SHELL-MODEL DIAGONALIZATION

Introduction

The main issue within the shell model (SM) is to attempt to include the effects of residual interactions into the independent-particle model (IPM). Usually the starting point is the IPM where a simple modified harmonic oscillator potential is used to generate single-particle wave functions, from which the wave function for the whole nucleus is constructed in a way consistent with the Pauli principle. This set of IPM wave functions are therefore the solutions to:

$$H_0\Phi_i = E_i^{(0)}\Phi_i.$$

The effects of residual interactions need to be included, so the realistic Hamiltonian is written:

$$H = H_0 + H'.$$

The term H' represents the effects of residual interactions and we'll refer to solutions of the Schödinger equation using this full Hamiltonian H as "exact". If it were a small perturbation, then first-order perturbation theory could be used. But this is really never the case and methods for incorporating larger perturbations on a Hamiltonian are needed. The following sketches out the general method of matrix diagonalization for such problems. The same methods are used in perturbation theory in the case of degenerate levels as discussed in Chapter 7 of A.M. Rae's book *Introduction to Quantum Mechanics*.

Method

We need to find the solutions to the full Hamiltonian:

$$H\Psi_i = E_i\Psi_i.$$

These exact wave functions Ψ_i can be expanded in terms of the complete orthonormal set of IPM wavefunctions Φ_i

$$\Psi_i = \sum_j a_{ji}\Phi_j$$

where a_{ji} are expansion coefficients with $a_{ji}^* a_{ji}$ being the probability of finding the nucleus with quantum numbers appropriate to Φ_j if it is in a state described by Ψ_i. If H' turns out to be very small for some reason, this series expansion will just be dominated by a single term. In order to find out what the exact wave functions are, we need to find the values of a_{ji} since we already know the IPM wave functions Φ_j.

Take this expansion and substitute it into the full Hamiltonian:

$$H \sum_j a_{ji} \Phi_j = E_i \sum_j a_{ji} \Phi_j.$$

Now multiply both sides by the conjugate of a particular IPM wave function Φ_k^*, and then integrate over all space. Using Dirac notation as a shorthand:

$$\langle \Phi_k | H | \sum_j a_{ji} \Phi_j \rangle = E_i \langle \Phi_k | \sum_j a_{ji} \Phi_j \rangle = E_i a_{ki}.$$

In the last step, orthogonality between particular IMP wave functions is used. Just to simplify the notation a little, write $H_{kj} \equiv \langle \Phi_k | H | \Phi_j \rangle$; these quantities are called $matrix\ elements$ for reasons that will become clear in two lines of alegbra.

We now have:

$$\sum_j H_{kj} a_{ji} = E_i a_{ki}.$$

This is the same as the following matrix equation:

$$\begin{pmatrix} H_{11} & H_{12} & \dots \\ H_{21} & H_{22} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_{1i} \\ a_{2i} \\ \vdots \end{pmatrix} = E_i \begin{pmatrix} a_{1i} \\ a_{2i} \\ \vdots \end{pmatrix}$$

Remember, we have the IPM solutions Φ_k and if we know the residual interaction we can therefore calculate the matrix elements $H_{kj} \equiv \langle \Phi_k | H_0 + H' | \Phi_j \rangle$. We need to find the set of expansion coefficients a_{ji} which will tell us the exact wave function and the energy of the level after the inclusion of the residual interaction E_i. Both of these can be found be solving this matrix equation, which is sometimes called the secular equation for the eigenvalues.

The equation only possesses solutions if, the determinant shown here is zero:

$$\begin{vmatrix} H_{11} - E_i & H_{12} & \dots \\ H_{21} & H_{22} - E_i & \dots \\ \vdots & \vdots & \ddots \end{vmatrix} = 0$$

Now, here a big problem. In general, in a nuclear system, there are an infinite number of Φ_j, so that the matrix dimensions are also infinite! But the physics of the problem is used to reduce the dimensions to a finite size. For example, at low energy we need not consider IPM levels with very high excitation energies. Often the IPM wave functions are restricted to a particular valence shell appropriate to the nucleus of interest, e.g. the fp orbitals. This process of reducing the matrix dimensions is needed not only to make the matrix finite, but also small enough

for a computer to hold in its memory, and is often referred to as *truncation of the model space*.

As an exercise, it is instructive to run through such a calculation for the simplistic case of two levels, the so-called *two-state mixing problem*. The determinant is then:

$$\begin{vmatrix} H_{11} - E & H_{12} \\ H_{21} & H_{22} - E \end{vmatrix} = 0$$

which has the solutions:

$$E = \frac{1}{2}\left[H_{11} + H_{22} \pm \left((H_{11} - H_{22})^2 + 4H_{21}H_{12}\right)^{1/2}\right]$$

giving the energies of the two levels after the inclusion of the interaction.

Substituting these two values back into the matrix equation yields the values of the expansion coefficients for the two wave functions (not difficult to do, but messy algebra), which turn out to be:

$$\Psi_1 = \frac{(E_2 - H_{22})\,\Phi_1 + H_{12}\Phi_2}{\left[(E_2 - H_{22})^2 + H_{12}^2\right]^2} \text{ and } \Psi_2 = \frac{(E_1 - H_{11})\,\Phi_2 + H_{12}\Phi_1}{\left[(E_1 - H_{11})^2 + H_{12}^2\right]^2}.$$

If there is no residual interaction then $H_{kj} = \langle\Phi_k|H_0|\Phi_j\rangle = E_j\delta_{kj}$. So the off diagonal matrix elements H_{12} will be zero, and $\Psi_1 = \Phi_1$ and $\Psi_2 = \Phi_2$ i.e. the IPM wave functions are unmixed. If you gradually turned the residual interactions on, then the values of H_{12} increase gradually mixing the two IPM wave functions.

If you have followed the two-state mixing example, you can understand the essence of many more complicated issues in nuclear physics. Go and read Chapter 1 of Casten's book *Nuclear Structure from a Simple Perspective* and Section 3.2.4 in Heyde's book *The Nuclear Shell Model*.

In reality matrix equations of very high dimensions must be solved and these can only be done using numerical methods by computers. You might by now be wondering why this process is called *matrix diagonalization*. In essence, by finding the set of expansion coefficients a_{ji}, you have found two matrices which can be used to reduce the matirx H_{kj} to a diagonal form (see relevant chapters of maths texts by Boas or Jordan and Smith):

$$\begin{pmatrix} a_{11} & a_{12} & \dots \\ a_{21} & a_{22} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} H_{11} & H_{12} & \dots \\ H_{21} & H_{22} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & \dots \\ a_{21} & a_{22} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} = \begin{pmatrix} E_1 & 0 & \dots \\ 0 & E_2 & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

This process can be run in reverse; if you can diagonalize the matrix by some other method, you can find the matrices of a_{ji}. Many numerical methods exist to diagonalize a large matrix that are employed in shell-model calculations, hence the name.