EFFECTIVE INTERACTIONS IN NUCLEAR STRUCTURE*

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Abstract

The theoretical justification of effective interactions for shell-model calculations is discussed in terms of t-matrix theory. A peculiar difficulty arises when t-matrix elements are fitted to energy levels, in that the single-particle basis functions are unknown. A criterion under which the t-matrix will act like a two-body interaction operator is presented, and the problem of relating the residual interaction to the phenomenological interaction is discussed.

1. Shell-Model Calculations from the t-Matrix Point of View

In this introduction we wish to review the use of the t-matrix in solving bound state problems [1], and the significance of these solutions in the nuclear shell model [2]. Let us start by outlining the solution to the eigenvalue problem

$$H\psi = E\psi \quad (1.1)$$

when H may be written as

$$H = H_0 + W, \quad (1.2)$$

and the eigenfunctions and eigenvalues of H_0 are known

$$H_0\phi_n = E_n\phi_n. \quad (1.3)$$

The solution of equation (1.1) may then be expressed by the series

$$\psi = \sum_n a_n \phi_n. \quad (1.4)$$

If one selects a normalization on ψ to be such that $a_0 = 1$ then equation (1.1) yields

$$E = E_0 + \langle \phi_0 | W | \psi \rangle \quad (1.5)$$

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and

$$a_n = \frac{\langle \varphi_n | W | \psi \rangle}{E - E_n} \quad (n \neq 0), \quad (1.6)$$

so that

$$\psi = \varphi_0 + \sum_{n \neq 0} \frac{\varphi_n \langle \varphi_n | W | \psi \rangle}{E - E_n}. \quad (1.7)$$

Repeated substitution of equation (1.7) into equation (1.5) yields the usual Brillouin-Wigner [3,4] perturbation series

$$E = E_0 + \langle \varphi_0 | W + W \frac{P}{E - H_0} W + W \frac{P}{E - H_0} W \frac{P}{E - H_0} W + \dots | \varphi_0 \rangle, \quad (1.8)$$

where

$$\frac{P}{E - H_0} \equiv \sum_{n \neq 0} \frac{|\varphi_n\rangle\langle\varphi_n|}{E - E_n} \quad (1.9)$$

The t -operator may now be defined as satisfying the relation

$$\langle \varphi_n | t | \varphi_0 \rangle = \langle \varphi_n | W | \psi \rangle \quad (1.10)$$

for all n , and is given implicitly by the operator equation

$$t = W + W \frac{P}{E - H_0} t, \quad (1.11)$$

in the basis φ_n .

The energy eigenvalue can then be expressed in terms of matrix elements of the zero-order unperturbed function φ_0 .

$$E = E_0 + \langle \varphi_0 | t | \varphi_0 \rangle. \quad (1.12)$$

Equation (1.12) has particular significance for the nuclear shell model, where the Hamiltonian is taken to represent a set of nucleons moving in a common external potential with a two-body interaction

$$H_{S.M.} = \sum_i [p_i^2/2m + V(r_i, p_i, \sigma_i)] + \sum_{i < j} V_{ij}. \quad (1.13)$$

This model Hamiltonian may presumably be obtained from a system where only two-body forces are present

$$H = \sum_i p_i^2/2m + \sum_{i < j} U_{ij} \quad (1.14)$$

rewriting H as

$$H = H_0 + W, \quad (1.14a)$$

where

$$H_0 = \sum_i [p_i^2/2m + V(r_i, p_i, \sigma_i)] \quad (1.14b)$$

and $W \equiv H - H_0$. It is then clear that the residual interaction in equation (1.13) should properly be the t -operator of the actual nuclear problem, if one truncates the Hilbert space in which V_{ij} is permitted to have non-vanishing matrix elements.

It is not clear that the t -operator so defined will be just a two-body operator. Effective many-body terms will arise in t , and it is hard to show that they are all small, or that there are cancellations among them. It has been demonstrated, in fact, that some three-body terms are significant in nuclear matter [5].

Most shell-model calculations retain only one- and two-body operators in the Hamiltonian, attempting to keep the theory as simple as possible. Many investigations avoid writing an explicit form for $H_{S.M.}$ altogether, and deal only with its matrix elements within the states defined by the configurations considered. In the $1p$ -shell [6,7], for example, one requires only two single-particle energies

$$\langle jm | H_0 | jm \rangle \quad j = 3/2, 1/2 \quad (1.15)$$

and fifteen two-body matrix elements

$$\langle p^2 L' S' J M | t | p^2 L S J M \rangle \quad (1.16)$$

to test the Hamiltonian over the entire shell. The method of fractional parentage coefficients, needed in deducing the energy levels and wave functions for the p^n configuration from these parameters, was introduced by Bacher and Goudsmit [8] and popularized by Racah [9] and Talmi [10]. Applications to atomic and nuclear systems are abundant, and several reviews have appeared on the subject [11-13].

A difficulty that has always been inherent in this procedure is that once one has obtained a good energy fit one has not always acquired exact knowledge of the single-particle basis functions. In atomic physics this seems to be fairly acceptable since the mixing of configurations from different major shells appears to be comparatively small, and therefore the t -operator cannot differ much from the phenomenological interaction. The basis functions should then be close to the Hartree-Fock orbitals. In nuclei configuration mixing can be large, so that the residual shell-model interaction is usually only expected to resemble the phenomenological interaction in form (i.e. both are expected to be invariant under time reversal, parity, etc.).

This difficulty is well known. What we wish to emphasize in this paper is that the problem is compounded in nuclear structure calculations by the fact that the t -matrix itself depends upon the basis functions selected in the calculation. In Section 2 we treat a simple analytic

problem by shell-model techniques, and illustrate how one might work back to the realistic interaction even when the t -matrix deduced is quite misleading. The t -matrix is usually determined in nuclei so that only its two-body part will contribute to the energy, and the conditions this places on the basis functions are examined in Section 3.

2. A Simple Analytic Example

The Schrodinger equation for the Stark effect in the harmonic oscillator

$$H = \frac{1}{2} \hbar \omega (p^2 + q^2) + \epsilon \cdot \mathbf{q} \quad (2.1)$$

is easily solved by making the coordinate translation

$$\mathbf{q}' = \mathbf{q} + \epsilon / (\hbar \omega), \quad (2.2)$$

to obtain

$$H = \frac{1}{2} \hbar \omega (p'^2 + q'^2) - \epsilon^2 / (2\hbar \omega). \quad (2.3)$$

The energy eigenvalues are then simply shifted uniformly away from those of the unperturbed oscillator

$$E_n = (N + 3/2) \hbar \omega - \delta, \quad (2.4)$$

where $\delta = \epsilon^2 / (2\hbar \omega)$. If we designate the eigenfunctions of

$$H_0 = \frac{1}{2} \hbar \omega (p^2 + q^2) \quad (2.5)$$

as $\varphi_n(\mathbf{q})$ then the eigenfunctions of H are obviously

$$\varphi_n(\mathbf{q}') = \exp \{ (\epsilon / \hbar \omega) \cdot \mathbf{grad} \} \varphi_n(\mathbf{q}) = \exp \{ -i(\epsilon / \hbar^2 \omega) \cdot \mathbf{p} \} \varphi_n(\mathbf{q}). \quad (2.6)$$

If the $\varphi_n(\mathbf{q})$ are used as the basis functions the t -operator is at once seen to be

$$t = \epsilon \cdot \mathbf{q} \exp \{ -i(\epsilon / \hbar^2 \omega) \cdot \mathbf{p} \}. \quad (2.7)$$

Now let us try to find the perturbation by shell-model methods. We will consider that H_0 is known, and that a full catalog of "experimental data" is at our disposal. The first thing a shell-model theorist would try is to fit a t -matrix to the energy levels. Since the perturbation shifts all levels by $-\delta$ he sees at once that

$$t' = -\delta \quad (2.8)$$

will do the job.

This effective interaction t' does not resemble the original perturbation ($W = \epsilon \cdot \mathbf{q}$) in any basic way. W conserves neither the parity nor the angular momentum of the oscillator, while t' obviously conserves both. Thus the effective interaction does not even have the same elementary symmetry properties as the actual interaction. Nevertheless t' is a perfectly proper t -operator of the problem. If one relabels the terms in the Hamiltonian:

$$H = H_0' + W', \quad (2.9)$$

here $W' = -\delta$, and

$$H_0' = \frac{1}{2} \hbar \omega (p'^2 + q'^2), \quad (2.9a)$$

then in the basis defined by $\phi_n(\mathbf{q}')$:

$$t' = -\delta - \delta \frac{P}{E - H_0} \quad t' = -\delta. \quad (2.10)$$

One has then correctly evaluated the t -operator by fitting matrix elements to the position energy levels, but little has been accomplished until the basis for this t -operator has been identified. To test the basis one must examine physical quantities other than the energy. It is easily seen that the static electric quadrupole moments are unaltered by the perturbation, since the wave functions can effectively be translated without further distortion. This would support the (erroneous) conclusion that the interaction is just $-\delta$ in the basis $\phi_n(\mathbf{q})$.

A clue to the proper basis is obtained when quantities relating to the $E1$ operator ($\mathbf{q}$) are considered. The perturbation induces a static electric dipole moment in the (nondegenerate) ground state, and thus one is made aware that t' is only an effective interaction. In this case the basis for t' may be found by strictly shell-model methods. One finds empirically that an effective $E1$ operator of the form

$$\mathbf{q}' = \mathbf{q} - \Delta \quad (2.11)$$

is needed to fit all electric dipole moments and transition rates. Further evidence that the basis for t' is just $\phi_n(\mathbf{q}')$ comes from the effective orbital angular momentum operator needed to fit $M1$ matrix elements:

$$\mathbf{l}' = \mathbf{l} - \Delta \times \mathbf{p}. \quad (2.12)$$

Since it is recognised that $\delta/(\hbar\omega) = \Delta^2/2$ the problem is easily solved.

Thus in this simple example both the interaction operator and the proper wave functions can be deduced by a "shell-model" analysis of the "experimental data".

3. Two-Body Interactions and Nuclear Spectra

Consider the Hamiltonian for a system of interacting particles, taking H_0 to be a sum of single-particle operators:

$$H_0 = \sum_i H_0(i) \quad (3.1)$$

and W to be a two-body interaction

$$W = \sum_{i < j} W_{ij}. \quad (3.2)$$

We want to examine the conditions under which the t -operator defined in the basis

$$H_0(i) \phi_{jm}(i) = E_j \phi_{jm}(i) \quad (3.3)$$

will be a two-body operator.

It will be convenient to work in the occupation representation

$$H_0 = \sum_{jm} E_j a_{jm}^+ a_{jm} . \quad (3.4)$$

$$W = \sum_{JM} V_J(j_1 j_2, j_3 j_4) A_{JM}^+(j_1 j_2) A_{JM}(j_3 j_4) , \quad (3.4a)$$

where

$$V_J(j_1 j_2, j_3 j_4) = \langle j_1 j_2 JM | W | j_3 j_4 JM \rangle \quad (3.4b)$$

and

$$A_{JM}(j_1 j_2) = \sum_{m_1+m_2=M} \langle j_1 j_2 JM | j_1 j_2 m_1 m_2 \rangle a_{j_1 m_1} a_{j_2 m_2} \quad (j_1 \neq j_2) \quad (3.4c)$$

$$A_{JM}(j^2) = \sqrt{2} \sum_{m_1 > m_2} \langle jj JM | jj m_1 m_2 \rangle a_{j m_1} a_{j m_2} . \quad (3.4d)$$

The a_α and a_α^+ are the familiar annihilation and creation operators for the orbital α , obeying the fermion anticommutation relations:

$$a_\alpha a_\beta + a_\beta a_\alpha = 0 \quad (3.5a)$$

$$a_\alpha^+ a_\beta^+ + a_\beta^+ a_\alpha^+ = 0 \quad (3.5b)$$

$$a_\alpha^+ a_\beta + a_\beta a_\alpha^+ = \delta_{\alpha\beta} . \quad (3.5c)$$

First we treat a system consisting of only two shell-model orbitals $\tilde{j}$ and j . We take these two orbitals to be of opposite parity in order to eliminate single-orbital excitations. The wave functions for a system with $2\tilde{j} + 1 + k$ particles may then be written in the form

$$\Psi_\alpha = \sum_n a_n^\alpha \phi_\alpha^{(n)}(\tilde{j}^{2\tilde{j}+1-n} j^{k+n}) , \quad (3.6)$$

where α denotes whatever absolute quantum numbers are required to completely specify the state.

If the normalization is chosen so that $a_0^\alpha \equiv 1$, then equation (1.5) tells us that

$$E_\alpha = \langle \varphi_\alpha^{(0)} | H_0 | \varphi_\alpha^{(0)} \rangle + \langle \varphi_\alpha^{(0)} | W | \psi_\alpha \rangle = E_0 + \langle \varphi_\alpha^{(0)} | W | \psi_\alpha \rangle, \quad (3.7)$$

where

$$E_0 = (2\tilde{j} + 1)E_{\tilde{j}} + kE_j. \quad (3.7a)$$

Since W is the sum of two-body operators it can excite no more than two particles at a time out of the ground state. Since $\varphi_\alpha^{(1)}$ cannot appear in ψ_α because of parity conservation we have

$$E = E_0 + \langle \varphi_\alpha^{(0)} | W | \varphi_\alpha^{(0)} \rangle + a_2^\alpha \langle \varphi_\alpha^{(0)} | W | \varphi_\alpha^{(2)} \rangle. \quad (3.8)$$

It is worth emphasizing that equation (3.8) is exact. This is related to the well recognized fact that the wave function ψ contains far more information about a physical system than is required to work most problems. In the current example only the two-body density matrix is needed to calculate the energy, and this point is well known. Alternatively, in the nuclear problem, one needs only the zero-order shell-model function and the amplitudes of the single-nucleon and two-nucleon excitations to compute the energy so long as one has only two-body forces.

Now consider the last term in equation (3.8)

$$\langle \varphi_\alpha^{(0)} | W | \varphi_\alpha^{(2)} \rangle = \langle \varphi_\alpha^{(0)} | \sum_{JM} V_J(\tilde{j}^2, j^2) A_{JM}^+(\tilde{j}^2) A_{JM}(j^2) | \varphi_\alpha^{(2)} \rangle. \quad (3.9)$$

It is evident that the only parts of $\varphi_\alpha^{(2)}$ which make a non-vanishing contribution to this matrix element are those that can be written in the form

$$\sum_{J'M'} \lambda_{J'} A_{J'M'}^+(j^2) A_{J'M'}(\tilde{j}^2) | \varphi_\alpha^{(0)} \rangle, \quad (3.10)$$

so that we can write

$$a_2^\alpha \langle \varphi_\alpha^{(0)} | W | \varphi_\alpha^{(2)} \rangle = \langle \varphi_\alpha^{(0)} | \sum_{JM} V_J(\tilde{j}^2 j^2) \lambda_{J'} A_{JM}^+(\tilde{j}^2) \quad (3.11)$$

$$\times A_{JM}(j^2) A_{J'M'}^+(j^2) A_{J'M'}(\tilde{j}^2) | \varphi_\alpha^{(0)} \rangle.$$

The coefficients $\lambda_{J'}$ are simply amplitudes for the appropriate components of direct two-orbital excitation out of the shell-model ground state. In general they will be complicated operators, but for any particular state it is possible to replace them by just a number.

The $A_{JM}^+(\tilde{j}^2)$ and $A_{JM}(j^2)$ in equation (3.11) are easily eliminated since they operate on a closed shell

$$a_2^\alpha < \varphi_\alpha^{(0)} | W | \varphi_\alpha^{(2)} > = < \varphi_\alpha^{(0)} | \sum_{JM} \lambda_J V_J(\tilde{j}^2 j^2) A_{JM}(j^2) A_{JM}^+(j^2) | \varphi_\alpha^{(0)} > , \quad (3.12)$$

and substituting into equation (3.8) yields

$$E = E_0 + < \varphi_\alpha^{(0)} | W + \sum_{JM} \lambda_J V_J(\tilde{j}^2 j^2) A_{JM}(j^2) A_{JM}^+(j^2) | \varphi_\alpha^{(0)} > \quad (3.13)$$

Equation (3.13) is again exact (when the proper values of λ_J are inserted), and has the desired form of a shell-model effective interaction in that only matrix elements for $\varphi_\alpha^{(0)}$ appear. The correction to the potential due to configuration mixing manifests itself as a "hole-hole" potential $A_{JM} A_{JM}^+$. This is readily inverted using the commutation relations in equation (3.5):

$$\sum_M A_{JM}(j^2) A_{JM}^+(j^2) = \sum_M A_{JM}^+(j^2) A_{JM}(j^2) - 2 \left(\frac{2J+1}{2j+1} \right) \sum_m a_{jm}^+ a_{jm} + (2J+1). \quad (3.14)$$

The effective shell-model interaction is then seen to be

$$W' = W + \sum_{JM} \lambda_J V_J(\tilde{j}^2, j^2) A_{JM}^+(j^2) A_{JM}(j^2) , \quad (3.15)$$

while the configuration mixing also provides a correction to the single particle energy

$$E'_j = E_j - 2 \sum_J \left(\frac{2J+1}{2j+1} \right) \lambda_J V_J(\tilde{j}^2, j^2) , \quad (3.16)$$

and a renormalization of the "core" energy

$$\sum_J (2J+1) \lambda_J V_J(\tilde{j}^2 j) . \quad (3.17)$$

The exact effective shell-model interaction derived above takes a particularly simple form in that nothing more complex than two-body operators are present. This is somewhat deceptive, however, since the λ_J are really state-dependent functions of the number operator. Simplicity is retained, however, if the λ_J have constant values in all levels throughout the shell. This is clearly not to be expected. Near the end of the shell the Pauli exclusion principle must inhibit configuration mixing more effectively than it does at the beginning (for $k = 2j + 1$ all $\lambda_J = 0$).

It is possible that this variation is balanced by the excitation of the j -orbitals up to higher shells, since the amplitude of these states should increase with k . Let us then introduce a third orbital $\bar{j}$ into our model, and consider the effect of the two-particle excitation $j^{k-2} \bar{j}^2$:

$$\varphi_{\alpha}^{(2)}(\tilde{j}^2 \tilde{j}^{+1} j^{k-2} \bar{j}^2) = \sum_{J'M'} \mu_J A_{J'M'}^+(\tilde{j}^2) A_{J'M'}(j^2) | \varphi_{\alpha}^{(0)} > . \quad (3.18)$$

is yields a correction to the t -matrix

$$\sum_{JM} \mu_J V_J(j^2, \bar{j}^2) A_{JM}^+(j^2) A_{JM}(j^2) , \quad (3.19)$$

th no contribution to the single-article energy. The excitations $j^2 j^{-1} j^k \bar{j}^2$ do nothing but normalize the core energy, and we take $\bar{j}$ to have parity opposite to j to eliminate states of e configuration $j^2 j^{-1} j^{k+1} \bar{j}$.

The matrix elements like

$$< j^2 j^{+1} j^k | W | j^2 j j^k \bar{j} > \quad (3.20)$$

ll produce corrections to the two-body interaction, single-particle energy, and core renormalization if they are not eliminated by imposing the Hartree-Fock condition. We have taken some re to avoid such single-particle excitations for several reasons. If the orbitals are the re-ult of a Hartree-Fock calculation then this matrix element is zero by definition. In any case or shells in the nucleus do alternate in parity, and this makes the excitation of a nucleon om one major shell to another energetically unfavorable. A recent paper by Kuo and Brown [14] onstrates nonetheless that such corrections to the energy are significant, and should prefer-ly be incorporated if one is not in a Hartree-Fock basis.

4. Conclusions

The dominant portion of configuration mixing in nuclei most likely comes from the pairing ffect. The excitation of zero-coupled pairs out of the shell-model ground state will modify e effective two-body interaction by (in the context of the limited model introduced in the eceding section):

$$[\lambda_0 V_0(\tilde{j}^2, j^2) + \mu_0 V_0(j^2, \bar{j}^2)] A_{00}^+(j^2) A_{00}(j^2) . \quad (4.1)$$

order for the effective interaction to be invariant throughout the shell the quantity

$$U_0 = V_0(j^2, j^2) + \lambda_0 V_0(\tilde{j}^2, j^2) + \mu_0 V_0(j^2, \bar{j}^2) \quad (4.2)$$

st remain constant. Similar conditions apply to the other components of the force.

Such conditions do not seem very realistic, and it is hard to see why they should even hold pproximately. Nonetheless many calculations have demonstrated the significance of effective interactions in the interpretation of nuclear spectra. The key to the success of these calcula-ions may come from the fact that the basis functions are not always precisely defined. When e attempts to fit matrix elements (or Slater integrals) to nuclear level positions the iterion for invariance of the $J_{12} = 0$ component of the force is that U_0 be constant for some

set of basis functions. It is evident that the orbitals of this basis can be represented by the fermion creation and annihilation operators a_{jm}^+ and a_{mj} to a good approximation. It does not follow, however, that these orbitals will be close to oscillator functions, the solutions of the Saxon-Woods potential, or even a Hartree-Fock basis.

Clearly the effective interaction can be useful only if one knows the basis in which it has been calculated. In Section 2 we presented an example of how one can define the basis by standard shell model procedures, when one insists that all experimental data must be fit. Thus if one can find effective moment operators which consistently work, one may establish clues to the basis functions.

Finally we must mention the disturbing possibility that the t -matrix may not have symmetry properties identical with the original potential. This is demonstrated in a rather striking manner in Section 2, where one starts with a potential $(\epsilon \cdot q)$ which does not conserve angular momentum, linear momentum, or parity, and derives a t -matrix which conserves all dynamical variables $(-\delta)$.

References

1. L.S. RODBERG, *Ann. Phys.* 2, 199 (1957).
2. H.A. BETHE, *Phys. Rev.* 103, 1353 (1956).
3. E.P. WIGNER, *Math. u. naturw. Anz. ungar. Akad. Wiss.* 53, 475 (1935).
4. L. BRILLOUIN, *J. Phys.* 4, 1 (1933).
5. H.A. BETHE, *Phys. Rev.* 138, B804 (1965).
6. S. COHEN and D. KURATH, *Nucl. Phys.* 73, 1 (1965).
7. D. AMIT and A. KATZ, *Nucl. Phys.* 58, 388 (1964).
8. R.F. BACHER and S. GOUDSMIT, *Phys. Rev.* 46, 948 (1934).
9. G. RACAH, *Farkas Memorial Volume*. Research Council of Israel, Jerusalem (1952).
10. I. TALMI, *Phys. Rev.* 107, 326 (1957); I. TALMI and I. UNNA, *Ann. Rev. Nucl. Sci.* 10, 353 (1960).
11. J.P. ELLIOTT and A.M. LANE, *Handbuch der Physik* (ed. by S. Flugge), Vol. 39, p. 241, Springer Verlag, Berlin (1957).
12. P. GOLDHAMMER, *Rev. Mod. Phys.* 35, 40 (1963).
13. B.R. JUDD, *Operator Techniques in Atomic Spectroscopy*. McGraw-Hill, New York (1963).
14. T.T.S. KUO and G.E. BROWN, Preprint.