Exercise 3

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1 How many Slater Determinants are possible

We have a three level system, with each level doubly degenerate. Given two particles, there are thus the equivalent of 6 independent states, each of which could have one single particle state. Hence there are $\binom{6}{2} = 15$ possible two body states. We thus have that there must be 15 possible slater determinants.

2 Properties of Hamiltonian

For this section we restrict our consideration only to the p=1,2 states.

We now consider a hamiltonian of the form

$$\hat{h_0}\psi_{p\sigma} = d \times p\psi_{p\sigma} \tag{1}$$

We also know that h_I merely has a constant value of -g between any two particle states, including between the same state. The total hamiltonian is of course then just

$$H = h_o + h_I \tag{2}$$

Now given this, we make one final assumption, which is that there will only be two slater determinants in play, namely those where the two particles are in the same level but different spins. Thus we can mark $|\psi_1\rangle, |\psi_2\rangle$ for each possibility, where both particles are in d=1 or d=2 respectively. Letting our basis then be

$$\begin{pmatrix} |\psi_1\rangle \\ |\psi_2\rangle \end{pmatrix} \tag{3}$$

It follows that, as there are two particles in each state

$$\hat{h_0} = \begin{pmatrix} 2p & 0 \\ 0 & 4p \end{pmatrix} \tag{4}$$

$$h_I = \begin{pmatrix} -g & -g \\ -g & -g \end{pmatrix} \tag{5}$$

We thus have that the overall hamiltonian must be

$$H = h_0 + h_I = \begin{pmatrix} 2p-g & -g \\ -g & 4p-g \end{pmatrix} \tag{6}$$

We can then trivially find the eigenvectors and the eigenvalues of this matrix in the normal fashion, setting the determinant to zero with a matrix $x\boldsymbol{I}$ subtracted from it.

$$\begin{vmatrix} 2p-g-x & -g \\ -g & 4p-g-x \end{vmatrix} = 0 \tag{7}$$

$$(2p-g-x)(4p-g-x) - g^2 = 0 \tag{8}$$

$$8p^2 - 2pg - 2px - 4pg + g^2 + gx - 4px + xg + x^2 = x^2 + x(-6p+2g) + 8p^2 - 6pg = 0 \tag{9}$$

$$x = (3p-g) \pm \sqrt{g^2+p^2} \tag{10}$$

So the eigenvalues are

$$\epsilon_1 = (3p-g) + \sqrt{g^2+p^2} \tag{11}$$

$$\epsilon_2 = (3p-g) - \sqrt{g^2+p^2} \tag{12}$$

We then can find the eigenvectors as:

$$\chi_1 = \begin{pmatrix} -g \\ p+\sqrt{g^2+p^2} \end{pmatrix} \tag{13}$$

$$\chi_2 = \begin{pmatrix} -g \\ p-\sqrt{g^2+p^2} \end{pmatrix} \tag{14}$$

We thus see that in the energy eigenstates there is a mixing of the p=2 state in the p=1 state of $-\frac{p\pm\sqrt{g^2+p^2}}{g}$

We see tha as p goes to zero this becomes close to 1, suggesting equal amounts of both states(as is sensible, since they would be degenerate states), or if g goes to zero it becomes ill definied(since of course in this case the eigenstates would revert to the basis states). That is, these eigenvectors more accurately represent the slater determinants in the form:

$$\chi_x = \begin{pmatrix} a & b \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = a\,|\psi_1\rangle + b\,|\psi_2\rangle \tag{15}$$

Where a and b are (normalized) constants defining the eigenvector of the corresponding matrix and the psi's are of course the slater determinants from part a.

3 Three states

We now consider the 3 level case(again only with the two particle on one level states considered.) We thus must have a matrix of the form:

$$\boldsymbol{H} = \begin{pmatrix} 2p - g & -g & -g \\ -g & 4p - g & -g \\ -g & -g & 6p - g \end{pmatrix} \tag{16}$$

However, this matrix is not easily diagonalizable in closed form, unless we provide numeric values for p and g. (In principle anything larger than 5x5 must be so as it will be equivalent to solving a general nth order polynomial, which becomes far more difficult for n¿2, and impossible for n¿5).

With this, I now consider a few cases in order to demonstrate features of the system. I first consider the uncoupled case, g=0. This trivially has no mixing with trivial eigenvalues of 2p,4p, and 6p.

Now in the case that $p = g = 1$, we have eigenvalues of .22, 3.3 and 5.5 corresponding to eigenvectors

$$\begin{pmatrix} -.87 \\ -.47 \\ -.14 \end{pmatrix} \begin{pmatrix} -.41 \\ .85 \\ -.32 \end{pmatrix} \begin{pmatrix} -.26 \\ .22 \\ .93 \end{pmatrix} \tag{17}$$

What we see is that we've decreased the energy of the first state from 2 to .28 by means of mixing, while decreasing the second to 3.325, and ever so slightly increasing the energy 6.4. There is much more substantial mixing in the first two eigenvectors, which makes sense as the mixing is more prominant relative to the base energy(ignoring the -g).

We now consider a case where $g > p$, which we will here do with $g = 10, p = 1$. Now in the case that $p = 1$, $g = 10$ we have eigenvalues of -26.1, 2.9 and 5.2 corresponding to eigenvectors

$$\begin{pmatrix} .62 \\ -.76 \\ -.2 \end{pmatrix} \begin{pmatrix} -.57 \\ .61 \\ -.54 \end{pmatrix} \begin{pmatrix} -.53 \\ -.22 \\ .81 \end{pmatrix} \tag{18}$$

We see here that as the p is made large relative to the value of g(so towards the third eigenvector), we see much more importance to the symmetry breaking of the energy of the single particle states, wheras in the case of the first two eigenvectors, since g¿¿p relatively speaking, there is much mixing, with the second state and first state being nearly equally ixed in the first eigenvector, with strong mixing of the third state in the second eigenvector.

We finally consider the case of $g = 1$, $p = 0$, we have eigenvalues of 0, 3 and 0 corresponding to eigenvectors

$$\begin{pmatrix} .82 \\ -.5 \\ 0 \end{pmatrix} \begin{pmatrix} -.41 \\ -.58 \\ -.707 \end{pmatrix} \begin{pmatrix} -.41 \\ -.58 \\ .707 \end{pmatrix} \tag{19}$$

4 Code for Working With Matricies

The code that follows interfaces with an underlying Fortran or C program(honestly I don't know which) in order to quickly work with matricies.

```
import numpy as np
g=10
p=1
H=np.mat([[2*p-g,-g,-g],[-g,4*p-g,-g],[-g,-g,6*p-g]])
print(np.linalg.eig(H))
```

ex3.py