3He . No converged Faddeev calculations exist for ^4He . Converged continuum calculations also exist for n-d scattering above breakup threshold[4].

4. Green’s Function Monte Carlo

The powerful Green’s Function Monte Carlo (GFMC) method was first applied to the few-nucleon systems in 1962[24]. In that work the integral form of the Schrödinger

equation for the three- and four-nucleon bound states was solved for spin- and isospin-independent square-well, Gaussian, and exponential potentials. The form of the equation which was solved is

$$\Psi = \lambda G_0 V \Psi,$$

where Ψ is the wave function for an *assumed* binding energy, G_0 is the (non-interacting) Green's function, and V is the nuclear potential. The eigenvalue λ of this restructured problem corresponds to the strength factor of the potential required to generate the assumed binding energy. Solutions for several binding energies can be easily interpolated to produce the value $\lambda = 1$ and the corresponding binding energy.

The equation above was solved by randomly sampling the distribution of nucleon coordinates in Ψ , performing the implicit integrals, and thus generating a new estimate for Ψ/λ . Iteration of this scheme (the power method) leads to the wave function corresponding to the largest value of $|1/\lambda|$. This is usually the ground state, although cases are known[1] where the iteration is dominated by *negative* values of λ , corresponding to the strongly repulsive parts of realistic nucleon-nucleon potentials. These "ghost states", which are not solutions of the original Schrödinger equation, nevertheless control the iteration, unless special care is taken.

The advantage of the Monte Carlo procedure is that it does not suffer from increasing dimensionality (as more nucleons are added) as much as traditional procedures do. Its disadvantage is that its solution is a set of random samples, and every calculated observable has an associated statistical error. Nevertheless, the method is very powerful and its advantages greatly outweigh its disadvantages.

The extension of this procedure to spin-dependent potentials was not immediate. Spin-independent potentials generate few-nucleon wave functions which are symmetric under the interchange of the spatial coordinates of any two nucleons. These space wave functions can then be coupled to a completely antisymmetric spin-isospin wave function to generate one which satisfies the requirements of the Pauli principle. Any dependence of the potential on spin or isospin generates wave function components which are not space symmetric. A similar situation exists for heavier nuclei, where the Pauli principle requires such wave function components, which have enhanced kinetic energy and reduce the binding. Relaxing the Pauli principle might lead to states which are more deeply bound. Iteration schemes such as the one previously described want to converge to the lowest state. Even if this state is a Pauli-principle-violating "ghost state", it can affect a Monte Carlo solution, because of its statistical nature. Although one can easily enforce that principle *in the mean*, the variance (statistical error) can increase uncontrollably, rendering the solution useless. This is typical of "Fermion" problems.

Carlson[2] was the first to show that the problem was not serious for few-nucleon systems. He used the time-dependent form of the Schrödinger equation continued to imaginary time ($t \rightarrow -i\tau$), which was first used for few-nucleon problems in 1962 [25]:

$$\Psi(\tau) = \exp(-H\tau)\Psi(0),$$

and which clearly converges for large τ to the lowest eigenvalue. This technique was originally applied to a variant of the Argonne potential[26] for the triton and the alpha particle. Subsequently[27], it was shown by direct computation using the Faddeev equations that there is no bound, symmetric triton state for Fermions corresponding to this potential, largely because OPEP is repulsive in such states. This fortuitous occurrence leads to stable iteration. The GFMC technique is currently the method of choice for the alpha particle.

5. Hyperspherical Techniques

The original impetus for this technique was supplied by Simonov[28], who recognized the geometric complexity of even the simplest light nuclei. The three-nucleon problem[18] has 3 intrinsic coordinates, usually taken to be the Jacobi coordinates: x , y , and θ , of which only one is an angle ($\cos(\theta) = \hat{x} \cdot \hat{y}$). By treating x and y as the Cartesian components of a two-dimensional vector and transforming to polar coordinates, the three intrinsic coordinates can be specified by a single length (the hyperradius) and two angles. The Schrödinger wave function of the triton can then be expanded in terms of a complete set of the angular variables and corresponding functions of the hyperradius.

Long before we had the ability to solve the Schrödinger equation for the triton, this scheme was extremely useful in providing insight into the Coulomb energy of ^3He , which provides the bulk of the binding energy difference of ^3He and ^3H . A truncated hyperspherical expansion[29] leads to the "magic formula", which relates the ^3He Coulomb energy to the charge densities of ^3He and ^3H , which can be taken from experiment. Although it is only an approximation, this relationship is accurate at the one percent level. In addition, hyperspherical variables are often used in Faddeev calculations[30], because the matrices one obtains by discretizing those equations are banded (*i.e.*, most elements are zero) in the hyperradius variable.

Extensive efforts to solve the hyperspherical equations have been only partially successful for realistic potentials, although they have been successful for other problems. Recently, large basis calculations for the Super Soft Core (C) potential[31] were reported[32], for which comparisons with other methods are possible. The reported binding energy differs from Faddeev calculations by less than 1 per cent. According to Ref. [32], the primary difficulty in achieving convergence is the (mixed-symmetry, s-wave) S' -state wave function component. The method chosen to solve the equations is also variational in nature.

An outgrowth of these methods is the integro-differential equation approach[33], which focuses on the important two-nucleon correlations in few- and many-body systems, and is equivalent to the s-wave Faddeev equations for the triton.

6. Hybrid Techniques

Some of the recent advances and new approaches have involved combinations of the somewhat arbitrary categories we have introduced (*e.g.*, a Faddeev wave function representation for a variational calculation). The methods discussed by the speakers in this session share this characteristic, and are applied to a variety of interesting problems, including purely Coulombic (*i.e.*, atomic physics) calculations. These methods therefore represent an interesting synthesis of fields, as well as techniques.

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