

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 accommodate 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 properties 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

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

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,

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

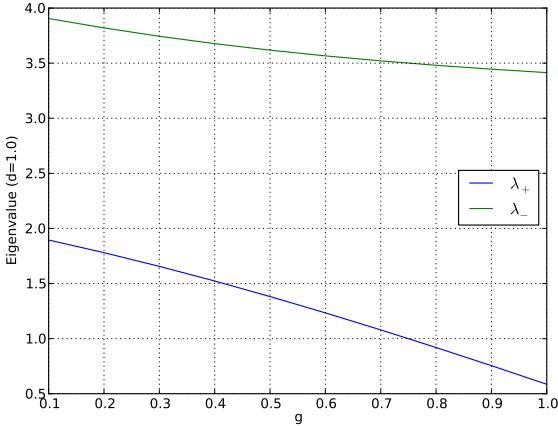
What is mixing of the state with two particles in $p = 2$ to the wave function with two-particles in $p = 1$? Discuss your results in terms of a linear combination of Slater determinants.

The actual wave functions for the assumed hamiltonian take the form

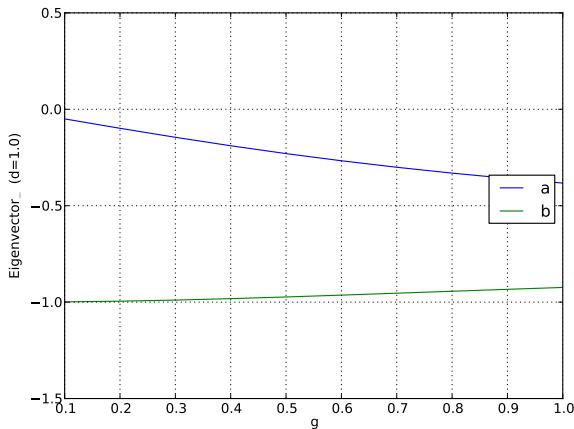
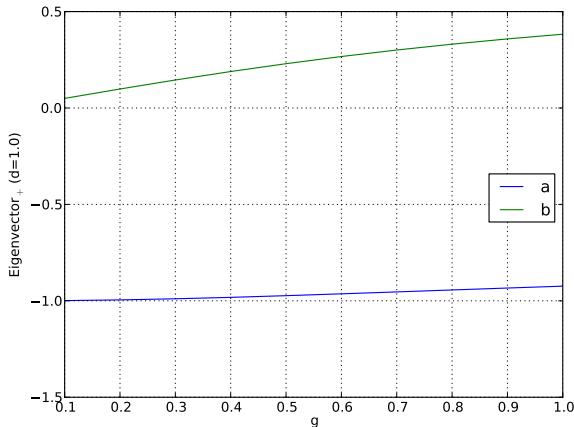
$$|\Psi_+\rangle = g * \Phi_1 + (d - \sqrt{g^2 + d^2}) |\Phi_0\rangle$$

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

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 coefficient 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 coefficient of Φ_1



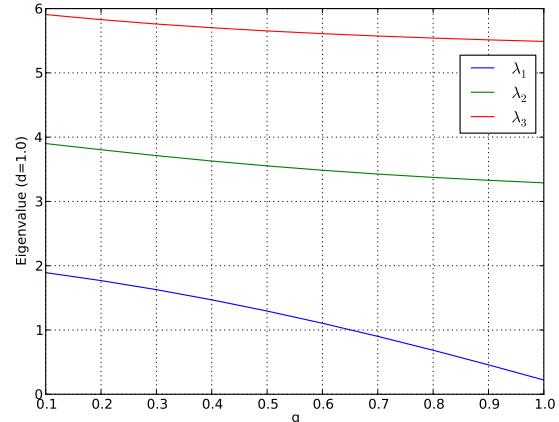
The lower component “b” varies linearly with g , while “a” varies nonlinearly away from 0 for the zero mixing case.

- 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 2×2 matrix as a subblock, with an additional component from the onebody part of the Hamiltonian, such that

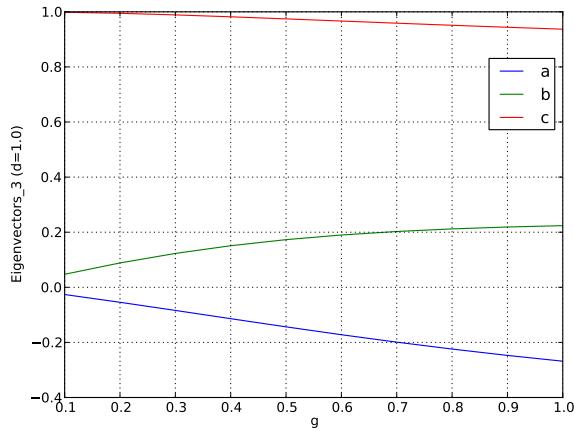
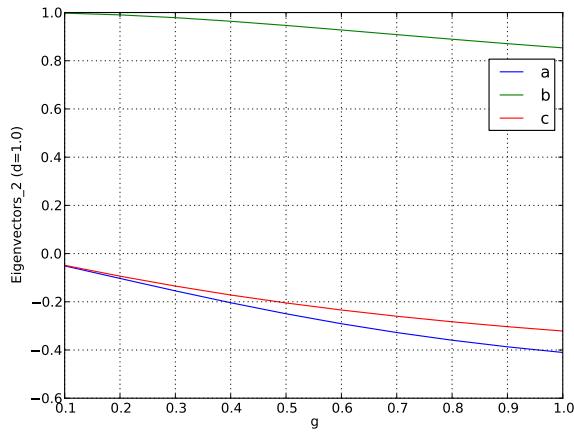
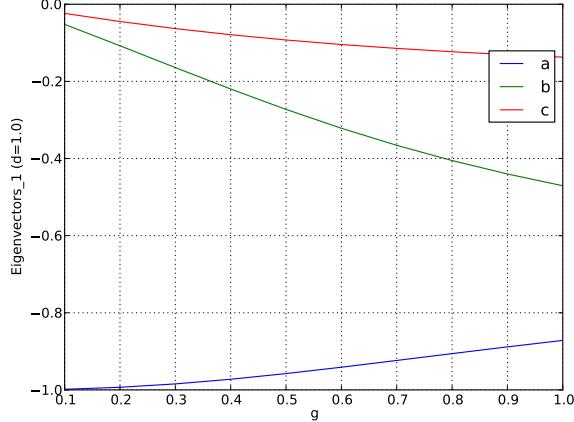
$$\hat{H} = \begin{pmatrix} 2d - g & -g & -g \\ -g & 4d - g & -g \\ -g & -g & 6d - g \end{pmatrix}$$

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



Here we see the eigenvalues of the 2×2 sub-block 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 components 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

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

$$\begin{aligned} & \sum_{i=1}^A \langle \delta\psi_{\alpha_i} | t + u | \phi_{\alpha_i} \rangle + \\ & \sum_{i \neq j=1}^N \{ \langle \delta\psi_{\alpha_i} \psi_{\alpha_j} | v | \psi_{\alpha_i} \psi_{\alpha_j} \rangle - \langle \delta\psi_{\alpha_i} \psi_{\alpha_j} | v | \psi_{\alpha_j} \psi_{\alpha_i} \rangle \} \end{aligned}$$

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

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

ORTHONORMALITY OF NEW BASIS:

$$\begin{aligned}\langle \psi_a | \psi_b \rangle &= \left\langle \sum_{\lambda'} c_{a\lambda'} \phi_{\lambda'} \middle| \sum_{\lambda} c_{b\lambda} \phi_{\lambda} \right\rangle \\ &= \sum_{\lambda \lambda'} c_{a\lambda'}^* c_{b\lambda} \langle \phi_{\lambda'} | \phi_{\lambda} \rangle \\ &= \sum_{\lambda \lambda'} c_{a\lambda'}^* c_{b\lambda} \delta_{\lambda \lambda'} \\ &= \hat{C}_a^* \cdot \hat{C}_b = \delta_{ab} \text{ B/C OF UNITARITY.}\end{aligned}$$

ANOTHER WAY TO WRITE THE UNITARY TRANS. ABOVE IS

$$\psi_a = \vec{c}_a \cdot \vec{\phi} \quad \text{AND FOR MANY STATES} \quad \Psi = C \phi$$

$$\Rightarrow \begin{pmatrix} \psi_1(x_1) & \psi_1(x_2) & \dots & \psi_1(x_A) \\ \psi_2(x_1) & \vdots & \ddots & \vdots \\ \vdots & & & \vdots \\ \psi_A(x_1) & & & \psi_A(x_A) \end{pmatrix} = \overline{\vec{C}} \begin{pmatrix} \phi_1(x_1) & \phi_2(x_1) & \dots & \phi_A(x_1) \\ \phi_1(x_2) & \vdots & \ddots & \vdots \\ \vdots & & & \vdots \\ \phi_1(x_A) & & & \phi_A(x_A) \end{pmatrix}$$

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

$$\boxed{\Psi = \det(C) \mathbb{I}}$$

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

#4 cont.

TAKING THE SD DEF TO USE $\Psi_0 = \frac{1}{\sqrt{A!}} \sum_p (-)^p P \prod_i^A \psi_{\alpha_i}(x_i)$, WE HAVE

$$\delta \Psi_0 = \sum_i \frac{\partial \Psi_0}{\partial \psi_{\alpha_i}} \delta \psi_{\alpha_i} = \frac{1}{\sqrt{A!}} \sum_p (-)^p P \sum_i^A \frac{\partial}{\partial \psi_{\alpha_i}} \left(\prod_j^A \psi_{\alpha_j}(x_j) \right) \delta \psi_{\alpha_i}$$

$$\delta \Psi_0 = \frac{1}{\sqrt{A!}} \sum_p (-)^p P \sum_i^A \prod_j^A \frac{\psi_{\alpha_j}(x_j) \delta \psi_{\alpha_i}(x_i)}{\psi_{\alpha_i}(x_i)} //$$

VARYING $\langle H \rangle$ WE HAVE $\langle \delta \Psi_0 | \sum_{i=1}^A \{t(x_i) + u(x_i)\} + \frac{1}{2} \sum_{i \neq j=1}^A v(x_i, x_j) | \Psi_0 \rangle$

①

②

① ONE BODY

$$\begin{aligned} & \frac{1}{A!} \left\langle \sum_p (-)^p P \sum_i^A \prod_j^A \frac{\psi_{\alpha_j} \delta \psi_{\alpha_i}}{\psi_{\alpha_i}} | \sum_n t_n + u_n | \sum_p (-)^p P \prod_i^A \psi_{\alpha_i} \right\rangle \quad A^2 = A = (A - \\ &= \frac{A!}{A!} \sum_n \left\langle \sum_i \frac{\delta \psi_{\alpha_i}}{\psi_{\alpha_i}} \prod_j^A \psi_{\alpha_j} | t_n + u_n | \prod_i^A \psi_{\alpha_i} \right\rangle \quad \text{From HW 1} \\ & \quad \langle z_i | h_i | z_i \rangle = \langle i | h_i | i \rangle \\ &= \sum_i \langle \delta \psi_{\alpha_i} | t_i + u_i | \psi_{\alpha_i} \rangle \prod_{\substack{j=1 \\ j \neq i}}^A \langle \psi_{\alpha_j} | \psi_{\alpha_j} \rangle \\ &= \sum_i \langle \delta \psi_{\alpha_i} | t(x_i) + u(x_i) | \psi_{\alpha_i} \rangle \end{aligned}$$

② TWO BODY

$$\begin{aligned} & \frac{1}{2A!} \left\langle \sum_p (-)^p P \sum_i^A \prod_j^A \frac{\psi_{\alpha_j} \delta \psi_{\alpha_i}}{\psi_{\alpha_i}} | \sum_{k \neq l=1}^A v_{kl} | \sum_p (-)^p P \prod_i^A \psi_{\alpha_i} \right\rangle \quad V \text{ CAN ONLY ACT ON TWO} \\ &= \frac{1}{2} \sum_{k,l} \langle \delta \psi_k \psi_l - \delta \psi_l \psi_k | v_{kl} | \psi_k \psi_l - \psi_l \psi_k \rangle \quad \text{STATES, THE OTHERS INTEGRAL OUT! SIMILAR TO } \langle i j | h_i | i j \rangle = \langle i j | h_j | i j \rangle \\ &= \langle \delta \psi_k \psi_l | v_{kl} | \psi_k \psi_l \rangle_{AS} \quad \text{JUST AS IN HW 1.} \end{aligned}$$