Exercises PHY981 Spring 2014

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The exercises are available at the beginning of the week and are to be handed in at the lecture the week thereafter on Wednesdays. This can be done electronically (as a pdf or postscript file) by email to hjensen@nscl.msu.edu or at the lecture. You can also send in a scanned version of your answer. The Friday lectures will be used to discuss the weekly exercises. The exercises will be graded and count 10% of the final mark.

Exercise 3

We will now consider a simple three-level problem, depicted in the figure below. This is our first and very simple model of a possible many-nucleon (or just fermion) problem and the shell-model. The single-particle states are labelled by the quantum number p and can accomodate up to two single particles, viz., every single-particle state is doubly degenerate (you could think of this as one state having spin up and the other spin down). We let the spacing between the doubly degenerate single-particle states be constant, with value d. The first state has energy d. There are only three available single-particle states, $p = 1$, $p = 2$ and $p = 3$, as illustrated in the figure.

a) How many two-particle Slater determinants can we construct in this space?

There should be six two-particle Slater determinants for this system,
$|1,1\rangle, |1,2\rangle, |2,2\rangle, |2,3\rangle, |3,3\rangle, |1,3\rangle$
If we don't consider spin then only $|1,2\rangle, |2,3\rangle, |1,3\rangle$ **can exist due to the pauli principle.**

b) We limit ourselves to a system with only the two lowest single-particle orbits and two particles, $p = 1$ and $p = 2$. We assume that we can write the Hamiltonian as

$$\hat{H} = \hat{H}_0 + \hat{H}_I,$$

and that the onebody part of the Hamiltonian with single-particle operator $\hat{h}_0$ has the property

$$\hat{h}_0 \psi_{p\sigma} = p \times d\psi_{p\sigma},$$

where we have added a spin quantum number σ. We assume also that the only two-particle states that can exist are those where two particles are in the same state p, as shown by the two possibilities to the left in the figure. The two-particle matrix elements of $\hat{H}_I$ have all a constant value, $-g$. Show then that the Hamiltonian matrix can be written as

$$\begin{pmatrix} 2d-g & -g \\ -g & 4d-g \end{pmatrix},$$

and find the eigenvalues and eigenvectors.

We have that $\hat{H}_0 = \sum_i^N \hat{h}_0(x_i)$**. Casting it on each of the states we are considering, we can write this as**

$$\begin{pmatrix} \langle\Phi_0|(h_1+h_2)|\Phi_0\rangle & \langle\Phi_0|(h_1+h_2)|\Phi_1\rangle \\ \langle\Phi_1|(h_1+h_2)|\Phi_0\rangle & \langle\Phi_1|(h_1+h_2)|\Phi_1\rangle \end{pmatrix}$$

$$\begin{pmatrix} \langle 12-21|(h_1+h_2)|12-21\rangle & \langle 12-21|(h_1+h_2)|21-12\rangle \\ \langle 21-12|(h_1+h_2)|12-21\rangle & \langle 21-12|(h_1+h_2)|21-12\rangle \end{pmatrix}$$

with $h_i = h_0(x_i)$**. From homework one using the onebody properites this is just**

$$\begin{pmatrix} d+d & 0 \\ 0 & 2d+2d \end{pmatrix} = \begin{pmatrix} 2d & 0 \\ 0 & 4d \end{pmatrix}.$$

Adding in the given $\hat{H}_I$ **we have**

$$\begin{pmatrix} 2d & 0 \\ 0 & 4d \end{pmatrix} + -g \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} 2d-g & -g \\ -g & 4d-g \end{pmatrix}.$$

To find the eigenvalues I will diagonalize the matrix using the characteristic equation $|A - \lambda I| = 0$**. This then yields the equation**

$$(2d - g - \lambda)(4d - g - \lambda) - g^2 = 0.$$

Thus the eigenvalues are $\lambda_\pm = 3d - g \pm \sqrt{g^2 + d^2}$ with

$$\begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}.$$

And after solving the eigenvalue problems,

$$\begin{pmatrix} 2d-g & -g \\ -g & 4d-g \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda_\pm \begin{pmatrix} a \\ b \end{pmatrix}$$

I find the eigenvectors to be,

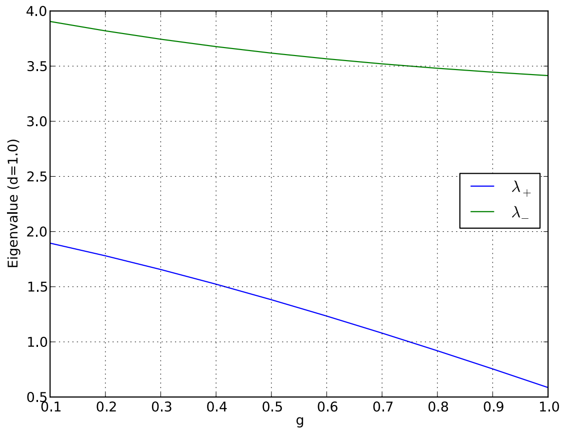
$$\begin{pmatrix} d \mp \sqrt{g^2+d^2} \\ g \end{pmatrix}.$$

What is mixing of the state with two particles in $p = 2$ to the wave function with two-particles in $p = 1$? Discuss your results in terms of a linear combination of Slater determinants.

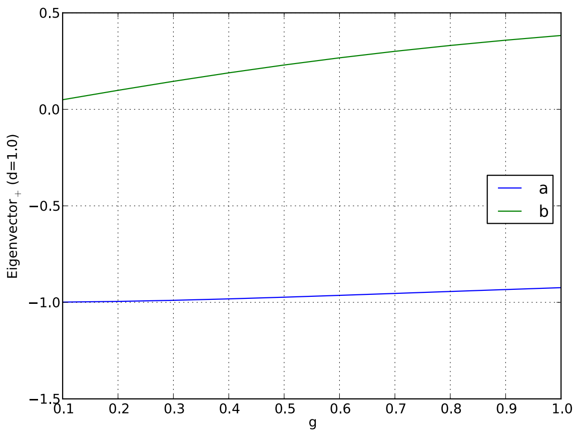
The actual wave functions for the assumed hamiltonian take the form

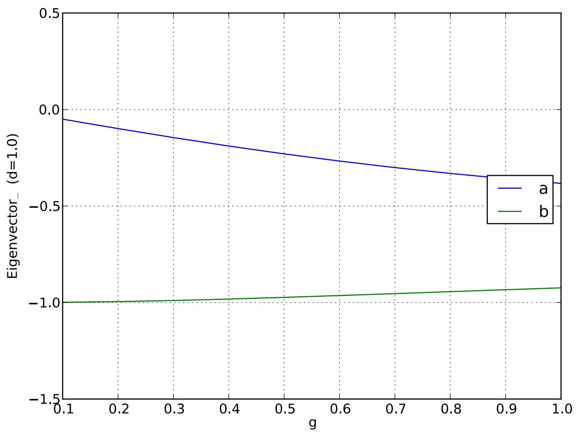
$$|\Psi_{+}\rangle = g * \Phi_1 + (d - \sqrt{g^2 + d^2})\,|\Phi_0\rangle$$
$$|\Psi_{-}\rangle = g * \Phi_1 + (d + \sqrt{g^2 + d^2})\,|\Phi_0\rangle$$

For d=1.0 I vary g from 0.1 to 1.0, and plot the eigenvalues vs g,



The eigenvalues appear to vary significantly with stronger mixing. Below are the components of each corresponding eigenvector, where a is the coeficient in front of the SD Φ_0, belonging to the basis of $\hat{H}_0$, in the expansion of the eigenvectors in terms of our old basis. b is the coeficient of Φ_1





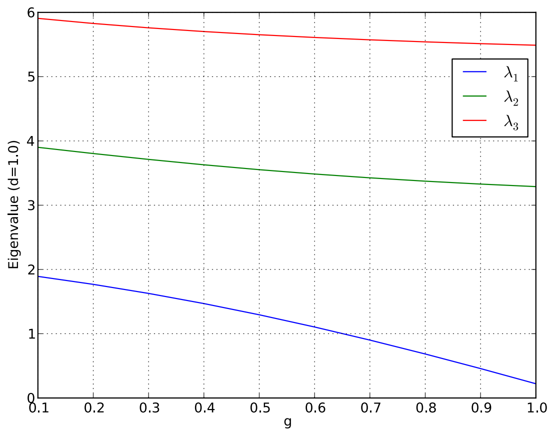
The lower component "b" varies linearly with g, while "a" varies nonlinearly away from 0 for the zero mixing case.

c) Add the possibility that the two particles can be in the state with $p = 3$ as well and find the Hamiltonian matrix, the eigenvalues and the eigenvectors. We still insist that we only have two-particle states composed of two particles being in the same level p. You can diagonalize numerically your 3×3 matrix.

Including the third level we have our original 2x2 matrix as a subblock, with an additional component from the onebody part of the Hamiltonian, such that

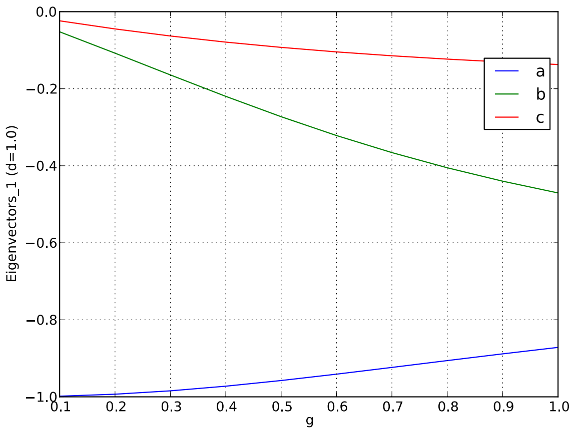
$$\hat{H} = \begin{pmatrix} 2d - g & -g & -g \\ -g & 4d - g & -g \\ -g & -g & 6d - g \end{pmatrix}$$

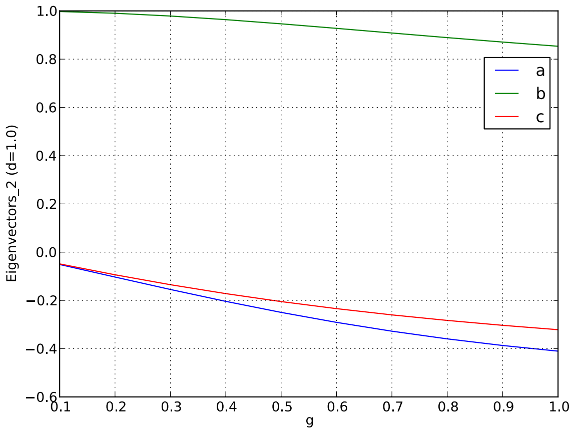
The eigenvalues as a function of the interaction strength (g) are again similar,

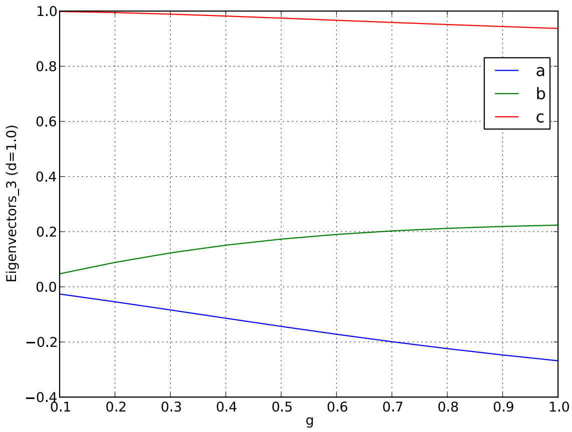


Here we see the eigenvalues of the 2x2 subblock are reproduced but with an additional eigenvalue of 6d which is only slightly mixed by the interaction hamiltonian. Plotting again numerical solutions for the eigenvector componets for each of the three eigen-

values we have,







This simple model catches several birds with a stone. It demonstrates how we can build linear combinations of Slater determinants and interpret these as different admixtures to a given state. It represents also the way we are going to interpret these contributions. The two-particle states above $p = 1$ will be interpreted as excitations from the ground state configuration, $p = 1$ here. The reliability of this ansatz for the ground state, with two particles in $p = 1$, depends on the strength of the interaction g and the single-particle spacing d. Finally, this model is a simple schematic ansatz for studies of pairing correlations and thereby superfluidity/superconductivity in fermionic systems.

Exercise 4

This exercise consists of two parts. The first part serves to convince you about the relation between two different single-particle bases, where one could be our new Hartree-Fock basis and the other a harmonic oscillator basis.

a) Consider a Slater determinant built up of single-particle orbitals ψ_λ, with $\lambda = 1, 2, \dots, A$.

The unitary transformation

$$\psi_a = \sum_\lambda C_{a\lambda}\phi_\lambda,$$

brings us into the new basis. The new basis has quantum numbers $a = 1, 2, \dots, A$. Show that the new basis is orthonormal. Show that the new Slater determinant constructed from the new single-particle wave functions can be written as the determinant based on the previous basis and the determinant of the matrix C. Show that the old and the new Slater determinants are equal up to a complex constant with absolute value unity. (Hint, C is a unitary matrix).

b) The last exercise deals with deriving the Hartree-Fock equations. Consider the Slater determinant

$$\Phi_0 = \frac{1}{\sqrt{A!}}\sum_p (-)^p P \prod_{i=1}^{A} \psi_{\alpha_i}(x_i).$$

How would you define a small variation in this function, that is

$$\delta\Phi_0 = ?$$

Show thereafter that the variation of the expectation value of the energy can be written as

$$\langle \delta\Phi_0 | \sum_{i=1}^{A} \{t(x_i) + u(x_i)\} + \frac{1}{2}\sum_{i\neq j=1}^{A} v(x_i, x_j) | \Phi_0 \rangle =$$

$$\sum_{i=1}^{A} \langle \delta\psi_{\alpha_i} | t + u | \phi_{\alpha_i} \rangle +$$

$$\sum_{i\neq j=1}^{N} \left\{ \langle \delta\psi_{\alpha_i}\psi_{\alpha_j} | v | \psi_{\alpha_i}\psi_{\alpha_j} \rangle - \langle \delta\psi_{\alpha_i}\psi_{\alpha_j} | v | \psi_{\alpha_j}\psi_{\alpha_i} \rangle \right\}$$

#4 CONSIDER A SD BUILT FROM SP STATES ψ_λ W/ $\lambda = 1, 2, \dots, A$

A UNITARY TRANS. $\psi_a = \sum_\lambda C_{a\lambda} \varphi_\lambda$ FORMS A NEW BASIS.

ORTHONORMALITY OF NEW BASIS:

$$\langle \psi_a | \psi_b \rangle = \left\langle \sum_{\lambda'} C_{a\lambda'} \varphi_{\lambda'} \middle| \sum_{\lambda} C_{b\lambda} \varphi_\lambda \right\rangle$$

$$= \sum_{\lambda\lambda'} C^*_{a\lambda'} C_{b\lambda} \langle \varphi_{\lambda'} | \varphi_\lambda \rangle$$

$$= \sum_{\lambda\lambda'} C^*_{a\lambda'} C_{b\lambda} \delta_{\lambda\lambda'}$$

$$= \hat{C}_a^* \cdot \hat{C}_b = \delta_{ab} \quad \text{B/C OF UNITARITY.}$$

ANOTHER WAY TO WRITE THE UNITARY TRANS. ABOVE IS

$$\psi_a = \vec{C_a} \cdot \vec{\varphi} \qquad \text{AND FOR MANY STATES} \qquad \Psi = C \varphi$$

$$\Rightarrow \begin{pmatrix} \psi_1(x_1) & \psi_2(x_1) & \cdots & \psi_a(x_1) \\ \psi_1(x_2) & \vdots & & \vdots \\ \vdots & & \ddots & \\ \psi_1(x_A) & & & \end{pmatrix} = \overleftarrow{\overline{C}} \begin{pmatrix} \varphi_1(x_1) & \varphi_2(x_1) & \cdots & \varphi_a(x_1) \\ \varphi_1(x_2) & \vdots & & \vdots \\ \vdots & & \ddots & \\ \varphi_1(x_A) & & & \end{pmatrix}$$

SINCE $\Psi = \frac{1}{\sqrt{A!}} \det(\psi) = \frac{1}{\sqrt{A!}} \det(C \cdot \varphi)$ WE HAVE THAT

$$\boxed{\Psi = \det(C)\, \Phi}$$

BECAUSE $\det(AB) = \det(A)\det(B)$

#4 CONT.

TAKING THE SD DEF TO TSE $\Phi_0 = \frac{1}{\sqrt{A!}} \sum_P (-)^P P \prod_i^A \psi_{\alpha_i}(x_i)$, WE HAVE

$$\delta\Phi_0 = \sum_i \frac{\partial \Phi_0}{\partial \psi_{\alpha_i}} \delta\psi_{\alpha_i} = \frac{1}{\sqrt{A!}} \sum_P (-)^P P \sum_i^A \frac{\partial}{\partial \psi_{\alpha_i}} \left(\prod_j^A \psi_{\alpha_j}(x_j) \right) \delta\psi_{\alpha_i}$$

$$\delta\Phi_0 = \frac{1}{\sqrt{A!}} \sum_P (-)^P P \sum_i^A \prod_j^A \frac{\psi_{\alpha_j}(x_j)\,\delta\psi_{\alpha_i}(x_i)}{\psi_{\alpha_i}(x_i)}$$

VARYING $\langle H \rangle$ WE HAVE $\langle \delta\Phi_0 | \underbrace{\sum_{i=1}^A \{t(x_i) + u(x_i)\}}_{1} + \underbrace{\frac{1}{2}\sum_{i \neq j = 1}^A v(x_i, x_j)}_{2} | \Phi_0 \rangle$

1 ONE BODY

$$\frac{1}{A!} \left\langle \sum_P (-)^P P \sum_i^A \prod_j^A \frac{\psi_{\alpha_j}\delta\psi_{\alpha_i}}{\psi_{\alpha_i}} \middle| \sum_n t_n + u_n \middle| \sum_P (-)^P P \prod_i^A \psi_{\alpha_i} \right\rangle$$

$A^2 = A = (A! \ldots$

$$= \frac{A!}{A!} \sum_n \left\langle \sum_i \frac{\delta\psi_{\alpha_i}}{\psi_{\alpha_i}} \prod_j^A \psi_{\alpha_j} \middle| t_n + u_n \middle| \prod_i^A \psi_{\alpha_i} \right\rangle$$

FROM HW 1
$\langle ij | \hat{h}_i | ij \rangle = \langle i | \hat{h} | i \rangle$

$$= \sum_i \langle \delta\psi_{\alpha_i} | t_i + u_i | \psi_{\alpha_i} \rangle \prod_{\substack{j=1 \\ j \neq i}}^A \langle \psi_{\alpha_j} | \psi_{\alpha_j} \rangle$$

$$= \sum_i \langle \delta\psi_{\alpha_i} | t(x_i) + u(x_i) | \psi_{\alpha_i} \rangle$$

2 TWO BODY

$$\frac{1}{2A!} \left\langle \sum_P (-)^P P \sum_i^A \prod_j^A \frac{\psi_{\alpha_j}\delta\psi_{\alpha_i}}{\psi_{\alpha_i}} \middle| \sum_{k \neq l = 1} v_{kl} \middle| \sum_P (-)^P P \prod_i^A \psi_{\alpha_i} \right\rangle$$

V CAN ONLY ACT ON TWO STATES, THE OTHERS INTEGR OUT! SIMILAR TO $\langle ij | h_i | ij \rangle = \langle i | h_i$ FOR THE ONE BODY CASE

$$= \frac{1}{2} \sum_{k,l} \langle \delta\psi_k \psi_l - \delta\psi_l \psi_k | V_{kl} | \psi_k \psi_l - \psi_l \psi_k \rangle$$

$$= \langle \delta\psi_k \psi_l | V_{kl} | \psi_k \psi_l \rangle_{AS}$$ JUST AS IN HW 1.