CALCULATIONS WITH REACTION MATRICES IN THE p–f SHELL

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Abstract

Elements of the shell-model reaction matrix have been calculated for the p–f shell with an exact treatment of the Pauli operator. These elements have been used in straightforward calculations of the energy levels of ^{42}Ca and ^{42}Sc and the binding energy of ^{40}Ca.

I. Introduction

Because of the strong short-range repulsive part of the free nucleon–nucleon interaction **v**, nuclear structure calculations with realistic potentials are generally based on perturbation expansions involving the energy-dependent nuclear reaction matrix $\mathbf{G}(\omega)$ which incorporates the "healing effects" of the Pauli principle. For closed shell nuclei, the Brueckner–Goldstone expansion (Baranger 1969) is used, while for open shell the appropriate expansion is that of Bloch and Horowitz as modified by Brandow (1967).

The reaction matrix is defined by the operator equation

$$\mathbf{G}(\omega) = \mathbf{v}+\mathbf{v}\{\mathbf{Q}/(\omega-\mathbf{H}_0)\}\mathbf{G}(\omega)\,, \tag{1}$$

where $\mathbf{H}_0$, the Hamiltonian generating the basis states, describes two non-interacting particles in a potential well. The starting energy ω and the Pauli operator **Q** are determined by the application.

Ideally we would like to choose $\mathbf{H}_0$, and hence the basis states, to give the most rapid convergence of the relevant perturbation series. In practice it is more convenient to take $\mathbf{H}_0$ to be the two-particle harmonic oscillator Hamiltonian because such wavefunctions are easily transformed into the relative-centre of mass (r.c.m.) coordinate system to facilitate numerical integrations. Unfortunately the Pauli operator **Q** is diagonal in the original coordinate system rather than in the r.c.m. system. Most authors (Wong 1967; Kuo and Brown 1968; Davies *et al.* 1969; Davies and Baranger 1970; Davies and McCarthy 1971) have therefore approximated **Q** by an operator which is diagonal in the r.c.m. system.

Recently, methods have been proposed (Lawson 1970; Truelove and Nicholls 1970; Barrett, Hewitt, and McCarthy 1971) for solving equation (1) for $\mathbf{G}(\omega)$ in a harmonic oscillator basis while treating **Q** exactly. Of these methods, the last is most suitable for calculations of properties of intermediate mass nuclei. In Section II of

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the present paper we give a brief description of this method. In Section III the method is applied to a calculation of the low-lying energy levels of ^{42}Ca and ^{42}Sc and in Section IV to a calculation of the binding energy of ^{40}Ca. The Hamada–Johnston (1962) potential is used throughout.

II. Calculation of Reaction Matrix

The operator equation (1) for the reaction matrix in a harmonic oscillator basis is usually solved by introducing the Bethe–Goldstone wavefunction $\Psi_\alpha^{\mathrm{BG}}(\omega)$ which "heals" onto the two-particle harmonic oscillator wavefunction Φ_α. The former wavefunction is defined by

$$\mathbf{v}\,\Psi_\alpha^{\mathrm{BG}}(\omega) = \mathbf{G}(\omega)\,\Phi_\alpha, \tag{2}$$

and hence satisfies the integro-differential equation

$$(\mathbf{H}_0+\mathbf{v}-\omega)\Psi_\alpha^{\mathrm{BG}}(\omega) = (\epsilon_\alpha-\omega)\Phi_\alpha + \sum_\mu (1-Q_\mu)\Phi_\mu\langle\Phi_\mu\,|\,\mathbf{v}\,|\,\Psi_\alpha^{\mathrm{BG}}(\omega)\rangle, \tag{3}$$

where the sum over μ is over all eigenfunctions of

$$\mathbf{H}_0\,\Phi_\mu = \epsilon_\mu\Phi_\mu. \tag{4}$$

Barrett, Hewitt, and McCarthy (1971) solve equation (3) by expanding $\Psi_\alpha^{\mathrm{BG}}$ in terms of the eigenfunctions Ψ_i of $\mathbf{H}_0+\mathbf{v}$, that is,

$$(\mathbf{H}_0+\mathbf{v})\Psi_i = E_i\,\Psi_i. \tag{5}$$

They show that $\mathbf{G}(\omega)$ satisfies the equation

$$\mathbf{G}(\omega) = \mathbf{G}^{\mathrm{R}}(\omega)-\mathbf{G}^{\mathrm{R}}(\omega)\{(1-\mathbf{Q})/(\omega-\mathbf{H}_0)\}\mathbf{G}(\omega), \tag{6}$$

where $\mathbf{G}^{\mathrm{R}}(\omega)$ is the "reference spectrum" matrix whose elements are given by

$$G^{\mathrm{R}}_{\beta\alpha}(\omega) = (\epsilon_\alpha-\omega)\left(\delta_{\alpha\beta} - (\epsilon_\beta-\omega)\sum_i^\infty b_{i\alpha}\,b_{i\beta}/(E_i-\omega)\right), \tag{7}$$

with

$$b_{i\alpha} = \langle\Psi_i\,|\,\Phi_\alpha\rangle. \tag{8}$$

The above equations are valid for both hard and soft core potentials.

Because $\mathbf{H}_0+\mathbf{v}$ is separable in r.c.m. coordinates, the eigenvalues E_i and eigenfunctions Ψ_i of equation (5) can be found numerically. The overlaps $b_{i\alpha}$ of equation (8) are then sums of products of radial overlap integrals and the usual Talmi–Moshinsky transformation coefficients (Moshinsky 1959). Once the above quantities have been found, it is possible to calculate the matrix elements $G^{\mathrm{R}}_{\beta\alpha}(\omega)$ using equation (7). The reaction matrix $\mathbf{G}(\omega)$ can then be obtained by inverting a subspace of the matrix equation (6). The convergence of the infinite sum over i in equation (7) and the sensitivity of the reaction matrix elements to the choice of the inversion space have been discussed by Barrett, Hewitt, and McCarthy (1971).

In the following calculations the harmonic oscillator well was taken to have $\hbar\Omega = 10{\cdot}5$ MeV. The Hamada–Johnston potential was used throughout for states with relative angular momentum $J \leqslant 3$; the potential **v** was set equal to zero for partial waves with $J > 3$ (see Barrett, Hewitt, and McCarthy 1971). Sufficient eigenstates of (5) were found to ensure that the cutoff point in the sum over i in equation (7), for all required $G^{\mathrm{R}}_{\beta\alpha}(\omega)$, occurred for E_i at least $6\,\hbar\Omega$ above the largest of ϵ_α, ϵ_β, or ω. The inversion subspace included all $\mathbf{Q} = 0$ states with single-particle quantum numbers satisfying $2n_1+l_1 \leqslant 10$ and $2n_2+l_2 \leqslant 10$.

III. Levels of $A = 42$ Nuclei

We consider a system of nucleons governed by the Hamiltonian

$$\mathscr{H} = \sum_i T_i + \sum_{i<j} v_{ij}, \tag{9}$$

where T_i is the kinetic energy operator for the ith nucleon and v_{ij} is the free nucleon–nucleon interaction. Using the Bloch–Horowitz degenerate perturbation theory developed by Brandow (1967) we write $\mathscr{H}$ as

$$\mathscr{H} = \mathscr{H}_0+\mathscr{H}_1, \tag{10}$$

where

$$\mathscr{H}_0 = \sum_i (T_i+U_i) \tag{11}$$

defines the unperturbed basis states and the perturbing Hamiltonian is

$$\mathscr{H}_1 = \sum_{i<j} v_{ij} - \sum_i U_i. \tag{12}$$

In the present calculation U_i is a harmonic oscillator potential.

If we select an A particle model space consisting of those states in which all single-particle states in the core are filled and the remaining particles are distributed over the valence orbitals, the energies of the system are of the form $E = E_{\mathrm{c}}+E_{\mathrm{v}}$, where E_{c} is the ground state energy of the core with the valence particles absent and E_{v}, the valence energies, are the eigenvalues of the energy-dependent operator $\mathbf{H}_0+\boldsymbol{\theta}_{\mathrm{v}}(E_{\mathrm{v}})$. The operator $\mathbf{H}_0$ is that part of $\mathscr{H}_0$ which refers to the valence particles and the effective interaction $\boldsymbol{\theta}_{\mathrm{v}}(E_{\mathrm{v}})$ is given by a perturbation series in the reaction matrix and the single-particle potential U. The Pauli operator to be used in calculating the G-matrix excludes all eigenstates of $\mathbf{H}_0$ with at least one particle in a core orbital or with both particles in the valence orbitals.

For the case of two valence particles, matrix elements of $\boldsymbol{\theta}_{\mathrm{v}}$ can be represented as the sum of a series of diagrams, some of which are shown in Figure 1. In this figure the waving lines represent G-matrix interactions and the dashed lines, interactions with the single-particle potential U. The external lines represent particles in the valence orbitals, coupled to a given total angular momentum J and isospin T.

For the ^{42}Ca and ^{42}Sc nuclei, we take the valence orbitals to be $0f_{7/2}$, $1p_{3/2}$, $1p_{1/2}$, and $0f_{5/2}$. The subset of diagrams with one nucleon line unconnected (e.g. (*b*) and (*c*) of Fig. 1) are included directly by inserting the experimental single-particle

excitations for the core plus one nucleon systems, namely 0·0, 2·1, 3·9, and 6·5 MeV (Kuo and Brown 1968). The theoretical results are then to be compared with experimental levels plotted so that the ground states of ^{42}Ca and ^{42}Sc are at −3·1 and −3·2 MeV respectively.

The convergence of the perturbation expansion for $\mathbf{\theta}_v$ has not yet been established. Kuo and Brown (1968) found that approximating $\mathbf{\theta}_v$ by their bare G-matrix elements plus the excitation energies gave results that were in poor agreement with experiment. They showed that agreement was improved considerably by including the "three-particle–one-hole" ($3p\,1h$) diagram (Fig. 1(d)); they did not investigate the $4p\,2h$ diagram (Fig. 1(e)) or higher order terms in the series. Barrett and Kirson (1970) have since shown that, in the case of ^{18}O, the $3p\,1h$ diagram is largely cancelled by the third-order core polarization diagrams and that the improved agreement found by Kuo and Brown was fortuitous. A subsequent paper (Kirson

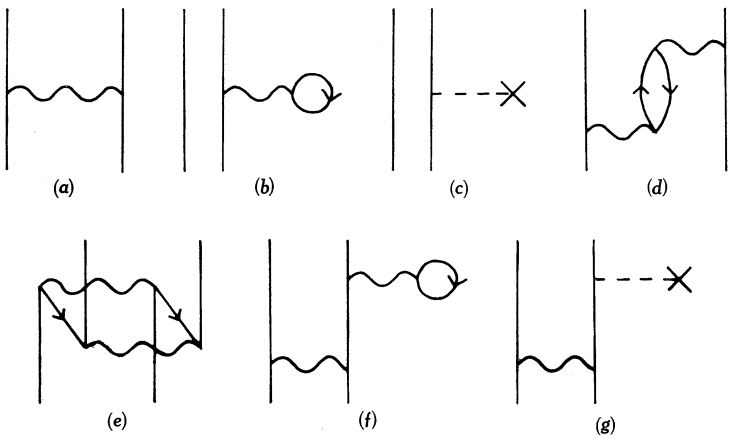

Fig. 1.—Some diagrams in the expansion of the effective interaction $\mathbf{\theta}_v(E_v)$ for the case of two valence nucleons.

1971) suggests that the sum of all core polarization diagrams in ^{18}O may in fact be small; we will therefore neglect all such diagrams. The bubble and potential insertion diagrams (e.g. (f) and (g) of Fig. 1) are usually neglected on the assumption that the harmonic oscillator potential used is approximately self consistent. We will also make this assumption, thereby approximating $\mathbf{\theta}_v$ by our bare G-matrix elements plus the experimental excitations.

A plot of the diagonalized effective interaction for the lowest $T = 0$ states of ^{42}Sc against energy E_v is shown in Figure 2. The eigenvalues of the energy-dependent operator $\mathbf{H}_0+\mathbf{\theta}_v(E_v)$ are given by the intersections of the curves with the line $E_v-94{\cdot}5$ MeV. For comparison, we also show in this figure Kuo and Brown's (KB) bare G-matrix results, which were calculated using an approximate Pauli operator and a plane wave intermediate state spectrum (that is, the energies of the intermediate states used in calculating the G-matrix were taken as the kinetic energy of the harmonic oscillator state, instead of the total harmonic oscillator energy). In Figure 3, our self-consistent (SC) levels and Kuo and Brown's levels are compared with the experimental values. Our levels are clearly well below experiment. The main

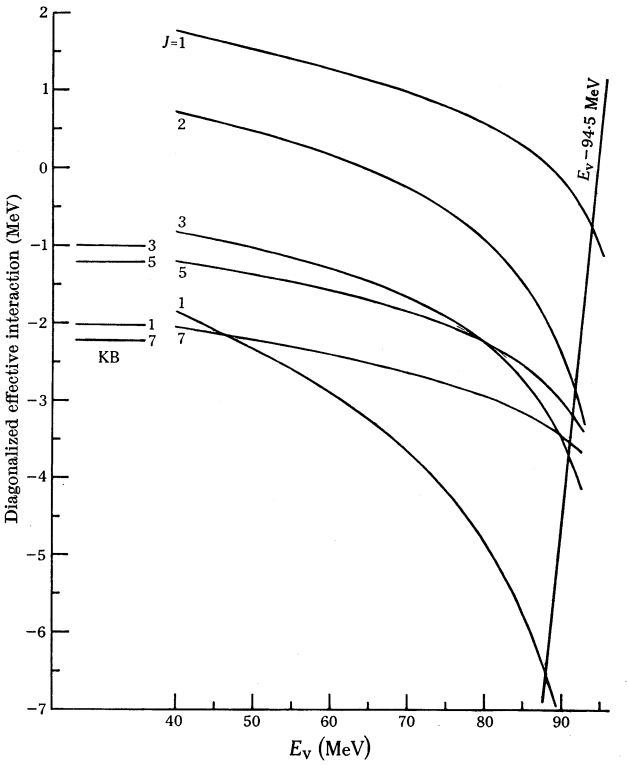

Fig. 2.—Diagonalized effective interaction as a function of the valence energy E_V for the lowest $T = 0$ states of ^{42}Sc. Also shown are the self-consistent line $E_V - 94{\cdot}5$ MeV and Kuo and Brown's (1968) diagonalized effective interaction (KB) derived from their bare energy-independent G-matrix.

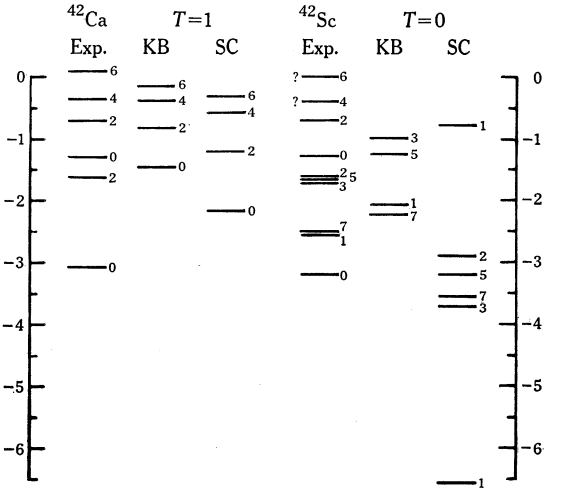

Fig. 3.—Comparison of self-consistent (SC) levels (eigenvalues E_V of $\mathbf{H}_0 + \boldsymbol{\theta}_V(E_V)$) and Kuo and Brown's (1968) bare G-matrix results (KB) with experimental levels for ^{42}Ca and ^{42}Sc. Both $T = 0$ and 1 theoretical levels apply for ^{42}Sc.

reason for this discrepancy seems to be that we do not have a properly self-consistent single-particle potential, that is, the bubble and single-particle potential insertions do not cancel. Inclusion of these effects tends to increase the energies of the intermediate state spectrum, which has the same effect as moving the curves in Figure 2 to the right. Since the line $E_v - 94{\cdot}5$ MeV is unchanged, the points of intersection move upwards to give improved agreement. Work is currently proceeding to include this correction.

The dependence of the $T = 1$ effective interaction on energy E_v is much weaker. The results for the low-lying ($T = 1$) levels of ^{42}Ca are compared with Kuo and Brown's (1968) bare G-matrix results and with experiment in the left-hand part of Figure 3. Better agreement is obtained in this case, but it is obviously still necessary to include higher order corrections, such as core polarization effects.

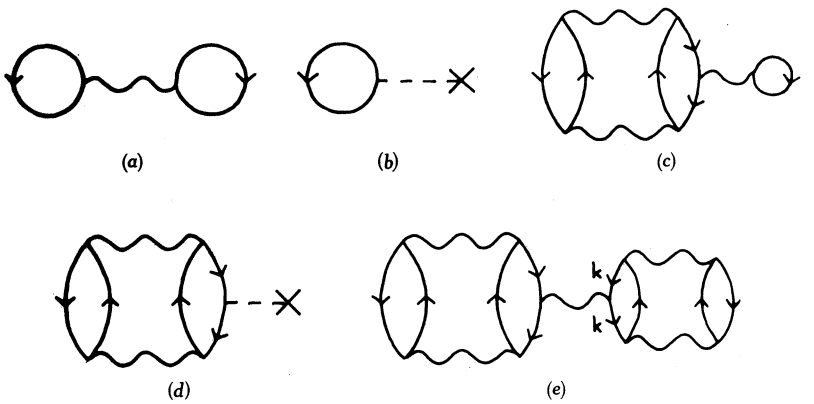

Fig. 4.—Diagrams representing the set of Bethe–Goldstone diagrams summed in the present calculation: (*a*) and (*b*) are the first-order contribution while (*c*), (*d*), and (*e*) are the first representatives of infinite sets of diagrams which are also included.

IV. Binding Energy of ^{40}Ca

As described in Section III, we can define the unperturbed Hamiltonian $\mathscr{H}_0$ and the perturbing Hamiltonian $\mathscr{H}_1$ for a system of nucleons. The total energy of the system is then given by the Brueckner–Goldstone perturbation series (Baranger 1969), which can be represented by a set of diagrams containing G-matrix interactions and single-particle insertions, as before. Some of the diagrams of the series are shown in Figures 4 and 5. In this case the diagrams have no external lines. The Pauli operator to be used for calculating the G-matrix excludes two-particle states where either particle occupies a core orbital.

Figure 4 indicates the set of diagrams included in this calculation: diagrams (*a*) and (*b*) are the first-order contribution to the binding energy, while additional diagrams such as (*c*) and (*d*) with any number of bubble and single-particle potential insertions in the hole lines are also included. This modifies the first-order calculation by requiring that self-consistent energies E_A, as defined by equations (14) and (15) below with P_B set equal to one, should replace the unperturbed energies in determining the starting energy of the G-matrix element in diagram (*a*). Finally, by using

occupation probabilities (Brandow 1970) we account for a further infinite set of diagrams, of which (*e*) is the first. The binding energy is then given by (Davies and Baranger 1970)

$$E = \sum_A \langle A \,|\, T \,|\, A\rangle + \tfrac{1}{2} \sum_{A,B} \langle AB \,|\, G(E_A+E_B) \,|\, AB\rangle P_A P_B + \sum_A (1-P_A)\langle A \,|\, U \,|\, A\rangle, \tag{13}$$

where

$$E_A = \langle A \,|\, T \,|\, A\rangle + \langle A \,|\, U \,|\, A\rangle, \tag{14}$$

$$\langle A \,|\, U \,|\, A\rangle = \sum_B \langle AB \,|\, G(E_A+E_B) \,|\, AB\rangle P_B, \tag{15}$$

$$P_A = \left\{1 - \sum_B \left(\frac{\partial}{\partial\omega}\langle AB \,|\, G(\omega) \,|\, AB\rangle\right)_{\omega=E_A+E_B} P_B\right\}^{-1}. \tag{16}$$

Here A and B are over all core orbitals, T is the kinetic energy, E_A is the single-particle self-consistent energy, and P_A is the occupation probability of the state A.

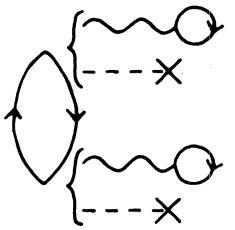

Fig. 5.—First of the infinite set of diagrams which would be included in a Brueckner–Hartree–Fock calculation.

TABLE 1

SELF-CONSISTENT ENERGY LEVELS AND OCCUPATION PROBABILITIES FOR CORE ORBITALS AND RESULTING BINDING ENERGY FOR ^{40}Ca

In (*a*) the unoccupied orbitals have unshifted harmonic oscillator energies while in (*b*) their unperturbed energies are shifted downwards by 10·5 MeV

Parameter	Orbitals						E	$-E/(A=40)$
	$0s_{1/2}$	$0p_{3/2}$	$0p_{1/2}$	$0d_{5/2}$	$1s_{1/2}$	$0d_{3/2}$	(MeV)	(MeV nucleon^{-1})
				(*a*) *Unshifted*				
E_A (MeV)	−38·09	−23·94	−22·30	−10·14	−9·22	−7·54	−94·09	2·35
P_A	0·837	0·862	0·861	0·887	0·882	0·884		
				(*b*) *Shifted*				
E_A (MeV)	−40·91	−26·35	−24·74	−12·14	−11·30	−9·60	−148·52	3·71
P_A	0·832	0·856	0·854	0·881	0·876	0·879		

A more complex calculation would also include an infinite set of diagrams, of which Figure 5 is the first, by requiring the occupied orbitals to be self-consistent in a Brueckner–Hartree–Fock calculation (Davies *et al.* 1969; Davies and McCarthy 1971). In using equations (13)–(16) we have assumed, however, that the self-consistent orbitals are well approximated by harmonic oscillator wavefunctions with $\hbar\Omega =$ 10·5 MeV.

The results of the procedure are presented in Table 1(*a*). Obviously our result is not in accord with the experimental binding energy of 8·55 MeV per nucleon.

It was found that occupation probabilities gave an effect in the right direction but increased the binding by only 0·25 MeV per nucleon, and so further refinements had to be considered. A large increase can be obtained by shifting the unperturbed energies of the unoccupied single-particle states. Table 1(*b*) demonstrates the effect of shifting all these states downwards by the oscillator spacing of 10·5 MeV. It is probable (McCarthy 1968) that such shifts reduce the contribution of the "three-body cluster" diagrams (those containing three hole lines). Since most of these are not included in the calculation, the results are improved. However, as no three-body diagrams have yet been calculated ,we are unable to choose the shifts so as to minimize them. Nevertheless it appears that physically reasonable values are sufficient to produce the desired binding.

V. Acknowledgments

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