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MICROSCOPIC THEORY OF MULTIPLE SCATTERING FOR OPEN SHELL NUCLEI

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Abstract

We consider the scattering of a distinguishable projectile from a nucleus assuming that the underlying interaction Hamiltonian is a sum of two-body potentials. We show that the effective interaction of the projectile with the nucleus in a truncated nuclear model space can be calculated as a linked cluster expansion. The shell-model interaction is required to be an energy-independent, hermitian potential; its expression in terms of the underlying two-body potential is given by folded diagrams. The terms in the expansion of the effective projectile-nucleus interaction must also contain folded diagrams but, unlike the shell-model potential, these are energy dependent in order to describe the singularities associated with the crossing of the scattering thresholds as the projectile energy is varied. Once the effective interaction is known, elastic and inelastic scattering may be evaluated numerically by solving a finite-dimensional coupled-channel equation.

I. Introduction

I want to tell you about some work that I have been doing with Mano Singham on multiple scattering theory and the shell model. We have in mind eventual applications to pion scattering, where experiments have established the sensitivities of the pion to nuclear structure (especially neutron/proton components of nuclear wave functions) in elastic and inelastic scattering, and established the unique possibilities provided by single and double charge exchange for calibrating the reaction theory. In order to capitalize on these successes, we want a theoretical framework in which nuclear structure and reaction theory can be brought together in a systematic fashion. Although frameworks exist that connect structure and reactions in an approximate (see, e.g., the DWIA¹ and coupled channel² approaches) and in a formally exact³ fashion, we have found none that is compatible with the microscopic techniques that have become both the language of the shell model^{4*} and

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the Green's function⁵ approach to scattering. The theory that I will discuss here is a first step in the desired direction. The work described here is more fully explained with examples in Ref. 4b.

The talk is organized as follows. In Section II we formally state the problem we wish to solve. In Section III we review limiting cases that have been developed previously in the literature and that we wish our theory to encompass: the optical model for closed shell nuclei plus projectile and the microscopic shell model for open shell nuclei with no projectile. In Section IV we obtain the main results of this paper, deriving the linked cluster expansion for the projectile-nucleus interaction for open-shell nuclei. Finally, in Section V we make a few concluding remarks.

II. Formal Statement of the Problem

We shall assume that we are given the Hamiltonian H that provides an exact description of the nucleus in its ground and excited states and that also describes the scattering of a spinless, neutral elementary projectile. Thus,

$$H = K_N + V_{NN} + K_P + V_{PN} \quad (\text{II.1})$$

where K_N is the kinetic energy of the nucleons, V_{NN} is the sum of the bare nucleon-nucleon interactions, K_P is the kinetic energy of the projectile, and V_{PN} is the sum of the bare projectile-nucleon interactions. We assume that the projectile is distinguishable from the constituents of the nucleus. Technical complications arise in the case of an indistinguishable projectile, but we believe that these can be overcome by a sufficiently careful analysis.

To complete the quantum mechanical description of the system we postulate the existence of a set of operators $\{\theta\}$ whose matrix elements give the observable properties of the nucleus. Thus, if

$$H_N | \mu_i \rangle = E_{\mu_i} | \mu_i \rangle \quad (\text{II.2})$$

where

$$H_N = K_N + V_{NN} \quad , \quad (\text{II.3})$$

then

$$\langle \mu_j | \theta | \mu_i \rangle \quad (\text{II.4})$$

gives all experimentally determinable information about the nucleus. $\{ | \mu \rangle \}$ represent the set of eigenstates of the true target Hamiltonian H_N with corresponding eigenvalues E_{μ} .

With the addition of the projectile, scattering amplitudes add to the accessible knowledge of the system through the T -matrix elements

$$\langle \mu_j, \mathbf{k}_j | V_{PN} | \Psi_i^{(+)} \rangle \quad (\text{II.5})$$

where $|\Psi_i^{(+)}\rangle$ is an outgoing-wave solution of the Schroedinger equation

$$(H_N + K_P + V_{PN}) |\Psi_i^{(+)}\rangle = E |\Psi_i^{(+)}\rangle \quad , \quad (II.6)$$

evolving from an incident state $|\mu_i, \mathbf{k}_i\rangle$, and $|\mu, \mathbf{k}\rangle$ is a state representing a projectile of asymptotic momentum \mathbf{k} and the nucleus in state $|\mu\rangle$.

For the purpose of constructing the effective interaction, it is useful to define a basis of states in terms of the single-particle Hamiltonian h_0

$$h_0 = t + u_0 \quad (II.7)$$

where t is the kinetic energy operator of a nucleon, and u_0 is a one-body potential. The set of eigenstates $|\alpha_i\rangle$ of h_0 is obtained as solutions of

$$h_0 |\alpha_i\rangle = \epsilon_{\alpha_i} |\alpha_i\rangle \quad . \quad (II.8)$$

We classify the eigenstates $|\alpha_i\rangle$ into active and passive orbitals as shown in Fig. 1. The definition of these orbitals is always with reference to the Fermi surface of the closed shell nucleus, even in the case where there are valence nucleons. We refer to the closed shell nucleus as the core. In keeping with the notation of Ref. 4a, α_i becomes a lower case Roman letter for states above the Fermi sea and an upper case Roman letter for states in the Fermi sea in Fig. 1.

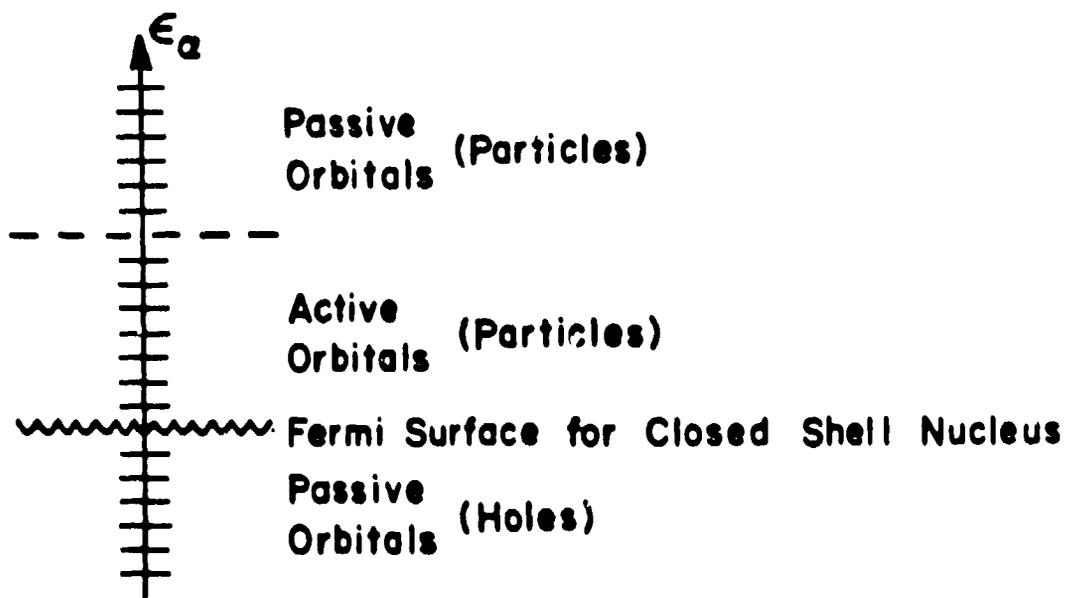


Figure 1. Classification of eigenstates of h_0 into passive and active orbitals. The number of active orbitals is assumed to be large but finite.

We now define H_0 and H_1 as

$$H_0 = K_N + U_0 \quad (\text{II.9})$$

$$H_1 = V_{N/N} - U_0 \quad (\text{II.10})$$

where

$$U_0 = \sum_i u_0(i) \quad (\text{II.11})$$

and the eigenstates and eigenvalues of H_0 are defined by

$$H_0 |\phi_i\rangle = (\Sigma \epsilon_{\alpha_j}) |\phi_i\rangle \quad , \quad (\text{II.12})$$

where $\{|\phi_i\rangle\}$ ($i = 0, \dots, N - 1$) represents all the possible states that can be constructed with n valence particles in active orbitals $\{\alpha_j\}_i$ outside a completely filled core,

$$|\phi_i\rangle = \mathcal{A} \prod_{\{\alpha_j\}_i} |\alpha_j\rangle \quad , \quad (\text{II.13})$$

where \mathcal{A} is the antisymmetrization operator. We define the valence model space M of dimension N to be the space spanned by the $|\phi_i\rangle$.

We can now state formally the object of the paper as follows. We want to find a subset of the observable properties of the true system by solving a quantum mechanical problem in the combined Hilbert space of the projectile and the truncated N -dimensional valence model space M . We will show how to construct an effective Hamiltonian \bar{H} and a set of effective operators $\{\bar{\theta}\}$ defined in this space, where

$$\bar{H} = H_0 + \bar{H}_1 + K_P + \Sigma(E) + \Delta\bar{\Sigma}(E) \quad . \quad (\text{II.14})$$

Here $\Sigma(E)$ is the one-body piece of the effective projectile-core interaction, which is closely related to the optical potential⁵ of the nucleus with no active nucleons. We define \bar{H}_N such that its discrete eigensolutions $|\bar{\mu}\rangle$ and \bar{E}_μ ,

$$\bar{H}_N |\bar{\mu}_i\rangle = \bar{E}_{\mu_i} |\bar{\mu}_i\rangle \quad , \quad (\text{II.15})$$

where

$$\bar{H}_N = H_0 + \bar{H}_1 \quad (\text{II.16})$$

bear a one-to-one relationship with a subset of the eigenstates of $H_N = H_0 + H_1$ such that for corresponding solutions

$$\bar{E}_{\mu_i} = E_{\mu_i} \quad (\text{II.17})$$

and

$$\langle \bar{\mu}_j | \bar{\theta} | \bar{\mu}_i \rangle = \langle \mu_j | \theta | \mu_i \rangle \quad . \quad (\text{II.18})$$

It was shown in Ref. 4a how to construct an \bar{H}_N having these properties. As in Ref. 4a, we establish a one-to-one correspondence between $|\bar{\mu}\rangle$ and $|\mu\rangle$ by assuming that they are both related to the same state $|\bar{\phi}_\mu\rangle$ in the limit of weak perturbations, where $|\bar{\phi}_\mu\rangle$ is a linear combination of model space eigenstates $|\phi_i\rangle$.

Furthermore, we require that the continuum eigenstates $|\bar{\Psi}_i^{(+)}\rangle$ of \bar{H} ,

$$\bar{H} |\bar{\Psi}_i^{(+)}\rangle = E |\bar{\Psi}_i^{(+)}\rangle \quad , \quad (\text{II.19})$$

where E is the total asymptotic energy of the projectile plus nucleus, bear the following relationship to the corresponding eigenstates $|\Psi_i^{(+)}\rangle$ of H

$$\langle \mu_f, \mathbf{k}_f | V_{PN} | \Psi_i^{(+)} \rangle = \langle \bar{\mu}_f, \mathbf{k}_f | \Sigma(E) + \Delta\bar{\Sigma}(E) | \bar{\Psi}_i^{(+)} \rangle \quad , \quad (\text{II.20})$$

i.e., that the scattering amplitudes of transitions between nuclear eigenstates described by \bar{H}_N are equal in the true and model problems.

III. Limiting Cases

The main object of this paper, to be attacked directly in the next section, is to develop a systematic procedure for obtaining $\Delta\bar{\Sigma}(E)$ in Eq. (II.14). In order to know how to accomplish this, it is necessary first to clearly state how $\Sigma(E)$ and \bar{H}_1 are constructed. Different definitions of these effective interactions can be found in the literature, and $\Delta\bar{\Sigma}(E)$ depends on the choice. Of special importance to us is keeping to a minimum the number of variables on which Σ and H_1 depend: we will choose those definitions that are compatible with the physics and that lead to the greatest convenience for the theorist who must do the calculations.

The important issue here is whether or not Σ and \bar{H}_1 are energy-dependent, i.e., depend on an energy variable (or variables) to be specified independently of the three momenta of the particles. Consider first \bar{H}_1 . In some theoretical frameworks an energy-dependence arises,⁶ but it is weak. The reason is that the shell model seeks to describe excitations over only a limited range of total energy, with the model space defined so that there is no possibility of the nucleus undergoing a transition between a state described by \bar{H}_1 to one not described by it in this energy range. Thus, all transitions to states outside the model space are virtual and occur over a limited time interval. It is therefore understandable why, in the phenomenological shell model,⁷ \bar{H}_1 can be taken as energy independent or instantaneous. The theoretical formulation that we choose and discuss briefly below gives rise to an energy-independent \bar{H}_1 .

In contrast to the case of \bar{H}_1 , there is a physical reason to give Σ an energy dependence. As the asymptotic energy of the projectile is raised, energy is made available to excite the nucleus. The changes in the physics as new thresholds are crossed give rise to singularities in the scattering amplitude or, equivalently, interactions with long time delays. It has been shown that in principle one can define energy-independent optical potentials.⁸ However, in practice, the energy-independent construction was shown to have serious shortcomings.⁹ For this reason and because phenomenological optical potentials¹⁰ generally have some energy dependence, the theoretical formulation that we choose and discuss briefly below is based on an energy-dependent $\Sigma(E)$.

A. Theory of the Optical Potential $\Sigma(E)$

The optical potential $\Sigma(E)$ describes the elastic scattering from the target core. In the case of no valence nucleons ($n = 0$), $\Sigma(E)$ may be obtained as the proper self energy of the projectile Green function $\mathcal{G}_{\mathbf{k}'\mathbf{k}}(t' - t)$,

$$\mathcal{G}_{\mathbf{k}'\mathbf{k}}(t' - t) = i^{-1} \langle 0 | \mathcal{T}(a_{\mathbf{k}'}(t') a_{\mathbf{k}}^+(t)) | 0 \rangle , \quad (\text{III.1})$$

where $|0\rangle$ is the exact target core ground state of energy E_0 (a solution of Eq. (II.2)) and $a_{\mathbf{k}}^+(t)$ is a creation operator in the Heisenberg representation,

$$a_{\mathbf{k}}^+(t) = e^{iHt} a_{\mathbf{k}}^+ e^{-iHt} , \quad (\text{III.2})$$

where $a_{\mathbf{k}}^+$ creates a projectile particle in momentum state \mathbf{k} , and where \mathcal{T} in Eq. (III.1) is the time-ordering operator. By applying standard many-body techniques one may obtain $\mathcal{G}_{\mathbf{k}'\mathbf{k}}$ as a sum of linked diagrams,¹¹ illustrated in Fig. 2. Time runs upward in our diagrams. The wiggly line refers to the projectile, and in the Feynman-Goldstone diagrams that we use here the projectile line extending from t to t' is represented by the individual propagator

$$\text{projectile: } \theta(t' - t) e^{-i\omega_{\mathbf{k}}(t' - t)} \quad (\text{III.3})$$

where $\omega_{\mathbf{k}} = k^2/2m$ is the projectile kinetic energy. The solid circle is the sum of all irreducible, proper self-energy insertions and it constitutes the optical potential $\Sigma(t', t)$. The times (t, t') at which the projectile lines attach to the circle need not be the same, which means that retardation is retained in the definition of $\Sigma(E)$ as an explicit energy dependence: in this case E is the Fourier transform variable related to (t, t') as

$$\Sigma(t', t) = i \int_{-\infty}^{+\infty} \frac{dE}{2\pi} \Sigma(E) e^{-iE(t' - t)} , \quad (\text{III.4})$$

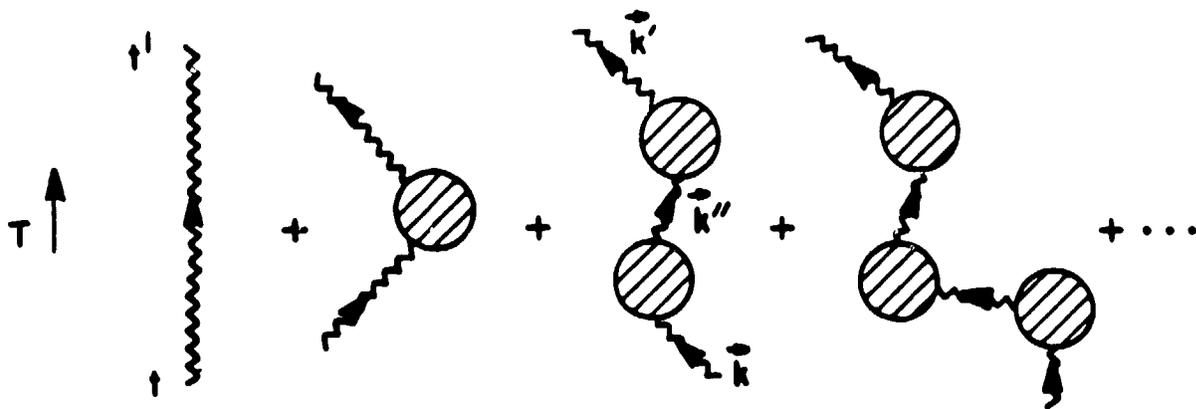


Figure 2. Diagrams of $\mathcal{G}_{k'k}(t' - t)$. The solid circle is irreducible (it will not break into two pieces when a projectile line is cut) and is identified with the optical potential $\Sigma(E)$.

$\Sigma(E)$ can be shown^{4b} to depend on n . For the case $n = 0$ we will denote $\Sigma(E)$ by $\Sigma_0(E - E_0)$, and the wave-function $\Psi_{\mathbf{k}}$ for the projectile with asymptotic momentum \mathbf{k} to scatter elastically from the core may be found by solving Schroedinger's equation

$$\left[\frac{-\nabla^2}{2m} + \Sigma_0(E - E_0) \right] \Psi_{\mathbf{k}} = (E - E_0) \Psi_{\mathbf{k}} \quad . \quad (\text{III.5})$$

The phase shifts (the observables) are related to $\Psi_{\mathbf{k}}$ in the usual manner.

B. Theory of the Shell Model Effective Interaction \bar{H}_1

In this case we have no projectile but n valence nucleons. As we have stated, the effective interaction \bar{H}_1 is strictly energy-independent, unlike the optical potential Σ . Such an \bar{H}_1 is given by the theory of folded Feynman diagrams, which is a diagrammatic formulation of degenerate Rayleigh-Schroedinger¹² perturbation theory applicable to the many-body problem. The early development of folded diagrams is traced back to the work of Morita¹³ and Brandow.¹⁴ In this subsection we wish to briefly review the folded diagram approach to \bar{H}_1 as developed in Ref. 4a, because some of the ideas will be applied to $\Delta\bar{\Sigma}$ in Section IV.

The idea of folded diagrams is to map a portion of the full space in which H_1 is defined onto the model space in which \bar{H}_1 is defined. This map is provided by the time evolution operators $T(t', t)$ and $\bar{T}(t', t)$ with time-dependent interactions. The time evolution operator $T(t', t)$ is defined as the solution to the equation

$$i \frac{d}{dt} T(t', t) = H(t) T(t', t) \quad . \quad (\text{III.6})$$

If H is time-independent, $T(t', t)$ has the explicit form

$$T(t', t) = e^{-iH(t'-t)} \quad . \quad (\text{III.7})$$

The time evolution operator for the true problem $T(t', t)$ is obtained with $H_1(t) = H_1 e^{-\eta|t|}$ while that in the model space $\bar{T}(t', t)$ is obtained with $\bar{H}_1(t) = \bar{H}_1 e^{-\eta|t|}$. The precise form of the time dependence is not important, but the turning off of the interaction should be sufficiently slow so as not to cause transitions between instantaneous eigenstates that evolve from states in the model space at $t = \pm\infty$ and those that do not. We then define corresponding states $|\psi_i(t)\rangle$ and $|\bar{\psi}_i(t)\rangle$ as those that evolve from the same model space state $|\phi_i(t)\rangle \equiv e^{iH_0 t} |\phi_i\rangle$

$$|\psi_i(t)\rangle \equiv T(t, -\infty) |\phi_i(-\infty)\rangle \quad (\text{III.8})$$

$$|\bar{\psi}_i(t)\rangle \equiv \bar{T}(t, -\infty) |\phi_i(-\infty)\rangle \quad (\text{III.9})$$

The states $|\bar{\phi}_\mu\rangle$ introduced below Eq. (II.18) would evolve into definite eigenstates $|\bar{\mu}\rangle$ and $|\bar{\mu}\rangle$; these states were not defined in Ref. 4a but will be useful in our discussion of scattering in Section IV. This mapping then permits one to prove the correspondence in Eqs. (II.17) and (II.18) provided that

$$\langle \bar{\psi}_\ell(t) | \bar{\theta} | \bar{\psi}_j(t) \rangle = \langle \psi_\ell(t) | \theta | \psi_j(t) \rangle, \quad (\text{III.10})$$

where the states in Eq. (III.10) are those defined in Eqs. (III.8) and (III.9). The proof is very simple^{4a} and obtained by expanding $|\psi\rangle$ and $|\bar{\psi}\rangle$ of Eq. (III.10) in eigenstates of H_N and \bar{H}_N . That $|\psi_\ell(t)\rangle$ is a linear superposition of only N eigenstates of H follows from the conditions stated below Eq. (III.7).

Also shown in Ref. 4a is how to define \bar{H}_1 and $\bar{\theta}$ such that Eq. (III.10) holds. We refer the interested reader to that paper for the complete discussion but we mention here a few of the important points. The first is that Eq. (III.10) holds if the following two conditions are met:

$$\bar{T}(+\infty, -\infty) = T(+\infty, -\infty) \quad (\text{III.11})$$

and

$$\bar{T}(+\infty, t) \bar{\theta} \bar{T}(t, -\infty) = T(+\infty, t) \theta T(t, -\infty) \quad (\text{III.12})$$

in the model space. These may be guaranteed by construction, i.e., \bar{H}_1 and $\bar{\theta}$ are defined perturbatively to satisfy these equalities.

We will next briefly review the diagrammatic procedure by which the equalities in Eqs. (III.11) and (III.12) are accomplished. We wish to stress that in applications there are two steps involved in implementing the theory. The first is to obtain \bar{H}_1 and $\bar{\theta}$ as outlined below, and the second is to diagonalize \bar{H}_N and obtain E_μ , and $\langle \bar{\mu}_j | \bar{\theta} | \bar{\mu}_i \rangle$.

Consider first Eq. (III.11). We use diagrammatic techniques for assuring this equality. Of course one needs to recognize that vertices of \bar{T} are expressed in terms of matrix elements of \bar{H}_1 and those of T in terms of matrix elements of H_1 . Diagrams shall be

considered different not only if they have a different topology (i.e., lines and vertices are connected differently), but also if they have the same topology but the sequence of times is different and/or the states that label the lines differ. So, in the end when one sums over all diagrams, one must sum over all topologies, all state labels, and all times with the integration

$$-i \int dt \quad . \quad (III.13)$$

Because we consider active nucleons to be in particle states only in this paper, we will be working with matrix elements of the form $\langle def | \bar{T}(t', t) | abc \rangle$, where the initial and final states refer to active particles. A typical diagram is shown in Fig. 3.

Diagrams for $T(t', t)$ appear as in Fig. 4. The rules are the same as for $\bar{T}(t', t)$ except now instead of matrix elements of \bar{H}_1 connecting the lines we have time-extended boxes. In order to be able to associate diagrams of \bar{T} with those of T , the definition of a box is very precise and is the following: a box is a connected set of passive lines, together with the vertices they join, plus any active particle lines drawn between two vertices already belonging to the box. With a box defined in this way, all diagrams of $T(t', t)$ between model space configurations can always be drawn as boxes connected by active particle lines only, and a one-to-one association made with diagrams of $\bar{T}(t', t)$. Examples of boxes are given in Fig. 5. Figures 5(a) and 5(d) are examples of two-body boxes, 5(b) and 5(c) three body-boxes, and 5(e) a zero-body box.

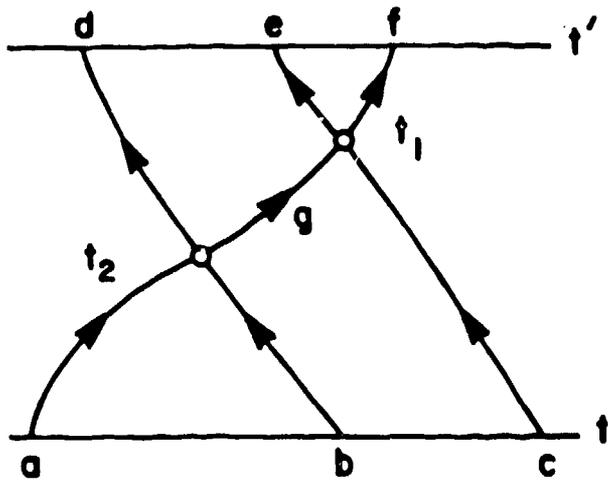


Figure 3. A Feynman-Goldstone diagram contributing to the matrix element $\langle def | \bar{T}(t', t) | abc \rangle$. The open circles are matrix elements of \bar{H}_1 .

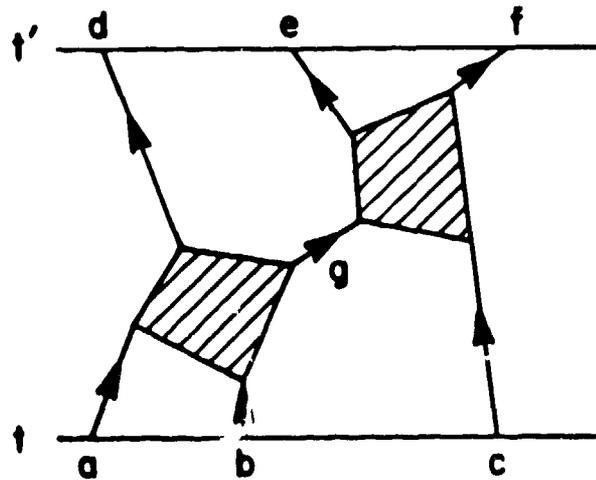


Figure 4. A Feynman-Goldstone diagram contributing to the matrix element $\langle def | T(t', t) | abc \rangle$.

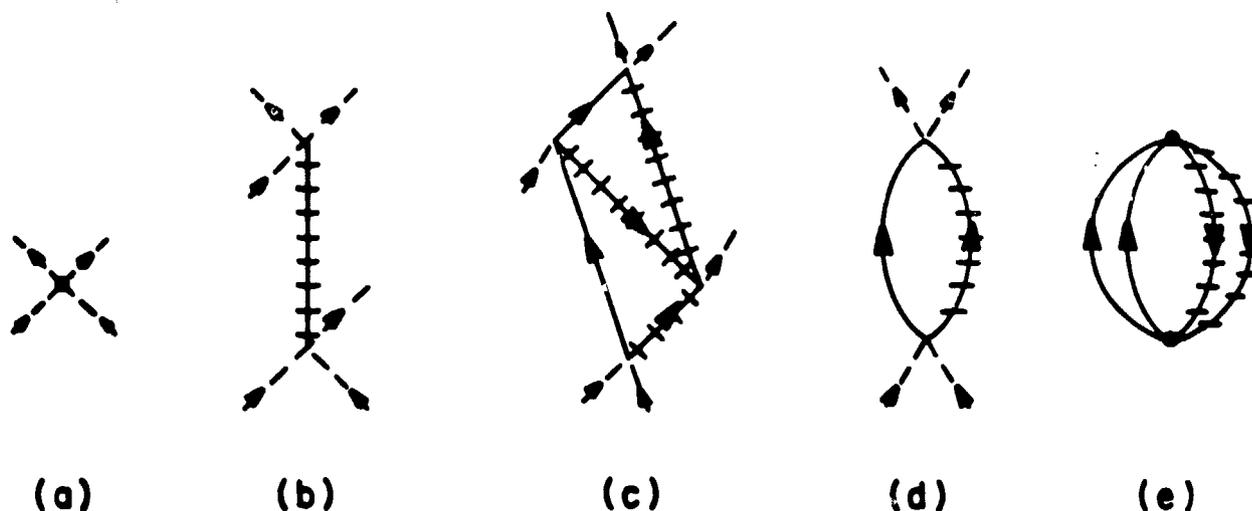


Figure 5. Examples of boxes. The crossed hatched lines are propagators corresponding to passive orbitals.

The diagrams of Fig. 3 and Fig. 4 are now to be made equal. This can be accomplished by equating the circles to the corresponding boxes. One such equality is shown in Fig. 6. To solve for the circle, each side of the equality in Fig. 6 is multiplied by the inverse of the propagators of the particle lines^{4a} that appear on the right-hand side of the equation. The time ordering $t'_1 > t_1$ is implicit in the figure so, for example, the inverse of the propagator for the particle line labeled d is $e^{-i\epsilon_d(t_0-t'_1)}$. We represent this by a line with its arrow pointing backward from its normal direction. It is easy to see, with this notation, that the solution to the equation in Fig. 6 is expressed diagrammatically as in Fig. 7.

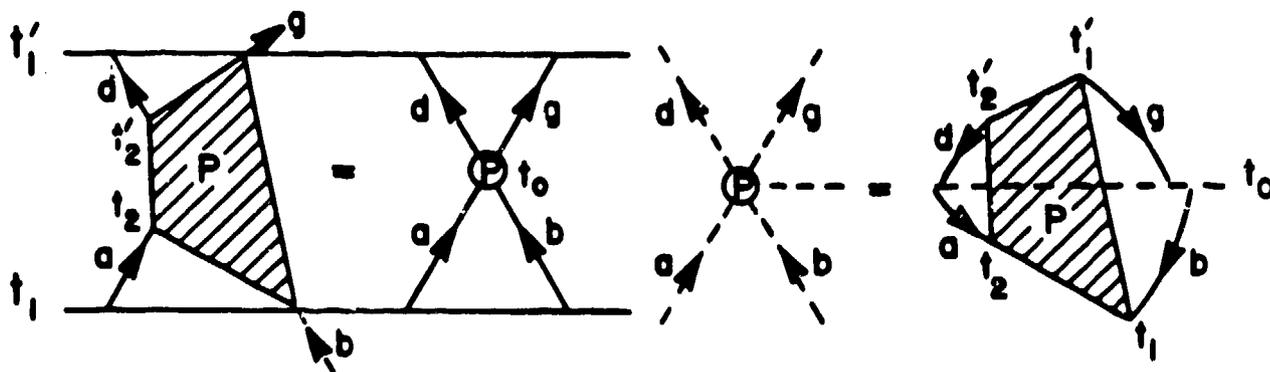


Figure 6. Establishing an equality between a box and its corresponding circle. The capital letter R designates the contents of the box.

Figure 7. Solution to the equation in Fig. 6.

\overline{H}_1 is thus a sum over contributions such as that shown in Fig. 7. The one-box contribution to $\langle dg | \overline{H}_1 | ab \rangle$ is the sum over all one-box folded diagrams. This sum includes an integration over all times, subject to the constraint that the time t_0 at which \overline{H}_1 acts (called the time base) is fixed in some way relative to $t'_2, t'_1, t_2,$ and t_1 . Internal labels on the lines are also summed over. The way to choose t_0 is discussed in detail in Ref. 4a; suffice it to say here that there is a great deal of flexibility in how to do this. One may exploit this flexibility to preserve symmetry between past and future, i.e., make \overline{H}_1 hermitian, which is a desirable feature for practical calculations. Hopefully, one can arrange perturbation theory such that the expansion converges rapidly in some appropriately chosen small parameter.

In order to ensure a complete equality between diagrams of $\overline{T}(+\infty, -\infty)$ and $T(+\infty, -\infty)$ one also must introduce zero-body, one-body, three-body, ..., n -body contributions to \overline{H}_1 , where n is the number of valence particles. Examples are given in Ref. 4a and Fig. 5. One hopes of course that the three- and higher-body forces will not be needed in practice.

Also, there will be multibox diagrams contributing to \overline{H}_1 . These need to be introduced in higher order because the boxes are extended in time and therefore cannot come arbitrarily close to one another whereas the circles are instantaneous and can.^{4a} When two boxes cannot be replaced by their corresponding circles without an active line running in an illegal direction this situation requires introducing a true-correcting diagram. If circles cannot be replaced by their corresponding boxes without making an active line run in an illegal direction, a model-correcting diagram is required. By "legal" and "illegal" we are referring of course to the time-direction established for particles and holes: particles must propagate forward in time and holes backward. Multibox diagrams are made into circles by repeating the construction illustrated in Figs. 6 and 7 for single-box diagrams. Examples of true- and model-correcting diagrams are given in Ref. 4a.

So, by following a rather straightforward algorithm one may define \overline{H}_1 to assure the equality in Eq. (III.11). The equality in Eq. (III.12) may be satisfied by again comparing diagrams of the left- and right-hand sides of this equation. Recognizing that the boxes and \overline{H}_1 have been defined already, the only remaining task is to define $\overline{\theta}$. One introduces new boxes for this purpose, wherein one vertex is the operator θ ; otherwise the box is defined as before. The final operator $\overline{\theta}$ contains zero-body, ..., n -body contributions. The only point that is a little different is that the time-base must be fixed to be the time at which the operator θ acts in its box. This restriction does not lead to a non-hermitian $\overline{\theta}$ as long as θ and \overline{H}_1 are hermitian.

Note that by construction we arrive at a *linked* cluster expansion for \overline{H}_1 . We are aided in arriving at the linked expansion by virtue of the individual particle propagator

formalism¹⁵ that we are using. This enables us to look at pieces of diagrams without having to consider whatever else is happening at the same time.

IV. Construction of the Transition Interaction $\Delta\bar{\Sigma}(E)$

We are ready to come to the new part of the problem, namely construction of the interaction between the projectile and the nucleus. So, we imagine that we have a projectile scattering from a nucleus with n valence particles in active orbitals.

In physical terms, the problem that we now solve is the following. We wish to evaluate the scattering amplitude of an energetic, spinless, distinguishable projectile from the ground state of the nuclear target to one of its low lying states. We do not know the exact eigenfunctions of the nucleus, but we do know the eigenstates $|\bar{\mu}\rangle$ of the model Hamiltonian \bar{H}_N . Can we construct $\Delta\bar{\Sigma}(E)$ perturbatively in terms of these states $|\bar{\mu}\rangle$ and the matrix elements of V_{NN} and V_{PN} of Eq. (II.1)? We again insist on a linked cluster expansion, but we expect that, unlike \bar{H}_1 , it will be necessary to introduce an energy dependence into $\Delta\bar{\Sigma}(E)$ to describe the opening of inelastic channels that we do not describe explicitly by our choice of model space.

The choice of model space for the combined problem is, of course, dictated by the decisions we already made in selecting $\Sigma(E)$ and \bar{H}_1 ; namely, we have a finite dimensional space (N) describing the nucleus and a complete set of plane wave states describing the projectile. The direct product of these two spaces forms the basis for the scattering problem. Again the implementation of the theory occurs in two steps. The first is to obtain $\Delta\bar{\Sigma}(E)$ (thus completely defining the effective Hamiltonian in Eq. (II.14)) and the second is to diagonalize \bar{H} by solving the appropriate coupled channel equations. We consider the former problem in this section.

A. Theory of $\Delta\bar{\Sigma}(E)$

The optical potential $\Sigma(E)$ and effective interaction \bar{H}_1 have already been defined and we do not want to change these. We will define $\Delta\bar{\Sigma}(E)$ so that the S -matrix elements are the same whether calculated with \bar{H} or H . We again consider the interaction switched off at large times, so that the S -matrix element for the projectile to induce a transition from μ_i to μ_f is

$$S_{f_i} \equiv \langle \tilde{\phi}_{\mu_f}(+\infty), \mathbf{k}_f | T(+\infty, -\infty) | \tilde{\phi}_{\mu_i}(-\infty), \mathbf{k}_i \rangle \quad . \quad (\text{IV.1})$$

The states $|\tilde{\phi}_{\mu}(-\infty)\rangle$ are specific linear combinations of the states in Eq. (II.13). The linear combinations are constructed so that $|\tilde{\phi}_{\mu}(-\infty)\rangle$ will evolve into the exact state $|\mu\rangle$ as interaction H_1 is slowly switched on in T . Similarly, $\langle\tilde{\phi}_{\mu}(+\infty)|$ is the state that $\langle\mu|$ evolves into as H_1 is turned off slowly in T . We want the interaction H_1 essentially fully turned on before the projectile begins to interact with the nucleus. This may be accomplished by turning V_{PN} on more slowly than H_1 or, even more simply, by arranging

for the projectile wave packet not to arrive at the target nucleus until $|\tilde{\phi}_\mu\rangle$ has evolved into $|\mu\rangle$. The corresponding S -matrix element in the model space is

$$\bar{S}_{fi} \equiv \langle \tilde{\phi}_{\mu_f}(+\infty), \mathbf{k}_f | \bar{T}(+\infty, -\infty) | \tilde{\phi}_{\mu_i}(-\infty), \mathbf{k}_i \rangle \quad (IV.2)$$

It follows from Eq. (65) of Ref. 4a that $|\tilde{\phi}_\mu\rangle$ is the same combination of $|\phi_i\rangle$ in both Eqs. (IV.1) and (IV.2). This means that S_{fi} can be made equal to \bar{S}_{fi} by equating the matrix elements of $\bar{T}(+\infty, -\infty)$ and $T(+\infty, -\infty)$ for any choice of initial and final configurations belonging to the model space. We define $\Delta\bar{\Sigma}(E)$ to establish this equality. We use the diagrams to define $\Delta\bar{\Sigma}(E)$, but in practice we obtain the S -matrix elements from the phase shifts in the scattered wave solutions of Schroedinger's equation.

An example of a diagram contributing to S_{fi} is shown in Fig. 8. As usual, we collect all passive lines into boxes, so that diagrams of S_{fi} appear as boxes connected by projectile and active nucleon lines. The boxes connecting the active lines alone are the same as for \bar{H}_1 . The new element of the theory at this level is the projectile-valence boxes that connect the projectile and the active nucleon lines. Examples of these boxes are given in Fig. 9. These are pieces of the two- and three-body boxes. The one-body box (no external valence lines) belongs to the optical potential $\Sigma(E)$.

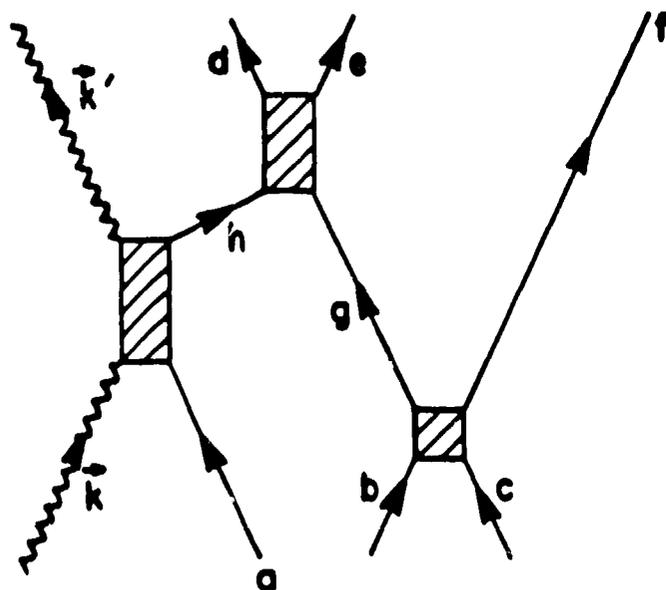


Figure 8. Example of a diagram contributing to S_{fi} .

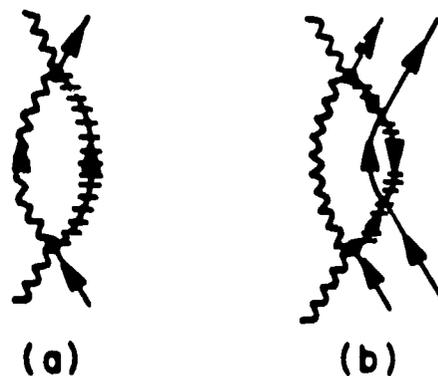


Figure 9. Examples of projectile-valence boxes.

Just as in Sect. III.B, we want to establish a one-to-one correspondence between diagrams of S_{fi} and \bar{S}_{fi} . But what do we mean by diagrams of \bar{S}_{fi} , now that \bar{H} in Eq. (II.14) is energy dependent? To answer this, we must first understand the meaning

of E in Eq. (II.19) and its relationship to $\Sigma(E)$ and $\Delta\bar{\Sigma}(E)$ in Eq. (II.14). Clearly E is to be identified with the total energy of the system. Such an identification can be shown to be preserved in $\Sigma(E)$ and $\Delta\bar{\Sigma}(E)$ if the diagrammatic units corresponding to them are defined *globally*, i.e., that they include everything that happens over the time interval $t' - t$ ($\Delta\bar{\Sigma}(E)$ is the Fourier transform of $\Delta\bar{\Sigma}(t' - t)$). This means that we have to specify a procedure for constructing $\Sigma(E)$ and $\Delta\bar{\Sigma}(E)$ out of the basic boxes and whatever else is happening over the interval $t' - t$. (One advantage of representing effective interactions by instantaneous potentials, as in the case of \bar{H}_1 , is that this complication is avoided.) We believe that it is easiest to do this directly in the diagrams that we draw for \bar{S}_{f_1} . It is important to do this carefully if we are to avoid a nasty difficulty that can arise when dealing with global propagators in perturbation theory, namely the appearance of disconnected diagrams. How our particular methods avoid this difficulty will be shown later.

We will represent the diagrams of \bar{S}_{f_1} as in Fig. 10, which shows valence particle propagators connected by circles (matrix elements of \bar{H}_1) and projectile propagators connecting projectile-valence *rectangles*, which are closely related to, but not identical with, $\Delta\bar{\Sigma}$. As discussed earlier, the interaction of the projectile with the nucleus develops over the full time interval $t' - t$, and the rectangle is drawn extended in time for this reason. However, we want to take the nuclear transition induced by the projectile to occur instantaneously at time t_0 , which is a reference time to be fixed relative to t' and t . Thus, the rectangles are also characterized by a single time t_0 at which the valence nucleon lines attach. All time orderings of the circles relative to t_0 are to be allowed, as long as particles and holes propagate in a legal direction. Note that the time base t_0 of the projectile-valence box is not an independent time variable. Otherwise, the considerations that go into the choice of t_0 here are identical to those that determine the time-base of interactions in \bar{H}_1 .

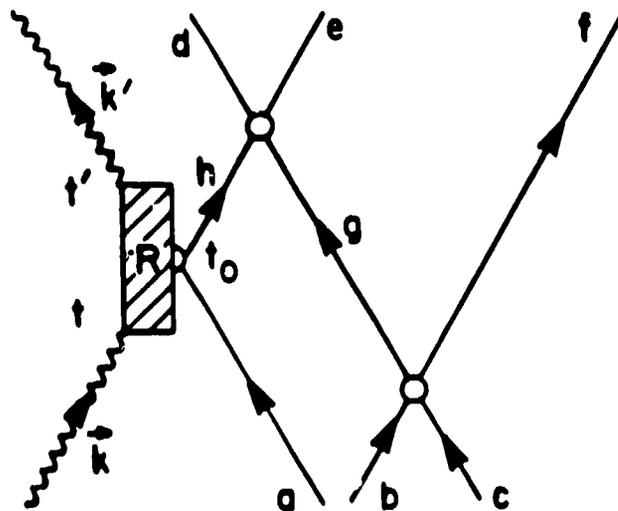


Figure 10. Example of diagrams contributing to \bar{S}_{f_1} .

In what follows we will first show how to determine the folded diagram expansion for the rectangles. Then we will describe the procedure for combining the rectangles with whatever else can occur over $t' - t$, to obtain $\Delta\bar{\Sigma}(t' - t)$.

Now that we know what diagrams of \bar{S}_{f_i} look like we can define the rectangles in order to establish an equality between the diagrams of S_{f_i} and the corresponding ones of \bar{S}_{f_i} . Compare, for example, the diagrams in Figs. 8 and 10. As before, we begin by equating the corresponding box to circle. The circle are then defined just as they were in Sect. III.B. The rectangle is related to its corresponding box by writing down an equation similar to that in Fig. 6 and then solving it for the rectangle. This is accomplished as before by removing the valence lines that are not a part of the definition of the rectangle. The result is shown in Fig. 11. The complete one-box contribution to the rectangle will entail a sum over all boxes, which will include an integration over all internal times (i.e., t' , t , and t_0 remain fixed). Projectile-valence contributions to it will contain $2, \dots, n$ body pieces. We can again achieve a one-to-one correspondence between all diagrams of S_{f_i} and \bar{S}_{f_i} by carefully and systematically introducing model-correcting and true-correcting projectile-valence diagrams.^{4b}

As we indicated earlier, our use of time-ordered projectile-valence diagrams should cause us to worry about unlinked diagrams. Consider, for example, Fig. 12. By virtue of retaining the time-dependence in $\Delta\bar{\Sigma}(t' - t)$, we are forced to consider all other processes that occur within the interval $t' - t$ as being part of $\Delta\bar{\Sigma}$. Since there is another interaction occurring during this time in Fig. 12 this constitutes a disconnected piece of the kernel $\Delta\bar{\Sigma}(t' - t)$. Fortunately the mathematical difficulties of the disconnected kernel can be overcome by the following rearrangement. Note that $e^{-i\bar{H}_N(t'-t)}$ is the sum of all possible diagrams involving propagating and interacting valence nucleons over the interval $t' - t$. Thus, we can take into account all possible actions of \bar{H}_1 by the following simple procedure. First eliminate all diagrams of the time-evolution operator \bar{T} containing explicit matrix elements of \bar{H}_1 . The

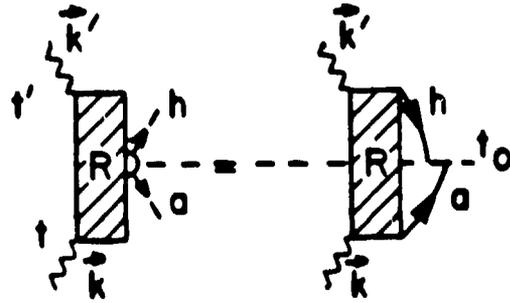


Figure 11. Definition of the projectile-valence rectangle contribution to $\Delta\Sigma(T)$ appropriate to Fig. 10.

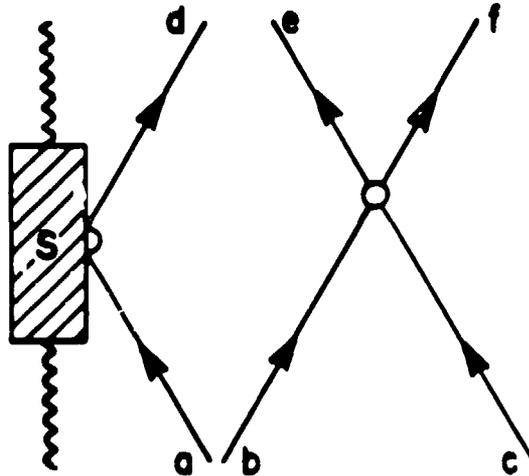


Figure 12. An unlinked contribution to $\Delta\bar{\Sigma}$.

resulting set of "skeletal" terms consists of iterated projectile and projectile-valence rectangles. They are connected by lines representing the unperturbed propagator of the projectile and by lines representing the unperturbed propagator of n valence nucleons. The latter consists of a series of propagators of the form

$$e^{-iH_0\Delta T_i} = \sum_{\alpha_1 \dots \alpha_n} |\alpha_1 \dots \alpha_n\rangle e^{-i(\epsilon_{\alpha_1} + \dots + \epsilon_{\alpha_n})\Delta T_i} \langle \alpha_1, \dots, \alpha_n | \quad (IV.3)$$

where $\Delta T_i = t_0(i+1) - t_0(i)$ is the time interval between the time-base of successive rectangles. The interaction $\Delta \bar{\Sigma}$ induces transitions from one unperturbed state $|\alpha_1 \dots \alpha_n\rangle$ to another $|\alpha'_1 \alpha'_2 \dots \alpha'_n\rangle$ at time $t_0(i)$. Second, make the replacement

$$\begin{aligned} e^{-i(\epsilon_{\alpha_1} + \dots + \epsilon_{\alpha_n})\Delta T_i} &= \langle \alpha_1 \dots \alpha_n | e^{-iH_0\Delta T_i} | \alpha_1 \dots \alpha_n \rangle \\ &\rightarrow \langle \alpha'_1 \dots \alpha'_n | e^{-i\bar{H}_N\Delta T_i} | \alpha_1 \dots \alpha_n \rangle \end{aligned} \quad (IV.4)$$

in Eq. (IV.3); these operators reintroduce the matrix elements of \bar{H}_1 in a compact and easily managed form. We now observe that the disconnected pieces illustrated in Fig. 12 disappear if we introduce the exact eigenvalues and the shell model states. The net result is that

$$\begin{aligned} e^{-iH_0\Delta T_i} &\rightarrow \sum_k \sum_{\alpha_1 \dots \alpha_n} \sum_{\alpha'_1 \dots \alpha'_n} |\alpha'_1 \dots \alpha'_n\rangle \langle \alpha'_1 \dots \alpha'_n | \bar{\mu}_k \rangle e^{-iE_{\mu_k}\Delta T_i} \\ &\quad \langle \bar{\mu}_k | \alpha_1 \dots \alpha_n \rangle \langle \alpha_1 \dots \alpha_n | \end{aligned} \quad (IV.5)$$

The conclusion is that the \bar{S} -matrix achieves a simple and relatively compact form if we calculate Σ and $\Delta \bar{\Sigma}$ in the shell-model basis

$$\begin{aligned} \langle \bar{\mu}_k | \Sigma + \Delta \Sigma | \bar{\mu}_\ell \rangle &\rightarrow \sum_m \sum_{\alpha_1 \dots \alpha_n} \sum_{\alpha'_1 \dots \alpha'_n} \langle \bar{\mu}_k | \alpha'_1 \dots \alpha'_n \rangle \langle \alpha'_1 \dots \alpha'_m | (\Sigma + \Delta \bar{\Sigma})_{m+1} | \alpha_1 \dots \alpha_m \rangle \\ &\quad \langle \alpha_1 \dots \alpha_n | \bar{\mu}_\ell \rangle e^{-iE_{\mu_k}(t'-t_0)} e^{-iE_{\mu_\ell}(t_0-t)} \end{aligned} \quad (IV.6)$$

where the phase factor $e^{-iE_{\mu_k}(t'-t_0)}$ is that portion of $e^{-iE_{\mu_k}\Delta T_i}$ in Eq. (VI.5) that extends from the time base t_0 to the end of the box at time t . Note that only m single particle states undergo a transition in Eq. (IV.6) when the $m+1$ -body piece of the effective interaction $(\Sigma + \Delta \bar{\Sigma})_{m+1}$ acts. The phase factors may be regarded as a contribution to the sum over all boxes that accounts for the valence-valence interactions occurring during the interval $t' - t$ over which the boxes Σ and $\Delta \bar{\Sigma}$ last. These phases give rise to a simple modification of the energy denominators of $\Delta \bar{\Sigma}(E)$. The final expression for Σ and $\Delta \bar{\Sigma}$ will thus be given in a hybrid form involving matrix elements of H_1 in the basis of H_0 , the unperturbed

eigenvalues of H_0 as well as the exact energies E_μ and the shell model wave functions $|\bar{\mu}\rangle$. How this looks in practice is examined by looking at examples in the next section.

We have now completed our demonstration of the existence of a linked cluster expansion of $\Delta\bar{\Sigma}(E)$. Actual evaluation of $\Delta\bar{\Sigma}(E)$ in practice requires care in order to choose the diagrams that represent the appropriate mix of nuclear structure and reaction dynamics. What we have demonstrated here is that $\Delta\bar{\Sigma}(E)$ does in fact depend on both these elements and therefore that in practical calculations to learn about either requires that $\Delta\bar{\Sigma}(E)$ will have to be chosen with some care.

B. Discussion

The theory that we have constructed leads to a set of coupled equations. If we project Eq. (II.19) onto a complete set of states $|\bar{\mu}_j\rangle$ we find, using Eqs. (II.14),

$$\sum_i \left[\left(\frac{-\nabla^2}{2m} + \Sigma_0(E - E_{\mu_i}) \right) \delta_{ij} + \langle \bar{\mu}_j | \Delta\bar{\Sigma}(E) | \bar{\mu}_i \rangle \right] \langle \bar{\mu}_i | \bar{\Psi}^{(+)} \rangle = (E - E_{\mu_j}) \langle \bar{\mu}_j | \bar{\Psi}^{(+)} \rangle, \quad (\text{IV.7})$$

where we have used the relationship^{4b} that $\langle \mu_i | \Sigma(E) | \mu_i \rangle = \Sigma_0(E - E_{\mu_i})$. Once the wave function $|\bar{\Psi}\rangle$ is found, the scattering amplitude $f_{\mu_f \mu_0}$ for scattering from the initial state $|\mu_0\rangle$ to the final state $|\mu_f\rangle$ is obtained from the boundary condition

$$|\bar{\Psi}^{(+)}(r)\rangle \xrightarrow{r \rightarrow \infty} |\bar{\mu}_0\rangle e^{ik_f r} + \sum_f \frac{e^{ik_f r}}{r} |\bar{\mu}_f\rangle f_{\mu_f \mu_0}. \quad (\text{IV.8})$$

Thus, for applications of the theory one proceeds in two steps. The first is the construction of \bar{H}_1 , Σ , and $\Delta\bar{\Sigma}$ using the mapping techniques discussed in Sections III and IV of this paper. The scattering information is then obtained as the solution of Eqs. (IV.7) and (IV.8).

The result in (IV.7) is a set of coupled equations for the wave function $|\bar{\Psi}\rangle$. In most cases the scattering to low lying nuclear states is a small part of the total cross section and one probably does not need the coupled channels as a practical matter. Coupled channels will be needed whenever (1) the leading order of the reaction requires several scatterings (e.g., pion double charge exchange); (2) a single step transition to a final state is possible but is strongly suppressed; or (3) the multistep processes are strongly enhanced by collectivity. These cases are exceptional and (2) and (3) can often be anticipated. In any case the coupled channel result is a convenient one because it collects into one place, and treats consistently, all the information that is available from the shell model and from studies of reaction dynamics. As a consequence, a comprehensive set of predictions of the model may be readily obtained.

Generally the most important channels are those of the continuum, e.g., quasielastic scattering. Since these channels are not included explicitly in Eq. (IV.7), one must incorporate them as a renormalization of the bare projectile-nucleon and nucleon-nucleon interaction. To see how this goes, consider Figs. 5 and 9, where the dots represent projectile-nucleon and nucleon-nucleon *bare* interactions. One may sum infinite classes of diagrams, the ladders to get the projectile-nucleon G -matrix and the nucleon-nucleon G -matrix. By insisting that at least one internal line of the box at each intermediate step be passive, the G -matrix becomes a box in its own right, and multiple-box diagrams can be built up in terms of these quantities. The necessity of using the G -matrices instead of the bare interactions is familiar in both nuclear matter¹⁶ and multiple scattering theory.¹⁷ Note that the projectile-nucleon G -matrix is different from the free space scattering amplitudes (T -matrix) because of the Pauli blocking of the intermediate states.

Based on developments¹⁹ that occurred during the late 1960's, it is not clear that a microscopic theory based on a perturbative treatment in a restricted space can be made to work, at least for the simple choice of H_0 used in most calculations. The problem is that intruder states, such as the low lying deformed $4p-4h$ 0^+ states in ^{16}O spoil the convergence of such expansions. The fact that, in spite of this, relatively simple perturbative microscopic descriptions²¹ of nuclear spectra exist gives us some confidence that successful treatments of $\Delta\bar{\Sigma}$ may be developed along similar lines. The results are suggestive that the expansions with which we are dealing are asymptotic expansions, for which evaluation of a few of the lowest orders in perturbation theory may suffice. Alternatively, one might explore different forms of H_0 that take the deformation into account.

Finally, let us mention the connection of our work to that of Feshbach,³ Mahaux and Weidenmüller,²² and Kuo, Osterfeld, and Lee.⁸

The Feshbach theory provides, just as ours, a partition of the scattering into two parts: the calculation of the optical potential and the subsequent calculation of the T -matrix. The structure of this theory as well as other formal approaches to multiple scattering²³ is simple because the *exact* nuclear eigenstates $|\mu\rangle$ of H_N are chosen as the basis for the formulation. However, this same feature makes the theory difficult to apply in practice, because one never knows $|\mu\rangle$ exactly. Knowledge of the formal structure provides little insight into the nature of the corrections that become necessary once a specific approximation to $|\mu\rangle$ is made.

Our model space M is, by contrast, built of a finite set of eigenstates of H_0 (see Eq. (II.9)). The scattering amplitudes are calculated from Σ and $\Delta\Sigma$ which, in contrast to the Feshbach theory, are given in terms of an expansion in the *known* quantities $|\mu\rangle$, $\langle\alpha|$, and matrix elements of V_1 in the basis of the e -states. The scattering solutions are thus expressed in such a way that permits systematic improvement. The corrections amount to the folded diagrams and other renormalizations to the free projectile nucleon T -matrix

as discussed in Sect. IV. Because our theory aims at calculating nuclear structure as well as scattering observables, it is more ambitious and appears more complicated than that of Feshbach.

Mahaux and Weidenmüller²² have developed a powerful calculational framework for evaluating the scattering of a nucleon from a nucleus in a model space. Their techniques enable them to include large numbers of basis states, but no more than one nucleon is allowed to be in the continuum. The residual interaction among the nucleons is taken to be the free nucleon-nucleon interaction or a simple phenomenological parameterization of it.

The work of Mahaux and Weidenmüller, as ours, is an attempt to fill in the gap between the formal multiple scattering theories and the traditional DWIA/coupled-channel prescriptions for calculating scattering with simplified nuclear wave functions. The main difference lies in how the residual interaction is chosen. The entire focus of our work is on constructing $\Delta\bar{\Sigma}$ consistent with the choice of Σ and \bar{H}_1 , while Mahaux and Weidenmüller require a $\Delta\bar{\Sigma}$ in order to apply their method. Thus, the two approaches are complementary. One might expect intuitively that as the dimensionality of the model space is increased, the importance of the renormalizations of the bare interaction leading to \bar{H}_1 , Σ , and $\Delta\bar{\Sigma}$ would decrease. Thus, for the large spaces within which Mahaux and Weidenmüller work, the appropriate renormalizations of Σ and $\Delta\bar{\Sigma}$ might be expected to be more easily calculated than in the more highly truncated model spaces appropriate to the phenomenological shell model.

Kuo, Osterfeld, and Lee⁸ have proposed a theory of an energy-independent optical potential to describe scattering. They have in mind eliminating the energy-dependence using the same technique of folded diagrams that has been used to remove the energy-dependence from the shell-model potential. Although they make a formal argument that an energy-independent optical potential could be defined in such a way as to describe elastic scattering, subsequent studies⁹ cast some doubt on the practicality of their proposal.

We stress that, in contrast to Kuo, Osterfeld, and Lee, our theory does not seek to eliminate the energy-dependence of Σ and $\Delta\bar{\Sigma}$. The reason is that the scattering to real inelastic intermediate states that lie outside the model space corresponds to boxes that last over long time intervals. This means that multiple-box folded diagrams, whose size is a measure of the time extent of the boxes involved, would become correspondingly more important. Thus, the folded diagram expansion replacing Σ and $\Delta\bar{\Sigma}$ by instantaneous interactions would probably not converge. Instead, we use the theory of folded diagrams to assure the compatibility of an energy-independent shell-model potential with the scattering operators Σ and $\Delta\bar{\Sigma}$, which remain energy-dependent. Our main interest is in obtaining the lowest-order perturbative corrections that arise from working in a model space in order to improve the reliability of the theory.

V. Concluding Remarks

We have shown how to bring together the shell model and multiple scattering theory in a consistent calculational framework. Beginning with an underlying true Hamiltonian H , which includes a description of the nucleus as well as the scattering of a distinguishable projectile (e.g., K^\pm , e , μ , ν) with the nucleus, we arrive at an effective interaction \bar{H} in a model space

$$\bar{H} = \bar{H}_N + K_P + \Sigma(E) + \Delta\bar{\Sigma}(E) \quad .$$

This is equivalent to H in the sense that (1) the discrete eigenstates of \bar{H}_N of energy E_μ correspond to a set of the discrete eigensolutions of H_N with the same eigenvalue, and that (2) the S -matrix elements for scattering between eigenstates of \bar{H}_N is the same as between corresponding eigenstates of H_N . Our effective interaction \bar{H}_N is energy independent and Hermitian, just like the familiar shell model potential. However, Σ and $\Delta\bar{\Sigma}$, which constitute respectively the one- and many-body pieces of the effective projectile-nucleus interaction, are energy dependent.

Implementation of the theory consists of two steps: (1) calculating the pieces \bar{H}_N , Σ , and $\Delta\bar{\Sigma}$. These are given by linked cluster expansions obtained by comparing diagrammatic expansions of the time-evolution operator in the true and model spaces; (2) solving for the scattering amplitude by evaluating the set of coupled channel equations in Eqs. (IV.7) and (IV.8).

As it now stands our theory does not apply to the scattering of all light hadrons, especially π , N , and \bar{N} . The reason is that our theory is applicable only to projectiles that are distinguishable from their counterparts in the nuclear wave function. A similar theoretical framework should exist to describe the scattering of these projectiles. Eventually, one would also like to relax our assumption that all particles interact through potentials, e.g., to permit an underlying field theoretical description. One might begin with one of the currently popular Bonn²³ or quantum hadronamic²⁴ meson-theoretical Hamiltonians.

We are hopeful that this approach will lend a firmer theoretical foundation to nuclear structure studies with light hadrons, because the familiar approximate DWIA/coupled channels descriptions of the scattering correspond to identifiable pieces of our theory (see, e.g., Sect. V). Thus, the corrections are easy to isolate and study, and one might be able to place theoretical limits on the accuracy with which nuclear structure and reaction dynamics can be deduced in any particular phenomenological study. The appropriate corrections to the bare interaction, which compensate for the truncations leading to the shell model built into the theory, have been already studied in the context of the microscopic shell model. We expect that this broad experience will be useful in the scattering problem.

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