Project 1, Lipkin Model

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a) **The Quasispin Operators**

$$\begin{aligned} J_+ &= \sum_p a^\dagger_{p+} a_{p-} \\ J_- &= \sum_p a^\dagger_{p-} a_{p+} \\ J_z &= \tfrac{1}{2} \sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma} \\ J^2 &= J_+ J_- + J_z^2 - J_z \end{aligned}$$

These operators must satisfy the usual commutation relations:

$$[J^2, J_z] = 0 \qquad [J_z, J_\pm] = \pm J_\pm \qquad [J_+, J_-] = 2J_z$$

We simply insert the definitions of the quasispin operators, and proceed using wick's theorem:

$$[J^2, J_z] = [J_+ J_-, J_z]$$

$$= \tfrac{1}{2} \sum_{pqr\sigma} \sigma (a^\dagger_{p+} a_{p-} a^\dagger_{q-} a_{q+} a^\dagger_{r\sigma} a_{r\sigma} - a^\dagger_{r\sigma} a_{r\sigma} a^\dagger_{p+} a_{p-} a^\dagger_{q-} a_{q+})$$

We are able to construct three separate non-zero single contractions in either of the operator strings, which leads to 5 non-vanishing terms in the wick expansion:

$$a^\dagger_{p+} a_{p-} a^\dagger_{q-} a_{q+} a^\dagger_{r\sigma} a_{r\sigma} = \left\{ a^\dagger_{p+} a_{p-} a^\dagger_{q-} a_{q+} a^\dagger_{r\sigma} a_{r\sigma} \right\}$$

$$+ \left\{ a^\dagger_{p+} \overbrace{a_{p-} a^\dagger_{q-}} a_{q+} a^\dagger_{r\sigma} a_{r\sigma} \right\} + \left\{ a^\dagger_{p+} \overbrace{a_{p-} a^\dagger_{q-} a_{q+}} a^\dagger_{r\sigma} a_{r\sigma} \right\}$$

$$+ \left\{ a^\dagger_{p+} a_{p-} a^\dagger_{q-} \overbrace{a_{q+} a^\dagger_{r\sigma}} a_{r\sigma} \right\} + \left\{ a^\dagger_{p+} \overbrace{a_{p-} a^\dagger_{q-}} \overbrace{a_{q+} a^\dagger_{r\sigma}} a_{r\sigma} \right\}$$

The terms generated on the second string look exactly the same, but they act on different operators, since they are rearranged. The first and second terms are immediately zero because we may permute the operator strings to look the same with an even permutation.

Evaluating the contractions we come to:

$$[J^2, J_z] = \tfrac{1}{2}\sum_{pqr}[(-\left\{a^\dagger_{p+}a^\dagger_{q-}a_{q+}a_{r-}\right\}\delta_{rp} + \left\{a^\dagger_{r-}a^\dagger_{p+}a_{p-}a_{q+}\right\}\delta_{rq})$$

$$+(\left\{a^\dagger_{p+}a_{p-}a^\dagger_{q-}a_{r+}\right\}\delta_{rq} - \left\{a^\dagger_{r+}a_{p-}a^\dagger_{q-}a_{q+}\right\}\delta_{rp})$$

$$+(\left\{a^\dagger_{p+}a_{r+}\right\}\delta_{pq}\delta_{rq} - \left\{a^\dagger_{r+}a_{q+}\right\}\delta_{rp}\delta_{pq})]$$

Evaluating these sums leads to the quick realization that everything may be permuted such that the commutator vanishes.

$$[J^2, J_z] = 0$$

$$[J_z, J_\pm] = \frac{1}{2}\sum_{pq\sigma}\sigma(a^\dagger_{q\sigma}a_{q\sigma}a^\dagger_{p\pm}a_{p\mp} - a^\dagger_{p\pm}a_{p\mp}a^\dagger_{q\sigma}a_{q\sigma})$$

Here there is only one non-zero term to worry about. After contractions we have:

$$[J_z, J_\pm] = \tfrac{1}{2}\textstyle\sum_{pq}(\pm\left\{a^\dagger_{q\pm}a_{p\mp}\right\} - \mp\left\{a^\dagger_{p\pm}a_{q\mp}\right\})\delta_{pq}$$

$$= \pm\textstyle\sum_p a^\dagger_{p\pm}a_{p\mp}$$

$$= \pm J_\pm$$

Similarly there is only one relevant term for the final commutator:

$$[J_+, J_-] = \textstyle\sum_{pq}(\left\{a^\dagger_{p+}a_{q+}\right\} - \left\{a^\dagger_{p-}a_{q-}\right\})\delta_{pq}$$

$$= \textstyle\sum_{p\sigma}\sigma a^\dagger_{p\sigma}a_{p\sigma}$$

$$= 2J_z$$

And thus it is confirmed that the quasispin operators obey the proper angular momentum algebra.

b) **Re-writing the Hamiltonian**

$$\begin{aligned} H = &\quad H_0 + H_1 + H_2 \\ H_0 = &\quad \tfrac{1}{2}\varepsilon \textstyle\sum_{\sigma p} \sigma a^\dagger_{\sigma p} a_{\sigma p} \\ H_1 = &\quad \tfrac{1}{2} V \textstyle\sum_{\sigma pq} a^\dagger_{\sigma p} a^\dagger_{\sigma q} a_{-\sigma q} a_{-\sigma p} \\ H_2 = &\quad \tfrac{1}{2} W \textstyle\sum_{\sigma pq} a^\dagger_{\sigma p} a^\dagger_{-\sigma q} a_{\sigma q} a_{-\sigma p} \end{aligned}$$

It is immediately noticeable that H_0 is in the form of J_z.

$$H_0 = \varepsilon J_z$$

H_1 causes two particle transitions between levels. The initial state of both particles is different from the final states, which translates mathematically into the freedom to anti-commute any creation or annihilation operators in H_1:

$$\begin{aligned} H_1 &= \tfrac{1}{2} V \textstyle\sum_{pq\sigma} a^\dagger_{\sigma q} a_{-\sigma q} a^\dagger_{\sigma p} a_{-\sigma p} \\ &= \tfrac{1}{2} V \textstyle\sum_{\sigma} (\sum_q a^\dagger_{\sigma q} a_{-\sigma q})(\sum_p a^\dagger_{\sigma p} a_{-\sigma p}) \\ &= \tfrac{1}{2} V (J_+^2 + J_-^2) \end{aligned}$$

H_2 may exchange the spins of two particles so long as they are in opposite spin states. it is then possible that the initial and final states will have at least one similar occupied orbital. Thus we must add a delta function when we permute to separate the sums:

$$\begin{aligned} H_2 &= \tfrac{1}{2} W \textstyle\sum_{\sigma pq} (a^\dagger_{-\sigma q} a_{\sigma q} a^\dagger_{\sigma p} a_{-\sigma p} - a^\dagger_{-\sigma q} a_{-\sigma p} \delta_{pq}) \\ &= \tfrac{1}{2} W \textstyle\sum_{\sigma} (\sum_q a^\dagger_{-\sigma q} a_{\sigma q})(\sum_p a^\dagger_{\sigma p} a_{-\sigma p}) - \tfrac{1}{2} W \textstyle\sum_{\sigma p} a^\dagger_{\sigma p} a_{\sigma p} \\ &= \tfrac{1}{2} W (J_+ J_- + J_- J_+ - N) \end{aligned}$$

Here N is the number operator.

c) **Conservation of Angular Momentum**

Demonstrating that $[J^2, H] = 0$ is equivalent to demonstrating that angular momentum is conserved by this Hamiltonian. This can be shown for H_0 trivially:

$$[J^2, H_0] = \varepsilon[J^2, J_z] = 0$$

Now a bit of commutator algebra:

$$[J^2, J_+] = J_+[J_-, J_+] + [J_z^2, J_+] - [J_z, J_+]$$

$$= -2J_+J_z + [J_z, J_+]_+ - [J_z, J_+]$$

$$= [J_z, J_+] - [J_z, J_+] = 0$$

So J_+ conserves angular momentum, and it should follow that it's hermitian conjugate J_- does as well. Immediately then we see that $[J^2, H_1] = 0$ and $[J^2, H_2] = -[J^2, N]$. Obviously particle number should be conserved under a rotation of the frame of reference, so we can safely assume $[J^2, N] = 0$ and therefore $[J^2, H_2] = 0$. Thus the Hamiltonian conserves angular momentum.

$$[J^2, H] = 0$$

d) **Construction of Irreducible Representation**

Suppose we have a state defined by the eigenvalues $J = J_z = 2$, given by

$$|\Phi_{J_z=-2}\rangle = a^\dagger_{1-}a^\dagger_{2-}a^\dagger_{3-}a^\dagger_{4-}\,|0\rangle = |1-, 2-, 3-, 4-\rangle$$

We can construct the rest of the $J = 2$ multiplet through application of J_+.

Lets consider the action of J_+ on some arbitrary state:

$$J_+\,|p\sigma_p, q\sigma_q, r\sigma_r, s\sigma_s\rangle = \sum_t a^\dagger_{t+}a_{t-}a^\dagger_{p\sigma_p}a^\dagger_{q\sigma_q}a^\dagger_{r\sigma_r}a^\dagger_{s\sigma_s}$$

We can re-write the right hand side of this equation using wick's theorem. Any string of normal ordered operators, other than one composed solely of creation operators, should return zero when acting on

the vacuum state. So we will consider only contractions which remove the single annihilation operator. We may construct non-zero contractions only between a_{t-} and creation operators with $\sigma = -$. The result of this contraction is the promotion of a particle from $\sigma = -$ to $\sigma = +$.

$$\sum_t \left\{ a^\dagger_{t+} \overbrace{a_{t-} a^\dagger_{p\sigma_p}} a^\dagger_{q\sigma_q} a^\dagger_{r\sigma_r} a^\dagger_{s\sigma_s} \right\} = \left\{ a^\dagger_{p+} a^\dagger_{q\sigma_q} a^\dagger_{r\sigma_r} a^\dagger_{s\sigma_s} \right\} \delta_{\sigma_p -}$$

$$\sum_t \left\{ a^\dagger_{t+} \overbrace{a_{t-} a^\dagger_{p\sigma_p}} a^\dagger_{q\sigma_q} a^\dagger_{r\sigma_r} a^\dagger_{s\sigma_s} \right\} = - \left\{ a^\dagger_{q+} a^\dagger_{p\sigma_p} a^\dagger_{r\sigma_r} a^\dagger_{s\sigma_s} \right\} \delta_{\sigma_q -}$$

$$= \left\{ a^\dagger_{p\sigma_p} a^\dagger_{q+} a^\dagger_{r\sigma_r} a^\dagger_{s\sigma_s} \right\} \delta_{\sigma_q -}$$

$+ etc \ldots$

So then we may proceed in this way, taking care to normalize our results using the relation:

$$J_+ \left| J, J_z \right\rangle = \sqrt{J(J+1) - J_z(J_z+1)} \left| J, J_z + 1 \right\rangle$$

The $J = 2$ multiplet:

$$|2, -2\rangle = |1-, 2-, 3-, 4-\rangle$$

$$|2, -1\rangle = \tfrac{1}{2}(|1+, 2-, 3-, 4-\rangle + |1-, 2+, 3-, 4-\rangle + |1-, 2-, 3+, 4-\rangle + |1-, 2-, 3-, 4+\rangle)$$

$$|2, 0\rangle = \tfrac{1}{\sqrt{6}}(|1+, 2+, 3-, 4-\rangle + |1+, 2-, 3+, 4-\rangle + |1+, 2-, 3-, 4+\rangle + |1-, 2+, 3+, 4-\rangle + |1-, 2+, 3-, 4+\rangle + |1-, 2-, 3+, 4+\rangle)$$

$$|2, 1\rangle = \tfrac{1}{2}(|1+, 2+, 3+, 4-\rangle + |1+, 2+, 3-, 4+\rangle + |1+, 2-, 3+, 4+\rangle + |1-, 2+, 3-, 4-\rangle)$$

$$|2, 2\rangle = |1+, 2+, 3+, 4+\rangle$$

This is not particularly surprising. The problem boils down to one of combinatorics.

e) **Evaluation of the Hamiltonian**

Construction of H_0 is trivial, as J_z is a good quantum number in this basis.

$$(H_0)_{ij} = \delta_{ij}\varepsilon(J_z)_i$$

Where the states are ordered from $J_z = -2$ to $J_Z = 2$. Now H_1 should only connect states which have J_z values differing by 2. By simply applying the definitions of $J_\pm$ for the $J = 2$ case, we arrive at:

$$(H_1)_{ij} = \tfrac{V}{2}(\delta_{i(j-2)}\sqrt{(6-(J_z)_j((J_z)_j+1))(6-((J_z)_j+1)((J_z)_j+2))}$$

$$+\delta_{i(j+2)}\sqrt{(6-(J_z)_j((J_z)_j-1))(6-((J_z)_j-1)((J_z)_j-2))})$$

H_2 is diagonal, despite looking rather complicated. The number operator should return four in all cases, being as there are four particles and the interaction conserves particle number. (Equal numbers of creation and annihilation operators). Once again by application of the definitions of $J_\pm$:

$$(H_2)_{ij} = \tfrac{W}{2}\delta_{ij}((6-(J_z)_i((J_z)_i-1)) + (6-(J_z)_i((J_z)_i+1)) - 4)$$

$$= W\delta_{ij}(4-(J_z)_i^2)$$

This Hamiltonian is constructed and diagonalized using the Fortran code *Lipkin_multiplet_solve.f90*. The results for the case of

$$\varepsilon = 2, \quad V = -1/3, \quad W = -1/4$$

are as follows:

$$E = (-4.2129, -2.9861, -0.9191, 1.4861, 4.1320)$$

The ground state energy is given by $E = -4.2129$. This state exhibits a weak mixing of the $J_z = 0$ and $J_z = 2$ states with the dominant $J_z = -2$ state, which highlights the fact that interaction can bring about two-particle transitions, but not single particle transitions.

For the case of:

$$\varepsilon = 2, \quad V = -4/3, \quad W = -1$$

we find:

$$E = (-7.7512, -7.4721, -1.5559, 1.4721, 5.3070)$$

In this case the ground state is now $E = -7.7512$ and we see that it contains a mixture of the same three states. However this time the ground state is mostly composed of the $J_z = 0$ channel, while $J_z = -2$ is also present to a large extent. $J_z = 2$ is still fairly suppressed. This is clearly a result of the four-fold increase in the interaction which raises transitions between these levels.

f) **Single Particle Basis**

We may use a unitary transformation to construct a new basis

$$|\phi_{\alpha p}\rangle = \sum_{\sigma=\pm 1} C_{\alpha\sigma} |u_{\sigma p}\rangle$$

characterized by $\alpha = \pm 1$ and p. Here p is not altered by the unitary transformation because the Hamiltonian does not induce transitions between different values of p. Equivalently, we might say that the degeneracy of the states is not broken by the inclusion of the interaction. If the degeneracy is not broken, there is no reason to mix different values of p.

Consider the overlap of two states in the new basis:

$$\langle \phi_{\beta q} | \phi_{\alpha p} \rangle = \textstyle\sum_{\sigma,\sigma'} C^*_{\beta\sigma'} C_{\alpha\sigma} \langle u_{\sigma' q} | u_{\sigma p} \rangle$$

$$= \textstyle\sum_{\sigma,\sigma'} C^*_{\beta\sigma'} C_{\alpha\sigma} \delta_{\sigma\sigma'} \delta_{pq}$$

$$= \textstyle\sum_{\sigma} C^*_{\beta\sigma} C_{\alpha\sigma} = \delta_{\alpha\beta}$$

Where in the last step we have used the definition of a unitary transformation:

$$C^\dagger C = \mathbb{1}$$

Thus the new basis is orthonormal.

g) **Expectation value of the Hamiltonian**

If we consider a slater determinant given in the new basis by:

$$|\Psi\rangle = \prod_{p=1}^{4} b^\dagger_{\alpha p} |0\rangle$$

where $b^\dagger_{\alpha p}\left|0\right\rangle = \left|\phi_{\alpha p}\right\rangle$. We could rewrite this slater determinant in terms of the old basis, but it is probably easier to write the Hamiltonian in terms of the new basis via the adjoint unitary transformation:

$$\left|u_{\alpha p}\right\rangle = \sum_{\alpha=\pm 1} C^*_{\alpha\sigma}\left|\phi_{\alpha p}\right\rangle$$

We will solve for the expectation value $\left\langle\Psi\right| H \left|\Psi\right\rangle$ in pieces.

$$\left\langle\Psi\right| H_0 \left|\Psi\right\rangle = \tfrac{1}{2}\varepsilon \textstyle\sum_{r,\sigma}\sum_{\lambda,\beta}\sigma C^*_{\lambda\sigma}C_{\beta\sigma}$$

$$\times \left\langle 0\right| b_{1\alpha}b_{2\alpha}b_{3\alpha}b_{4\alpha}b^\dagger_{r\lambda}b_{r\beta}b^\dagger_{4\alpha}b^\dagger_{3\alpha}b^\dagger_{2\alpha}b^\dagger_{1\alpha}\left|0\right\rangle$$

One possible set of contractions which lead to a non-zero matrix element are:

$$\left\{ b_{1\alpha}b_{2\alpha}b_{3\alpha}b_{4\alpha}b^\dagger_{r\lambda}b_{r\beta}b^\dagger_{4\alpha}b^\dagger_{3\alpha}b^\dagger_{2\alpha}b^\dagger_{1\alpha} \right\}$$

There are four other sets of contractions which may be chosen as the quantum numbers of Ψ are fixed. Each gives the same result:

$$= \tfrac{1}{2}\varepsilon \textstyle\sum_{r,\sigma}\sum_{\lambda,\beta}\sigma C^*_{\lambda\sigma}C_{\beta\sigma}\delta_{\lambda\alpha}\delta_{\beta\alpha}\delta_{r4}$$

$$= \tfrac{1}{2}\varepsilon \textstyle\sum_{\sigma}\sigma|C_{\alpha\sigma}|^2$$

Adding these together gives:

$$\left\langle\Psi\right| H_0 \left|\Psi\right\rangle = 2\varepsilon\sum_{\sigma}\sigma|C_{\alpha\sigma}|^2$$

The two body parts of the Hamiltonian can similarly be re-written as:

$$H_1 = \tfrac{1}{2}V\textstyle\sum_{\sigma,p,q}\sum_{\beta,\gamma,\mu,\lambda} C^*_{\beta\sigma}C^*_{\gamma\sigma}C_{\mu-\sigma}C_{\lambda-\sigma}b^\dagger_{\beta p}b^\dagger_{\gamma q}b_{\mu q}b_{\lambda p}$$

$$H_2 = \tfrac{1}{2}W\textstyle\sum_{\sigma,p,q}\sum_{\beta,\gamma,\mu,\lambda} C^*_{\beta\sigma}C^*_{\gamma-\sigma}C_{\mu\sigma}C_{\lambda-\sigma}b^\dagger_{\beta p}b^\dagger_{\gamma q}b_{\mu q}b_{\lambda p}$$

$$H_{int} = \tfrac{1}{2}\textstyle\sum_{\sigma,p,q}\sum_{\beta,\gamma,\mu,\lambda} C^*_{\beta\sigma}C_{\lambda-\sigma}(VC^*_{\gamma\sigma}C_{\mu-\sigma} + WC^*_{\gamma-\sigma}C_{\mu\sigma})b^\dagger_{\beta p}b^\dagger_{\gamma q}b_{\mu q}b_{\lambda p}$$

Once again we find that there are a very limited number of sets of contractions which lead to non-zero matrix elements. Now we must

choose two particles to interact. This can be done in six different ways, and again each choice leads to the exact same result:

$$= \tfrac{1}{2} \sum_{\sigma,p,q} \sum_{\beta,\gamma,\mu,\lambda} C^*_{\beta\sigma} C_{\lambda-\sigma} (V C^*_{\gamma\sigma} C_{\mu-\sigma} + W C^*_{\gamma-\sigma} C_{\mu\sigma})$$

$$\times \delta_{\alpha\beta}\delta_{\alpha\gamma}\delta_{\alpha\mu}\delta_{\alpha\lambda}(\delta_{4p}\delta_{3q} + \delta_{3p}\delta_{4q})$$

$$= \sum_\sigma C^*_{\alpha\sigma} C_{\alpha-\sigma} (V C^*_{\alpha\sigma} C_{\alpha-\sigma} + W C^*_{\alpha-\sigma} C_{\alpha\sigma})$$

$$= \sum_\sigma [V (C^*_{\alpha\sigma})^2 (C_{\alpha-\sigma})^2 + W |C_{\alpha-\sigma}|^2 |C_{\alpha\sigma}|^2]$$

adding all terms together gives:

$$\langle \Psi | \, H_{int} \, | \Psi \rangle = 6 \sum_\sigma [V (C^*_{\alpha\sigma})^2 (C_{\alpha-\sigma})^2 + W |C_{\alpha-\sigma}|^2 |C_{\alpha\sigma}|^2]$$

and thus:

$$\langle \Psi | \, H \, | \Psi \rangle = \sum_\sigma (6[V (C^*_{\alpha\sigma})^2 (C_{\alpha-\sigma})^2 + W |C_{\alpha-\sigma}|^2 |C_{\alpha\sigma}|^2] + 2\varepsilon\sigma |C_{\alpha\sigma}|^2)$$

$$= (12[V (C^*_{\alpha\sigma=1})^2 (C_{\alpha\sigma=-1})^2 + W |C_{\alpha\sigma=1}|^2 |C_{\alpha\sigma=-1}|^2] + 2\varepsilon(|C_{\alpha\sigma=1}|^2 - |C_{\alpha\sigma=-1}|^2))$$

With the added simplification that all coefficients are real, we arrive at:

$$\langle \Psi | \, H \, | \Psi \rangle = 12(V+W)(C_{\alpha\sigma=1})^2 (C_{\alpha\sigma=-1})^2 + 2\varepsilon((C_{\alpha\sigma=1})^2 - (C_{\alpha\sigma=-1})^2)$$

h) **Calculation of the Variational Minimum**

Consider the energy functional derived in the previous section:

$$E[\Psi] = 12(V+W) C^2_{\alpha\sigma=1} C^2_{\alpha\sigma=-1} + 2\varepsilon (C^2_{\alpha\sigma=1} - C^2_{\alpha\sigma=-1})$$

Noting the orthonormality of the unitary transformation C, we may re-write this as:

$$E[\Psi] = 12(V+W) C^2_{\alpha\sigma=1} (1 - C^2_{\alpha\sigma=1}) + 2\varepsilon (2C^2_{\alpha\sigma=1} - 1)$$

$$= 12(V+W)(C^2_{\alpha\sigma=1} - C^4_{\alpha\sigma=1}) + 2\varepsilon (2C^2_{\alpha\sigma=1} - 1)$$

Minimizing with respect to $C_{\alpha 1}$:

$$\frac{\partial E[\Psi]}{\partial C_{\alpha 1}} = 0 = 12(V+W)(2C_{\alpha\sigma=1} - 4C^3_{\alpha\sigma=1}) + 8\varepsilon C_{\alpha\sigma=1}$$

$$\Rightarrow 3(V+W)(1 - 2C^2_{\alpha\sigma=1}) + \varepsilon = 0$$

$$\Rightarrow 2C^2_{\alpha\sigma=1} = \frac{\varepsilon}{3(V+W)} - 1$$

$$\Rightarrow C^2_{\alpha\sigma=1} = \frac{1}{2}(\frac{\varepsilon}{3(V+W)} + 1)$$

Note here that $C_{\alpha\sigma=1} = 0$ is also a extrema in the functional, which corresponds with no change of basis. For an attractive interaction, i.e. $(V+W) < 0$, the condition of real coefficients C applies the constraint that

$$\frac{\varepsilon}{3(V+W)} + 1 < 0$$

or:

$$\frac{\varepsilon}{3} < -(V+W)$$

For a repulsive interaction, i.e. $(V+W) > 0$, our coefficients must not be greater than unity.

$$\frac{\varepsilon}{3(V+W)} + 1 < 2$$

or

$$\frac{\varepsilon}{3} < (V+W)$$

For a repulsive interaction, the local minimum is the Lipkin basis given by $C = 0$. However this is a very poor approximation of the true energy.

For an attractive interaction, the variational minimum is found at:

$$C_{\alpha+} = \pm\sqrt{\frac{1}{2}(\frac{\varepsilon}{3(V+W)} + 1)}$$

and

$$C_{\alpha-} = \pm\sqrt{\frac{1}{2}(1 - \frac{\varepsilon}{3(V+W)})}$$

The unitary transformation C should be the transformation from the Lipkin basis to the Hartree Fock basis.

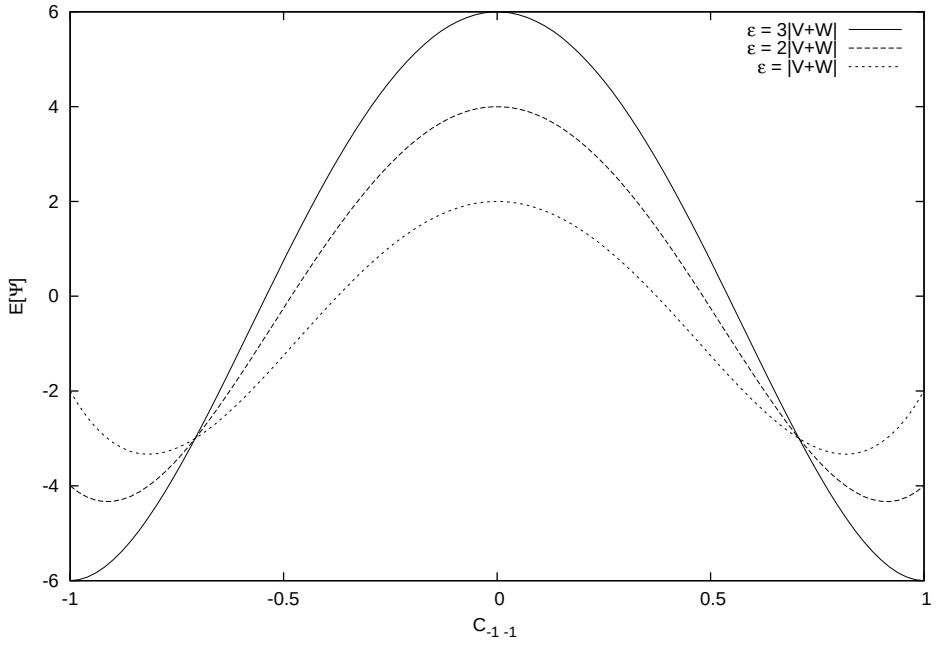

Figure 1: Energy functional for varying attractive interaction strengths

Consider our results from the exact diagonalization:
Case 1:

$$\varepsilon = 2, \quad V = -1/3, \quad W = -1/4 \quad E = -4.2129$$

Case 1 violates our condition for a HF minimum energy. The best possible energy is obtained by using the Lipkin Basis, i.e. $C_{\alpha-} = 1$. The energy functional returns $E_{HF} = E_{LIP} = -4.0000$ in this case, which leaves us with roughly 5% error. This isn't a terrible approximation.

Case 2:

$$\varepsilon = 2, \quad V = -4/3, \quad W = -1 \quad E = -7.7512$$

This case meets our condition for a minimum. The optimized basis exists at $C_{\alpha-} = .8018$, and gives an energy of $E_{HF} = -7.5714$, which is 2% error. The Lipkin Basis gives $E_{LIP} = -4.0000$, which is obviously a very poor approximation to the true ground state. Here we see the advantage of calculations in the HF basis; we have much smaller correlation energies, so higher order methods do not need to work as hard to converge.

i) **Numerical Hartree Fock Calculation**

We may verify the results of the previous section through a self-consistent diagonalization of the fock matrix:

$$F_{\alpha\beta} = \langle\alpha|H_0|\beta\rangle + \sum_{j=1}^{A}\sum_{\gamma\delta} C^*_{j\gamma}C_{j\delta}\langle\alpha\gamma|H_1 + H_2|\beta\delta\rangle_{AS}.$$

where j refers to the Hartree Fock basis and α refers to the Lipkin basis. More accurately we may write:

$$F_{\alpha\beta} = \langle p_\alpha\sigma_\alpha|\, H_0\, |p_\beta\sigma_\beta\rangle + \sum_{p_j=1}^{4}\sum_{\sigma_\gamma\sigma_\lambda} C_\gamma C_\lambda\, \langle p_\alpha\sigma_\alpha p_j\sigma_\gamma|\, H_1 + H_2\, |p_\beta\sigma_\beta p_j\sigma_\lambda\rangle$$

where we have made use of the fact that different p values do not mix. This allows us to ignore p in the coefficients. Because the HF ground state should reside within one orbital, (degeneracy is still four), we may only include one index on the coefficients, referring to an orbital σ in the Lipkin basis.

matrix elements of use:

$$\langle p_\alpha \sigma_\alpha | \, H_0 \, | p_\beta \sigma_\beta \rangle = \tfrac{1}{2} \varepsilon \sigma_\alpha \delta_{p_\alpha p_\beta} \delta_{\sigma_\alpha \sigma_\beta}$$

$$\langle p_\alpha \sigma_\alpha p_j \sigma_\gamma | \, H_1 \, | p_\beta \sigma_\beta p_j \sigma_\lambda \rangle = V(\delta_{p_\alpha p_\beta} - \delta_{p_\alpha p_j} \delta_{p_\beta p_j}) \delta_{\sigma_\alpha - \sigma_\beta} \delta_{\sigma_\alpha \sigma_\gamma} \delta_{\sigma_\alpha - \sigma_\lambda}$$

$$\langle p_\alpha \sigma_\alpha p_j \sigma_\gamma | \, H_2 \, | p_\beta \sigma_\beta p_j \sigma_\lambda \rangle = W \delta_{\sigma_\alpha - \sigma_\gamma} \delta_{\sigma_\beta - \sigma_\lambda} (\delta_{p_\alpha p_\beta} \delta_{\sigma_\alpha - \sigma_\beta} - \delta_{p_\alpha p_j} \delta_{p_\beta p_j} \delta_{\sigma_\alpha \sigma_\beta})$$

Applying these to the definition of the fock matrix gives:

$$F_{\alpha\beta} = \delta_{p_\alpha p_\beta} [\delta_{p_\alpha p_\beta} (\frac{1}{2} \varepsilon \sigma_\alpha - W (C_{(-\alpha)})^2) + \delta_{p_\alpha p_\beta} ((3V + 4W) C_\alpha C_{(-\alpha)})]$$

The common $\delta_{p_\alpha p_\beta}$ term tells us that F is block diagonal, and as a result, we can reduce the scale of the problem from 8×8 to 2×2. We must start with a guess for C, diagonalize, and then re-calculate F, with our new C, until nothing changes any more. This will mark HF convergence. The Lipkin model offers the peculiar case of $C = \mathbb{1}$ being a stationary point in the energy functional. This is not necessarily the minimum, so we must perturb our initial conditions from this traditional guess, or we will not be able to move along the functional.

Once we are converged, we must calculate our HF energy.

$$E_{HF} = \sum_{j=1}^{N} \epsilon_j - \frac{1}{2} \sum_{i,j=1}^{N} \langle ij | \, V \, | ij \rangle$$

our conserved degeneracy also alters this expression:

$$E_{HF} = 4\epsilon_- - 12(V + W) C_- C_+$$

The code *Lipkin_HF.f90* solves this problem, and reproduces the results of the previous section. Our HF eigenvectors are exactly those which minimize the energy functional from the previous section.