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The Foundations of the Shell Model — Revisited*

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In 1993 fall semester I was asked to lecture on nuclear structure — and in due course and relatively early I came to the section on the shell model. The shell model is a marvelous creation, especially when one realizes that it exists, in spite of the relatively strong nucleon–nucleon forces. We now realize that this mean field feature is characteristic of complex systems and relatively independent of the character of the interparticle forces. What I needed to present to the students was a simple derivation of the shell model together with a way for estimating the error in making the mean field approximation and thus quantitatively guaranteeing its validity. I must be careful here — I did not do a literature search and what I will present to you may not be new. But at least it is not currently in the books on nuclear structure or in presentations in conferences on the shell model. Serendipitously, Claude Mahaux wrote me to ask some questions on my discussion of the Pauli principle for the optical model — he is writing a review article on the mean field. I realized that my 1962 [1] derivation of the optical model potential, simplified in the paper on doorway states with Kerman and Lemmer [2] was in fact also a derivation of the shell model. Moreover the error could be expressed as a matrix element whose evaluation could be performed using techniques Kerman, Koonin (FKK) and I had developed in a paper on statistical multi-step reactions [3]. These developments, optical model derivation, doorway states, and multi-step reactions are in my recent work on nuclear reactions [4].

This derivation of the mean field depends essentially on two elements. The first: As in the case of the optical model the shell model potential is an energy average of the many body Hamiltonian. The second: The error can be calculated using the assumption that the matrix elements for highly excited states are random. Energy averaging removes the complicated modes of motion and retains the simpler excitations upon which the shell model is based. The assumption of randomness is expected to be valid when a state or the states involved in the matrix element are highly excited. This assumption greatly simplifies the calculation of the error in the shell model.

We begin by using the projection operator analysis. Let

$$\Psi = P\Psi + Q\Psi \tag{0.1}$$

where

$$P^2 = P \ , \quad PQ = 0 \ , \quad Q^2 = Q \ , \quad P + Q = 1$$

The operator P projects the sub-Hilbert space consisting of the Slater determinants formed from single particle wave functions. Q subtends all the remaining states. The many body Schrödinger equation

$$H\Psi = E\Psi \tag{0.2}$$

upon substituting Eq. (0.1) becomes the coupled equations

$$(E - H_{PP})(P\Psi) = H_{PQ}(Q\Psi) \tag{0.3}$$
$$(E - H_{QQ})(Q\Psi) = H_{QP}(P\Psi) \tag{0.4}$$

where

$$H_{PP} = PHP \ , \quad H_{PQ} = PHQ \quad etc.$$

The operator H_{PP} is the Hartree Fock potential. To go beyond the Hartree Fock approximation we reduce the coupled equations Eq. (0.3) and Eq. (0.4) to a single equation in P space by taking energy averages. The energy average of Eq. (0.3), indicated by angular brackets, is

$$(E - H_{PP})\langle P\Psi\rangle = H_{PQ}\langle Q\Psi\rangle \tag{0.5}$$

or

$$\langle P\Psi\rangle = \psi_0 + \frac{1}{E - H_{PP}} H_{PQ}\langle Q\Psi\rangle \tag{0.6}$$

where $(E - H_{PP})\psi_0 = 0$. To obtain $\langle Q\Psi\rangle$ we turn to Eq. (0.4). Substituting Eq. (0.3) into Eq. (0.4) yields

$$(E - H_{QQ} - W_{QQ})(Q\Psi) = H_{QP}\psi_0 \tag{0.7}$$

where

$$W_{QQ} = H_{QP}\frac{1}{E - H_{PP}} H_{PQ} \tag{0.8}$$

Therefore

$$Q\Psi = \frac{1}{E - H_{QQ} - W_{QQ}} H_{QP}\psi_0 \tag{0.9}$$

Averaging, one obtains

$$\begin{aligned}\langle Q\Psi\rangle &= \left\langle \frac{1}{E - H_{QQ} - W_{QQ}} \right\rangle H_{QP}\psi_0 \\ &= \left\langle \frac{1}{e_Q} \right\rangle H_{QP}\psi_0 \end{aligned} \tag{0.10}$$

where

$$e_Q \equiv E - H_{QQ} - W_{QQ}$$

Eq. (0.6) can now be written

$$\langle P\Psi\rangle = \psi_0 + \frac{1}{E - H_{PP}} H_{PQ}\left\langle \frac{1}{e_Q} \right\rangle H_{QP}\psi_0 \tag{0.11}$$

or

$$(E - H_{PP})\langle P\Psi\rangle = H_{PQ}\left\langle \frac{1}{e_Q} \right\rangle H_{QP}\psi_0 \tag{0.12}$$

Solving Eq. (0.11) for ψ_0 and substituting in Eq. (0.12) yields an equation for $\langle P\Psi\rangle$:

$$(E - H_{PP})\langle P\Psi\rangle = H_{PQ}\rangle\left\langle \frac{1}{e_Q} \right\rangle H_{QP}\frac{1}{1 + \frac{1}{E - H_{PP}} H_{PQ}\left\langle \frac{1}{e_Q} \right\rangle H_{QP}}\langle P\Psi\rangle$$

A little bit of algebraic manipulation reduces this equation to

$$\left(E - H_{PP} - H_{PQ}\frac{1}{\left\langle \frac{1}{e_Q} \right\rangle^{-1} + W_{QQ}} H_{QP}\right)\langle P\Psi\rangle = 0 \tag{0.13}$$

This then is a mean field potential in which the effect of the excitations not included in the shell model space are included by an averaging procedure. This potential varies slowly with energy and therefore can be represented by a non-local potential operating in P space. We shall not go into the detailed evaluation of $\left(\frac{1}{e_Q}\right)^{-1}$. Suffice it to say that when the energy of excitation of the shell model state is large as is the case for the hole state formed in $(e, e'p)$ or $(p, 2p)$ reactions it will be complex and thus the shell model potential will have an imaginary component. On the other hand when we consider a low lying state the average of $\frac{1}{e_Q}$ should be real. This version of the shell model potential makes a straightforward transition with increasing energy to the optical model potential which has the same form as that given by Eq. (0.13).

An estimate of the error accompanying the shell model potential of Eq. (0.13) can be obtained as below. Following Kawai, Kerman, and McVoy (0.5) one can show that the exact equations can be written as follows:

$$(E - \bar{H})\psi_P = V_{PQ}\psi_Q \tag{0.14a}$$

$$(E - H_{QQ})\psi_Q = V_{QP}\psi_P \tag{0.14b}$$

where $\bar{H}$ is the shell model potential and V is a renormalized interaction. Let ϕ_0 be a solution of Eq. (0.15):

$$(\bar{E}_0 - \bar{H})\phi_0 = 0 \tag{0.15}$$

where we shall take $\bar{H}$ to be hermitian. Secondly we note that

$$\psi_Q = \frac{1}{E - H_{QQ} - \bar{W}_{QQ}} V_{QP}\phi_0 \tag{0.16}$$

where

$$\bar{W}_{QQ} = V_{QP}\left(\frac{1}{E - \bar{H}}\right)' V_{PQ} \tag{0.17}$$

The prime indicates that in the expansion of $\left(\frac{1}{E-\bar{H}}\right)'$ in terms of the eigenstates of $\bar{H}$ the term proportional ϕ_0 is to be omitted a requirement which is equivalent to the condition $\langle\phi_0, \psi_P\rangle = 1$.

Multiplying Eq. (0.14a) from the left yields

$$\langle\phi_0, (E - \bar{H})\psi_P\rangle = E - E_0 = \langle\phi_0 V_{PQ}\psi_Q\rangle$$

Substituting Eq. (0.16) for ψ_Q one obtains

$$\Delta E \equiv E - \bar{E} = \left\langle \phi_0 V_{PQ}\frac{1}{E - h} V_{QP}\phi_0 \right\rangle \tag{0.18}$$

where

$$h = E - H_{QQ} - \bar{W}_{QQ}$$

The average of ΔE in Eq. (0.18) is zero by construction. To make this explicit it is convenient to replace Eq. (0.18) by

$$\Delta E = \left\langle \phi_0 V_{PQ} \frac{1}{E-h} V_{QP} \phi_0 \right\rangle - \left\langle \phi_0 V_{PQ} \frac{1}{E-h} V_{QP} \phi_0 \right\rangle_{AV} \tag{0.19}$$

But the average of the square of ΔE

$$\left[(\Delta E)^2\right]_{AV} = \left\{ \left[\left\langle \phi_0 V_{PQ} \frac{1}{E-h} V_{QP} \phi_0 \right\rangle \right] \right\}_{AV} - \left[\left\langle \phi_0 V_{PQ} \frac{1}{E-h} V_{QP} \phi_0 \right\rangle_{AV} \right]^2 \tag{0.20}$$

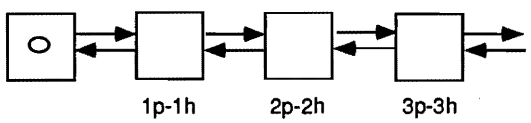
is not. It is a measure of the error in the shell model of this paper.

One notes the close relationship of the matrix element Eq. (0.18) with the starting point of the statistical multi-step compound reaction theory of FKK [3]. In ref. [4] it is given as (V.5.33):

$$\mathcal{J}_{fi}^{(msc)} = \left\langle \phi_f^{(-)} V_{PQ} \frac{1}{E-h} V_{QP} \phi_i^{(+)} \right\rangle \tag{0.21}$$

where $\mathcal{J}_{fi}^{(msc)}$ is the multistep transition amplitude for the reaction $i \to f$. As in the case being considered here $\langle \mathcal{J}_{fi}^{(msc)} \rangle_{AV} = 0$ but the average of the square is not. The similarity of Eq. (0.21) and Eq. (0.18) suggests that the methods employed by FKK to evaluate the square magnitude of $\mathcal{J}_{fi}^{msc}$ can be employed here.

As a first step we partition the Hilbert space into classes of increasing complexity: initial state, $1p-1h$ states, $2p-2h$ states, *etc.* The initial state is a solution of $(E_0 - \bar{H})\phi_0 = 0$. The action of the interaction is to induce transitions to states of increasing complexity as



indicated by the diagram. Using the analysis of FKK the matrix element in Eq. (0.18) can be rewritten as follows:

$$\Delta E = \sum_m (\Delta E)_m$$

where m is the maximum number of particle-holes:

$$(\Delta E)_m = \langle \phi_0 V_{01} G_1 V_{02} G_2 \ldots V_{m-1,m} G_m V_{m,m-1} G_{m-1} \ldots V_{21} G_1 V_{10} \phi_0 \rangle - \langle\ \rangle_{AV} \tag{0.22}$$

where

$$V_{m,m-1} = Q_m V Q_{m-1} \tag{0.23}$$

The propagators G_μ satisfy

$$G_\mu = \frac{1}{E - h_{\mu,\mu} - V_{\mu,\mu+1} G_{\mu+1} V_{\mu+1,\mu}} = \frac{1}{E - \mathcal{H}_\mu} \tag{0.24}$$

In Eq. (0.22) we now insert the eigenfunctions of G_μ^{-1}

$$\mathcal{H}_\mu \psi_{\mu,\alpha} = \xi_{\mu,\alpha} \psi_{\mu,\alpha} \tag{0.25}$$

We write out the first two terms of Eq. (0.21)

$$\begin{aligned}
\Delta E_1 &= \langle \phi_0 V_{01} G_1 V_{10} \phi_0 \rangle - \langle \phi_0 V_{01} G_1 V_{10} \phi_0 \rangle_{AV} \\
&= \sum_\alpha \frac{\langle \phi_0 V \psi_{1,\alpha} \rangle \langle \psi_{1,\alpha} V \phi_0 \rangle}{E - \xi_{1,\alpha}} - \langle \Delta E_1 \rangle_{AV} \\
&= \sum_\alpha \frac{|\phi_0 V \psi_{1,\alpha}|^2}{E - \xi_{1,\alpha}} - \langle \Delta E_1 \rangle_{AV} \\
\Delta E_2 &= \langle \phi_0 V_{01} G_1 V_{12} G_2 V_{21} G_1 V_{10} \phi_0 \rangle \\
&= \sum_{\alpha,\beta,\gamma} \frac{\langle \phi_0 V \psi_{1,\alpha} \rangle \langle \psi_{1,\alpha} V \psi_{2\beta} \rangle \langle \psi_{2\beta} V \psi_{1,\gamma} \rangle \langle \psi_{1,\gamma} V \phi_0 \rangle}{(E - \xi_{1\alpha})(E - \xi_{2\beta})(E - \xi_{1\gamma})} - \langle \Delta E_2 \rangle_{AV}
\end{aligned} \tag{0.26}$$

Using the random phase approximation $\gamma = \alpha$

$$= \sum_{\alpha,\beta} \frac{|\langle \phi_0 V \psi_{1,\alpha} \rangle|^2 \, |\langle \psi_{1\alpha} V \psi_{2\beta} \rangle|^2}{(E - \xi_{1\alpha})^2 (E - \xi_{2\beta})} - \langle \Delta E_2 \rangle_{AV} \tag{0.27}$$

We shall stop at this point as the numerical evaluation has not yet been performed. You will note that our goal is a modest one. We are not attempting to determine the residual interaction. We are only providing an estimate of the error in using the mean field model.

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