

# PHYSICAL REVIEW C

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### Practical Approach to the Continuum Shell Model\*

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A second quantized version of the Lane-Robson reaction formalism is applied to the continuum shell-model problem. The dynamical equations have a matrix structure which differs from that encountered in the conventional shell model only through the addition of a relatively small number of states and the presence of complex, energy-dependent boundary-condition parameters. Oscillator basis states may be used throughout. All matrix elements may be evaluated by existing shell-model codes. The equations provide a practical basis for dynamical studies of resonance phenomena in single-nucleon scattering channels. An extension of the model to include cluster channels is suggested.

#### I. INTRODUCTION

The nuclear shell model provides a powerful tool for the description of nuclear bound states. Recent large scale calculations<sup>1</sup> based on realistic interactions build many of the important microscopic correlations into the nuclear wave function and achieve very satisfactory agreement with observation. However, direct application of the conventional shell model to states which can decay via nucleon emission is hindered by the fact that the basis states are localized, whereas continuum states contain components which extend indefinitely far from the nucleus. If the coupling to possible decay channels is neglected, the observed resonance structure of the unbound states is represented incorrectly by a sequence of quasibound levels of zero width.

A number of reaction formalisms have been given in the literature<sup>2-5</sup> which, in principle, enable reaction channels to be correctly incorporated into the shell-model framework. Many of these formalisms turn out to be quite hard to implement in practice, with the result that there have been few, if any, numerical calculations which attempt to use the full power of the shell-model representation for the investigation of resonance phenomena.

In this note, we use a second quantized version of the Lane-Robson reaction formalism to reduce the dynamical equations of the continuum shell model<sup>6</sup> to an extremely simple and elegant form. The resulting equations are expressed directly in shell-model terms. The various many-body matrix elements which occur can readily be calculated by existing shell-model codes.

As a result, we have here a powerful new approach to the investigation of many interesting physical phenomena. A partial list might include<sup>6</sup>: elastic and inelastic scattering of nucleons, single-nucleon charge-exchange reactions, single-particle (potential resonance) and many-body resonance phenomena and their interference, doorway states and intermediate structure, isobaric-analog resonances, photonuclear emission and absorption, etc. In addition, the model can be used<sup>7</sup> to supply single-nucleon-transfer form factors and spectroscopic factors for comparison with experiment via distorted-wave Born-approximation calculations. It can also provide an arena for the testing of more approximate models, e.g. the Pinkston-Satchler<sup>8,9</sup> approach to the form-factor problem, and for the clarification of various technical or conceptual questions, e.g., the influence of antisymmetry on reaction processes, the mech-

anism by which conventional shell-model states are shifted and broadened by interaction with the open channels etc. Many of the above questions have already received attention<sup>6</sup> within other formulations. The present formalism may lead to some new insights. At the very least, the greater simplicity of the present calculational scheme will permit larger problems to be tackled.

In common with previous formulations of the continuum shell-model problem, the present formulation has certain limitations. Although it is able to couple in any number of single-nucleon channels, it is not capable of describing either breakup channels in which multinucleon clusters separate, or many-body breakup channels. Thus it cannot be used directly to investigate transfer reactions. In common with the conventional shell model, the present model will be most definite at relatively low excitation energies.

The present derivation is carried out within the framework of second quantization which conveniently ensures that all states are fully antisymmetric. For simplicity of notation, the angular momentum coupling in the single-nucleon channels is not displayed, although it would be trivial to include it. Of course, no coupling is required if the states of the residual nucleus have zero spin. A simple numerical example of the present model has appeared in Ref. 10. Other more thoroughgoing calculations are in progress.

## II. FORMALISM

The so-called continuum shell model<sup>6</sup> is based upon a second quantized trial state<sup>7</sup>

$$|T\rangle = \sum_{\alpha=1}^N S_{\alpha}^{\dagger} |A_{\alpha}\rangle + \sum_{\beta=1}^{N'} c_{\beta} |B_{\beta}\rangle \quad (1)$$

which may be assumed to have definite total angular momentum. The second term in the trial function represents the localized component of the state and is described by the conventional shell model. The first term represents the various single-nucleon channels which are to be included in the model. The model unknowns are the amplitudes  $c_{\beta}$  and the single-nucleon creation operators  $S_{\alpha}^{\dagger}$ . Thus, for example, in an application of the model to  $^{17}\text{O}$ , one might choose the (trivial) representation  $|A_{\alpha}\rangle = |^{16}\text{O}(\text{cs})\rangle$ ,  $|B_{\beta}\rangle = |^{16}\text{O}(\text{cs})v^1 JM\rangle$  in which  $|^{16}\text{O}(\text{cs})\rangle$  is simply the closed-shell state of  $^{16}\text{O}$  and  $v^1$  implies a configuration of one nucleon in an appropriate valency orbit ( $1d_{5/2}$  or  $2s_{1/2}$ , say). Alternatively, one might employ the more ambitious model<sup>11</sup>  $|A_{\alpha}\rangle \sim |^{12}\text{C}(\text{cs})v^4 J_{\alpha} M_{\alpha}\rangle$ ,  $|B_{\beta}\rangle \sim |^{12}\text{C}(\text{cs})v^5 JM\rangle$  in which there are 4 and 5 nucleons, respectively, distributed across the  $1p_{1/2}$ ,  $1d_{5/2}$ , and  $2s_{1/2}$  orbits. Intermediate assumptions

are also possible. In any case, however, the state  $|A_{\alpha}\rangle$  represents a state of the residual nucleus which remains after a nucleon has been removed. It is, therefore, necessary<sup>7</sup> that the states  $|A_{\alpha}\rangle$  be *eigenfunctions* of the nuclear Hamiltonian within the shell-model space allotted to the residual nucleus. The states  $|B_{\beta}\rangle$ , on the other hand, can be taken to be unmixed shell-model basis states.

Dynamical equations were obtained from this trial state in Ref. 7 by overlapping the Schrödinger equation for  $|T\rangle$  with various elements of the model space. The resulting coupled integrodifferential equations were found to be exceedingly cumbersome. We now show that application of the Lane-Robson formalism<sup>5</sup> to the same equations leads to a set of algebraic equations which are scarcely more involved than the conventional shell model itself.

We start by introducing the channel radius  $a$  which is to be chosen such that the nuclear interaction between separating fragments vanishes for  $r \geq a$ . In practice, this means that the radius  $a$  must be greater by at least the range of the nuclear interaction than the radius beyond which the nuclear density has become negligible (see Fig. 1.). The operators  $S_{\alpha}^{\dagger}$  are represented by single-particle shell-model functions within the region  $0 \leq r \leq a$ . To this end we introduce functions  $\phi_m(x)$  defined by

$$\begin{aligned} \phi_m(x) &= \psi_m(x), & 0 \leq r \leq a, \\ \phi_m(x) &= 0, & r > a, \end{aligned} \quad (2)$$

where  $\psi_m(x)$  is a standard single-particle shell-model basis function. This artifice is used only to demonstrate that the operators  $a_m^{\dagger}$ , which correspond to creation of a nucleon in states  $\phi_m$ , do

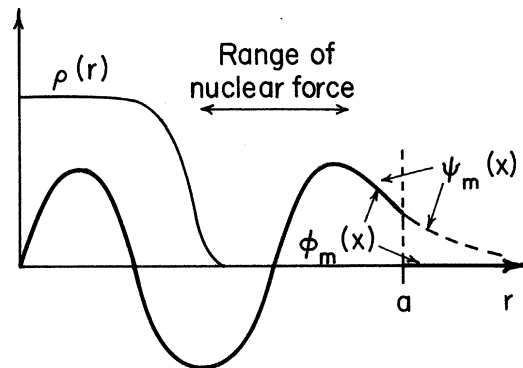


FIG. 1. Illustration of the manner in which the supplementary functions span the region between the conventional shell-model functions (represented by a typical nuclear density) and the external region.

not produce orthogonal functions. Instead, we have

$$\langle 0 | a_m a_m^\dagger | 0 \rangle = \int \phi_m^*(x) \phi_m(x) dx \equiv \mathcal{O}_{mm}. \quad (3)$$

The expansion of  $S_\alpha^\dagger$  can now be written as

$$S_\alpha^\dagger = \sum_m c_{\alpha m} a_m^\dagger \quad (\text{valid within } r \leq a). \quad (4)$$

The choice of states  $m$  which are to be included in the sum needs careful handling. Clearly, we should not introduce too many new amplitudes or the resulting equations will become unmanageable. Explicit calculations<sup>10, 12</sup> which have made use of this representation suggest that some 4 to 6 amplitudes in each channel may normally be sufficient. However, this question is still under investigation. In order to avoid redundancy problems,<sup>7</sup> it is necessary to exclude from the sum any amplitudes which refer to states already represented among the states  $|B_\beta\rangle$ . Thus, for example, if we are working with the  $s_{1/2}$  channel in  $^{17}\text{O}$ , the core and valency orbits already include the  $1s_{1/2}$  and  $2s_{1/2}$  functions, so that the sum over  $m$  should begin with the  $3s_{1/2}$  state (and possibly terminate with the  $7s_{1/2}$  state). Since the orbits  $m$  lie outside the valency space of the conventional shell model, we shall refer to them as "supplementary orbits." Their purpose is to form a link between the conventional orbits and the external region which begins at  $r = a$ .

The dynamical equations of the model can now be written as

$$\langle A_\alpha | a_m [H + L(b) - E] | T \rangle = \langle A_\alpha | a_m L(b) | T \rangle, \quad (5)$$

$$\langle B_\beta | (H - E) | T \rangle = 0, \quad (6)$$

where  $L(b)$  is the boundary-condition operator, given in second quantized form by

$$L(b) \equiv \sum_\alpha \int dx \psi^\dagger(x) | A_\alpha \rangle (\hbar^2/2\mu) \delta(r - a) \times \left[ \frac{d}{dr} - (b_\alpha - 1)/a \right] \langle A_\alpha | \psi(x). \quad (7)$$

The operator  $\psi(x)$  annihilates a nucleon at coordinate position  $x$ . The reason for the introduction of the operator  $L(b)$  into Eq. (5) is fully discussed in Ref. 5. We may understand it at an intuitive level as follows. The amplitudes  $c_{\alpha m}$  in Eq. (4) are determined by the dynamical equations in such a manner that the form factor  $f_\alpha(x) \equiv \langle A_\alpha | \psi(x) | T \rangle$ , which is sensitive to  $S_\alpha^\dagger$ , is represented as accurately as possible within the model space. It does not follow that the expansion in Eq. (4) reproduces the *derivative* of the form factor accurately. Indeed, explicit calculations show that many more terms are required in the sum if the

derivative is to be accurately represented near the edge of the interior region. The kinetic energy term in the Hamiltonian contains derivatives which may be reduced by application of Green's theorem to derivatives at the boundary  $r = a$ . The latter derivatives are canceled by those in the operator  $L(b)$ . Thus, it will be permissible to use the expansion (4) on the left side of Eq. (5) but not on the right. Equation (6) might also include an operator  $L(b)$ , but the vanishing of the shell-model state  $|B_\beta\rangle$  at  $r = a$  (in any coordinate) ensures that its contribution is zero.

When Eq. (7) is inserted into the right-hand term of Eq. (5), we find

$$\langle A_\alpha | a_m L(b) | T \rangle = (\hbar^2/2\mu) \int dx \phi_m^*(x) \delta(r - a) \times \left[ \frac{d}{dr} - (b_\alpha - 1)/a \right] f_\alpha(x). \quad (8)$$

This expression vanishes if we make the "natural choice" of  $b_\alpha$ ,

$$b_\alpha(E) = \left( \frac{r}{u_\alpha} \frac{du_\alpha}{dr} \right)_{r=a}, \quad (9)$$

where  $u_\alpha(r)$  is just  $r$  times the radial part of the form factor. The parameter  $b_\alpha(E)$  occurs also on the left-hand side of Eq. (5) and carries into that equation the influence of the spatial region beyond  $r = a$ .

The model equations may now be written out in more detail as

$$\sum_{\alpha' m'} \left\{ \langle A_\alpha | a_m (H - E) a_m^\dagger | A_{\alpha'} \rangle + (\hbar^2/2\mu) u_m^*(a) \times \left[ \left( \frac{du_{m'}}{dr} \right)_{r=a} - \frac{b_{\alpha'}(E)}{a} u_{m'}(a) \right] \delta_{\alpha\alpha'} \right\} c_{\alpha' m'} + \sum_{\beta'} \langle A_\alpha | a_m H | B_{\beta'} \rangle c_{\beta'} = 0, \quad (10)$$

$$\sum_{\alpha' m'} \langle B_\beta | H a_m^\dagger | A_{\alpha'} \rangle c_{\alpha' m'} + \sum_{\beta'} \langle B_\beta | H - E | B_{\beta'} \rangle c_{\beta'} = 0. \quad (11)$$

This pair of equations embodies the main formal result of this paper. The amplitudes  $c_{\alpha m}$  and  $c_\beta$  are solutions of homogeneous algebraic equations with coefficients which form a symmetric matrix. The elements of this matrix are energy-independent except where shown explicitly.

The matrix  $\langle B_\beta | H - E | B_{\beta'} \rangle$  is that encountered in the conventional shell-model problem. The coupling between the conventional shell-model states and the single-nucleon channels is represented by matrix elements of form  $\langle B_\beta | H a_m^\dagger | A_\alpha \rangle$ . Since this matrix element contains only one sup-

plementary orbit, contributions to it will all come from within the interaction region. It may, therefore, be evaluated by standard shell-model tech-

niques without regard to the fact that the orbit  $\phi_m(x)$  does not exist beyond  $r=a$ . The final matrix element may be put into standard form by

means of Wick's theorem. The result is

$$\begin{aligned} \langle A_\alpha | a_m(H-E)a_m^\dagger | A_{\alpha'} \rangle = & \left[ (E_\alpha - E)\mathcal{O}_{mm'} + \int_0^a dx \psi_m^*(x)t(x)\psi_{m'}(x) \right] \delta_{\alpha\alpha'} \\ & + \int dx \phi_m^*(x) \langle A_\alpha | \int dx' \psi^\dagger(x')v(x,x')(1-P_{xx'})\psi(x') | A_{\alpha'} \rangle \phi_{m'}(x), \end{aligned} \quad (12)$$

where  $E_\alpha \equiv \langle A_\alpha | H | A_\alpha \rangle$ , and  $P_{xx'}$  is the operator which exchanges coordinates  $x$  and  $x'$ . The last term in Eq. (12) represents the interaction between the supplementary orbit and the various occupied core and valency orbits in the residual nucleus. It is simply the usual many-body matrix element of the two-body part of the interaction with the interactions among core and valency orbits deleted. It may be evaluated in standard fashion for all components of the interaction save the direct component of the Coulomb interaction. A method for handling the Coulomb contribution is detailed in Ref. 10. The single-body matrix element of the kinetic energy which appears in Eq. (12) is not in itself symmetric in  $m$  and  $m'$ , but it gives a symmetric contribution when combined with the explicit derivative term in Eq. (10).

Although all matrix elements in Eqs. (10) and (11) can be evaluated by standard shell-model techniques, the solutions of these equations involve features not encountered within the conventional shell model. Bound states may occur at energies such that all channel energies  $E - E_\alpha$  are negative. The parameters  $b_\alpha(E)$  are then all real (and negative) so that the amplitudes satisfy an eigenvalue equation described by a real symmetric matrix. The matrix is energy-dependent through the boundary-condition parameters so that simple matrix diagonalization can no longer be used to obtain all the eigenvalues simultaneously. This will not present a serious drawback if the number of bound states for any given total angular momentum is small.

If only one channel is open, and if the Hamiltonian is taken to be real (no absorption), the parameter  $b_\alpha(E)$  of the open channel will also be real. Equations (10) and (11) can now be solved at any energy. They constitute an eigenvalue equation for the boundary-condition parameter of the open channel. The behavior of this parameter as a function of energy determines the resonance structure of the scattering solution.

If an absorptive term is included in the Hamiltonian (to approximate the effect of omitted open

channels), if several channels are open, or even if there is only one open channel but the residual nucleus has a nonzero spin, the parameters  $b_\alpha(E)$  will in general take on complex values, representing the propagation of net flux along the open channels. In such cases the amplitudes will also be complex in general. In such cases, also, solutions have to be found which reproduce the desired asymptotic form of the total wave function. These solutions may be conveniently constructed<sup>13</sup> as a superposition of particular solutions  $|T_{\alpha_0}\rangle$  defined to have unit incoming flux in the  $\alpha_0$  channel only. The boundary conditions in the open channels of  $|T_{\alpha_0}\rangle$  are specified by

$$u_\alpha(r) \underset{r \rightarrow \infty}{\sim} v_\alpha^{-1/2} [\mathcal{G}_\alpha(r)\delta_{\alpha\alpha_0} - S_{\alpha\alpha_0}\mathcal{O}_\alpha(r)], \quad (13)$$

where  $\mathcal{G}_\alpha(r) \equiv G_{l_\alpha}(k_\alpha r) - iF_{l_\alpha}(k_\alpha r)$  is the usual incoming combination of standard Coulomb functions,<sup>14</sup>  $\mathcal{O}_\alpha(r) \equiv \mathcal{G}_\alpha^*(r)$  and  $v_\alpha \equiv \hbar k_\alpha/\mu$  is the asymptotic relative velocity in channel  $\alpha$ .

The desired particular solutions may be obtained as follows.<sup>12</sup> If  $\alpha$  is one of the open channels, the term in  $b_\alpha(E)$  in Eq. (10) is taken to the right and treated formally as a source. Equations (10) and (11) now have the structure

$$Ac = g, \quad (14)$$

where the real, symmetric matrix  $A$  is a fully defined function of energy, and the source vector  $g$  has elements

$$g_{\alpha m} = \frac{\hbar^2}{2\mu} u_m^*(a) \left( \frac{du_\alpha}{dr} \right)_{r=a} \sum_{\alpha' \text{ open}} \delta_{\alpha\alpha'}, \quad g_\beta = 0 \quad (15)$$

which evidently contain, via Eq. (13), the unknown collision matrix elements. The formal solution of Eq. (14) may be combined with the identity

$$\sum_m c_{\alpha m} u_m(a) = u_\alpha(a) \quad (16)$$

to provide an explicit expression for the collision matrix<sup>13</sup>

$$S = \rho^{1/2} \mathcal{O}^{-1} (1 - RL)^{-1} (1 - RL^*) \mathcal{G}_\rho^{-1/2}. \quad (17)$$

The matrices  $\mathcal{G}$ ,  $\mathcal{O}$ ,  $L$ , and  $\rho$  which appear in Eq.

(17) are diagonal, with elements  $\mathcal{G}_\alpha \equiv \mathcal{G}_\alpha(a)$ ,  $\Theta_\alpha \equiv \Theta_\alpha(a)$ ,  $L_\alpha \equiv a\Theta'_\alpha(a)/\Theta_\alpha(a)$ ,  $\rho_\alpha \equiv k_\alpha a$ , and the  $R$  matrix is defined by

$$R_{\alpha\alpha'} \equiv \sum_{mm'} \gamma_m (A^{-1})_{\alpha m, \alpha' m'} \gamma_m^*, \quad (18)$$

where  $\gamma_m \equiv (\hbar^2/2\mu a)^{1/2} u_m(a)$ . Once the collision matrix has been obtained, it may be used in conjunction with Eq. (14) to provide a complete specification of the trial state  $|T_\alpha\rangle$  associated with any incident channel  $\alpha$ . The procedure is quite straight-forward and is noniterative. It must be carried out afresh at every energy of interest, however.

Another novel feature of the present formalism as compared to the conventional shell model is that it employs more single-particle orbits so that a larger set of two-body matrix elements is needed. It is not difficult to evaluate such two-body matrix elements if a suitable phenomenological interaction is given, but the corresponding "realistic" two-body matrix elements may be harder to pin down.<sup>15</sup> In addition to the matrix elements between the supplementary orbits and the valency orbits, it is necessary to know the interaction between the supplementary orbits and the core. These matrix elements might be estimated by introducing a conventional Woods-Saxon well. Alternatively, a detailed summation over two-body matrix elements can be performed, as described in Ref. 10.

The question as to how many open channels need be explicitly included in any given calculation must be answered in terms of the physics. If the channel threshold energy  $E_\alpha$  lies much higher than the energy of interest, the corresponding amplitudes  $c_{\alpha m}$  automatically become very small, and it will be permissible to omit all reference to that channel. Thus, for example, a low-energy calculation carried out for  $^{17}\text{O}$  might include only the  $^{16}\text{O}(\text{g.s.}) + \text{neutron}$  channel. The channel based on the  $^{16}\text{O}$  first excited state opens<sup>16</sup> 6.06 MeV higher in energy; that based on the  $^{16}\text{N}$  ground state opens<sup>16</sup> 9.64 MeV higher. If these channels

are ignored, it is likely that only some 4 to 6 states are required in addition to those already present in the conventional shell model.

Many remarks have been made in the past about the advantages or disadvantages occasioned by the presence of a radius parameter in a reaction theory. In the present instance, it is clear that the amplitudes  $c_{\alpha m}$  will depend both upon the choice of  $a$ , and upon the number of supplementary functions allotted to channel  $\alpha$ . The optimum representation, determined by solution of the dynamical Eqs. (10) and (11), depends upon the region over which the representation is to be valid and the particular set of functions which have been made available. On the other hand, the form factors  $f_\alpha(x)$  will be independent of these details, provided only that the set of supplementary functions is large enough. From these remarks it follows that the amplitudes  $c_\beta$  are independent of the channel radius if the choice of supplementary functions is adequate.

We hope that the ideas presented in this paper will provide a stimulus for further research with regard both to specific numerical applications of the model and to extensions of the formalism to include cluster channels and many-body breakup channels within the shell-model framework. The addition of deuteron and possibly even  $\alpha$ -particle channels appears to be formally possible by techniques similar to those employed here. But it is not yet clear to the author that these extensions will be realizable in practice. The deuteron threshold lies only 2.23 MeV below the neutron-proton three-body breakup channel, so that the latter should be important whenever the former becomes significant. Improved calculations of two-nucleon-transfer form factors may be feasible. The  $\alpha$ -particle channel requires supplementary functions to describe four nucleons. Although the number of functions thus introduced into the model appears to be quite large, the physical importance of the  $\alpha$  channel suggests that this representation will warrant very careful study.

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## Effective Interaction in Nuclei

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An equivalent potential is derived by best fitting the Sussex matrix elements. The derived equivalent potential is compared with the equivalent Yale potential obtained in a similar manner and with central effective potentials in widespread current use. Remarks are made about the general nature of the effective nuclear force.

### I. INTRODUCTION

In any nuclear structure calculation the choice of the interaction is crucial. Recently there has been much emphasis on calculating the various nuclear properties using the realistic interactions such as Hamada-Johnston, Yale, and Tabakin. The first two of these have a hard core. This makes the perturbation treatment more difficult starting from the independent particle wave functions. In actual practice, one uses the reaction matrix  $G$  instead. The calculation of the  $G$  matrix from these potentials is possible only within certain approximations,<sup>1,2</sup> and the convergence of the perturbation expansion should also be taken into account.<sup>3</sup> This difficulty of the infinitely repulsive hard core may be avoided by the use of a separable nonlocal potential e.g., the Tabakin potential. The principal drawback of such a potential is that it does not approach the one-pion-exchange potential at large distances. The Sussex group<sup>4</sup> has derived the relative matrix elements of the nucleon-nucleon interaction directly from the observed nucleon-nucleon phase shifts. Thus the usual intermediate step of first deriving the potential from the scattering data is eliminated. This has the special advantage that the deficiencies in one's treatment of the many-body problem are not hidden by the adjustment of the free parameters of the interaction to fit some particular properties. Various properties of nuclear systems, such as deuteron properties,<sup>5</sup> spin-orbit splittings,<sup>6</sup> binding energies, rms

radii, single-particle energies, etc.,<sup>7</sup> have been calculated using the Sussex matrix elements and the results are in good agreement with experiment and with other realistic interactions.

On the other hand, there are numerous nuclear structure calculations using the phenomenological effective interactions, generally central potentials of smooth shape. In fact, before the separation technique of Moszkowski and Scott<sup>8</sup> became available for use with the hard-core problem of realistic interactions, the calculations were possible only for nonsingular effective interactions so that perturbation theory could be used directly. In these, the effective interaction is taken as a suitable combination of the conventional exchange forces such as Wigner, Majorana, Bartlett, and Heisenberg. The parameters of the effective interaction are adjusted to best reproduce the energy levels and other properties of the nuclei considered. This approach has been very useful and has given us much information about the nature of the effective nuclear force. However, the effective interaction is dependent on the configuration space chosen and includes renormalizations from the admixture of the various configurations. Thus, there is always a danger that the description of the relevant states might not be correct and that, a wrong configuration having been chosen, the good agreement might have been forced by adjusting the various parameters of the interaction. This has been very strongly pointed out by Cohen, Lawson, and Soper<sup>9</sup> in their calculations on the "pseu-