### Midterm exam fall 2012 FYS-KJM4480/9480, deadline Monday October 15 at 12pm (noon). It counts 30% of the final mark. Use your student number only.

# Hand in an individual answer only with your student number. The box for handing in the answer is at the reception of the Department of Physics (see letter box marked fys-kjm4480/9480.)

This midterm exam is based partly on exercise 13 Fall 2012, parts a), b) and c). The system is however that of electrons confined in two dimensions by a harmonic oscillator potential, normally called quantum dots. Strongly confined electrons offer a wide variety of complex and subtle phenomena which pose severe challenges to existing many-body methods. Quantum dots in particular, that is, electrons confined in semiconducting heterostructures, exhibit, due to their small size, discrete quantum levels. Small confined systems, such as quantum dots, have become very popular for experimental study. Beyond their possible relevance for nanotechnology, they are highly tunable in experiments and introduce level quantization and quantum interference in a controlled way. The possibility to manufacture systems with a tailored electronic structure, may improve electrical or optical properties of materials, a reason why quantum dots are good candidates as components in quantum computers, optimized solar cells, laser technology and medical imaging, to name a few.

We will consider a system of two and six electrons. These represent both so-called closed shell systems. The numbers two and six, together with N = 12, N = 20, N = 30, N = 42, etc define magic numbers for quantum dots in much the same way as we have for atoms and nuclei.

Our Hilbert space will be defined by the three lowest harmonic oscillator single-particle states. In total, when we add spin, we have 12 single-particle states. Without spin, the spatial coordinates are represented by six single-particle states (see below).

Ou Hamiltonian for N electrons takes the following form

$$\hat{H} = \sum_{i=1}^{N} t(x_i) + \sum_{i=1}^{N} \frac{1}{2} m_e \omega^2 r_i^2 + \sum_{i< j}^{N} \frac{ke^2}{r_{ij}}$$

with k = 1.44 eVnm. Throughout this midterm exam we will use atomic units, this means that  $\hbar = c = e = m_e = 1$ . The constant k becomes also equal 1. We will also set the oscillator frequency  $\omega$  to one.

We can rewrite our Hamiltonians as

$$\hat{H} = \hat{H}_0 + \hat{H}_I = \sum_{i=1}^N \hat{h}_0(x_i) + \sum_{i< j}^N \frac{1}{r_{ij}},\tag{1}$$

where we have defined  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$  and  $\hat{h}_0(x_i) = \hat{t}(x_i) + \frac{r_i^2}{2}$  The variable x contains both the spatial coordinates and the spin values. The first term of Eq. (1),  $H_0$ , is the sum of the N one-body Hamiltonians  $\hat{h}_0$ . Each individual Hamiltonian  $\hat{h}_0$  contains the kinetic energy operator of an electron and its harmonic oscillator potential. The second term,  $H_I$ , is the sum of the N(N-1)/2 two-body interactions between each pair of electrons. Note that the double sum carries a restriction i < j.

As basis functions for our calculations we will use harmonic oscillator functions for the single-particle functions. This means the onebody operator is diagonal in this basis for states i, j with quantum numbers  $nm_lm_s$ . The expectation value is

$$\langle i|\hat{h}_0|j\rangle = e_i\delta_{i,j} = e_{n_im_{l_i}} = \hbar\omega(2n_i + |m_{l_i}| + 1).$$

The quantum numbers  $n_i$  refers to the number of nodes of the wave function, while the quantum numbers  $m_{l_i}$  represent the projection of the orbital momentum. Observe that this expectation value is independent of spin. Throughout this midterm exam we employ  $\hbar\omega = 1$  a.u.

In the calculations you will need the Coulomb interaction with matrix elements involving the orbits we discussed above. The single-particle functions are given by the so-called generalized Laguerre polynomials (with  $\alpha = \sqrt{m\omega/\hbar}$ )

$$\psi_{nm_l}(r,\theta) = \alpha \exp(im\theta) \sqrt{\frac{n!}{\pi(n+|m|)!}} (\alpha r)^{|m|} L_n^{|m|} (\alpha^2 r^2)) \exp(-\alpha^2 r^2/2),$$
(2)

with eigenenergy  $\hbar\omega(2n+|m|+1)$ . Here  $L_n^{|m|}$  are the so-called Laguerre polynomials. For the system we will study, we need only  $L_0^{|m|}(x) = 1$  and  $L_1^0(x) = -x + 1$ . These functions can then be used to compute the integral that the define the two-body matrix elements stemming from the repulsive Coulomb interaction (with no spin degrees of freedom)

$$\langle \alpha\beta|V|\gamma\delta\rangle = \int r_1 dr_1 d\theta_1 \int r_2 dr_2 d\theta_2 \psi^*_{n_\alpha m_{l_\alpha}}(r_1,\theta_1) \psi^*_{n_\beta m_{l_\beta}}(r_2,\theta_2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \psi_{n_\gamma m_{l_\gamma}}(r_1,\theta_1) \psi_{n_\delta m_{l_\delta}}(r_2,\theta_2).$$

The explicit values for these matrix elements are found in the appendix of this midterm exam. Note well that these matrix elements do not include spin. When setting up the final antisymmetrized matrix elements you need to consider the spin degrees of freedom as well.

We will also, for both two and six electrons assume that the many-particle states we construct have always a total projection of the orbital momentum M = 0 and the same total spin projection  $M_S = 0$ . This means that if we excite one or two particles from the ground state, the spins and projections of the orbital momenta of the various single-particle states should always sum up to zero.

1a) We start with the two-electron system and define our single-particle Hilbert space to consist of the single-particle orbits  $(n = 0, m_l = 0)$ ,  $(n = 1, m_l = 0)$ ,  $(n = 0, m_l = \pm 1)$  and  $(n = 0, m_l = \pm 2)$ , with their corresponding spin degeneracies, see Fig. 1. Without spin we have thus six single-particle states. Adding the two spin degeneracies, we end up with 12 states.

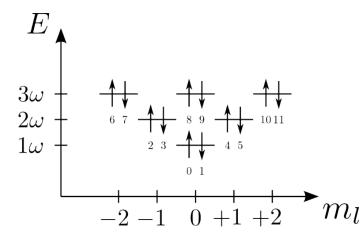


FIG. 1: Quantum spectrum for an electron in a two-dimensional oscillator well using a so-called Darwin-Fock representation. Here we show the states and their oscillator energies for three major shells. The oscillator energies are given by  $e_{nm_l} = \hbar\omega(2n + |m_l| + 1)$ . The single-particle states are ordered according to the quantum numbers  $n, m_l = 0, \pm 1, \pm 2$  and  $m_s = \pm 1/2$ .

Set up the ansatz for the ground state  $|\Phi_0\rangle$  in second quantization and define a table of single-particle states. Construct thereafter all possible one-particle-one-hole excitations  $|\Phi_i^a\rangle$  where *i* refers to levels below the Fermi level (define this level) and *a* refers to particle states. Define particles and holes. The Slater determinants have to be written in terms of the respective creation and annihilation operators. The two-particle states you construct should all have total spin projection  $m_{s_1} + m_{s_2} = M_S = 0$  and orbital momentum projection  $m_{l_1} + m_{l_2} = M = 0$ . The sub-indices refer to electron one and two, respectively. Construct also all possible two-particle-two-hole states  $|\Phi_{ij}^{ab}\rangle$  in a second quantization representation for the same total quantum numbers (for the two-particle system having the same values of M and  $M_S$ ).

1b) Define the Hamiltonian in a second-quantized form and use this to compute the expectation value of the ground state (defining the so-called reference energy and later our Hartree-Fock functional) of the two-electron quantum dot. Show that it is given by

$$E[\Phi_0] = \langle \Phi_0 | \hat{H} | \Phi_0 \rangle = \sum_i \langle i | \hat{h}_0 | i \rangle + \frac{1}{2} \sum_{ij} \left[ \langle ij | \frac{1}{r} | ij \rangle - \langle ij | \frac{1}{r} | ji \rangle \right].$$

Define properly the sums keeping in mind that the states ij refer to all quantum numbers  $nm_lm_s$ . Use the values for the various matrix elements listed at the end of this exam.

1c) Hereafter we will limit ourselves to a system which now contains only one-particle-one-hole excitations beyond the chosen state  $|\Phi_0\rangle$ . Using the possible Slater determinants from exercise a) for the two-electron quantum dot, compute also the expectation values (without inserting the explicit values for the matrix elements first) of

$$\langle \Phi_0 | H | \Phi_i^a \rangle$$
,

and

$$\langle \Phi_i^a | H | \Phi_j^b \rangle$$

Represent these expectation values in a diagrammatic form, both for the onebody part and the two-body part of the Hamiltonian.

Insert then the explicit values for the various matrix elements and set up the final Hamiltonian matrix and diagonalize it using for example Octave, Matlab, Python, C++ or Fortran as programming tools.

Compare your results from those of exercise b) and comment your results. The exact energy with our Hamiltonian is 3 atomic units for the two-electron quantum dot. This means that an infinite single-particle (in terms of the harmonic oscillator basis) basis is used.

1d) compute also the expectation values (without inserting the explicit values for the matrix elements first) for the two-electron system by including all possible 2p - 2h Slater determinants by adding to the Hamiltonian matrix from the previous exercise the expectation values

$$\begin{split} &\langle \Phi_0 | \hat{H} | \Phi^{ab}_{ij} \rangle, \\ &\langle \Phi^a_i | \hat{H} | \Phi^{bc}_{jk} \rangle, \end{split}$$

and

 $\langle \Phi_{ij}^{ab} | \hat{H} | \Phi_{kl}^{cd} \rangle.$ 

Represent again these expectation values in a diagrammatic form, both for the onebody part and the two-body part of the Hamiltonian.

Insert then the explicit values for the various matrix elements and set up the final Hamiltonian matrix and diagonalize it using for example Octave, Matlab, Python, C++ or Fortran as programming tools.

Compare your results from those of exercise c) and comment your results.

1e) We repeat exercises b) and c) but now for the six electron quantum dot. Define the ansatz for  $|\Phi_0\rangle$  and limit yourself again to one-particle-one-hole excitations. Compute the reference energy  $\langle \Phi_0 | \hat{H} | \Phi_0 \rangle$ . Thereafter you will need to set up the appropriate Hamiltonian matrix which involves also one-particle-one-hole excitations. Diagonalize this matrix and compare your eigenvalues with  $\langle \Phi_0 | \hat{H} | \Phi_0 \rangle$  and comment the result. The best numerical result for our Hamiltonian is obtained with Diffusion Monte Carlo calculations, and for  $\hbar\omega = 1$  the energy for the ground state is 20.1597 atomic units for the six electron quantum dot, see for example Lohne Pedersen *et al*, Physical Review B **84**, 115302 (2011).

With a given energy functional, we can perform at least two types of variational strategies.

- Vary the Slater determinant by changing the spatial part of the single-particle wave functions themselves.
- Expand the single-particle functions in a known basis and vary the coefficients, that is, the new function single-particle wave function  $|p\rangle$  is written as a linear expansion in terms of a fixed basis  $\phi$  (harmonic oscillator, Laguerre polynomials etc)

$$\psi_p = \sum_{\lambda} C_{p\lambda} \phi_{\lambda},$$

Both cases lead to a new Slater determinant which is related to the previous via a unitary transformation. Below we will set up the Hartree-Fock equations using the second option. We assume that our basis is still formed by the hydrogen-like wave functions.

1f) Consider a Slater determinant built up of single-particle orbitals  $\phi_{\lambda}$  where the indices  $\lambda$  refer to specific single-particle states.

The unitary transformation

$$\psi_p = \sum_{\lambda} C_{p\lambda} \phi_{\lambda},$$

brings us into the new basis  $\psi$ . 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). Which assumptions are you making in order to obtain this result?

1g) Minimizing with respect to  $C_{p\alpha}^*$ , remembering that  $C_{p\alpha}^*$  and  $C_{p\alpha}$  (and that the indices contain all single-particle quantum numbers including spin) are independent and defining

$$h_{\alpha\gamma}^{HF} = \langle \alpha | h | \gamma \rangle + \sum_{p} \sum_{\beta\delta} C_{p\beta}^* C_{p\delta} \langle \alpha\beta | V | \gamma\delta \rangle_{AS},$$

show that you can write the Hartree-Fock equations as

$$\sum_{\gamma} h_{\alpha\gamma}^{HF} C_{p\gamma} = \epsilon_p^{\rm HF} C_{p\alpha}.$$

Explain the meaning of the different terms and define the Hartree-Fock operator in second quantization. Write down its diagrammatic representation as well. The greek letters refer to the wave functions in the original basis (in our case the harmonic oscillator functions) while roman letters refer to the new basis.

Discuss the stability of the Hartree-Fock equations and find out whether the matrix elements listed at the end of the midterm exam result in a stable procedure (consider the two- and six-electron cases).

1h) The Hartree-Fock equations with a variation of the coefficients  $C_{p\alpha}$  lead to an eigenvalue problem whose eigenvectors are the coefficients  $C_{p\alpha}$  and eigenvalues are the new single-particle energies. Use the single-particle states of Fig. 1 and set up the Hartree-Fock matrix for both the two-electron and the six electron systems. Find after the first diagonalization the new single-particle energies and the new ground state energy. Compare these results with those you obtained by diagonalizing the Hamiltonian matrices in c) for the two-electron systems and e) for the six electron system. Comment yur results.

When setting up the Hartree-Fock matrix in the first iteration, our guess for the coefficients  $C_{p\beta}$  etc. is  $C_{p\beta} = 1$  for  $p = \beta$  and zero else.

1i) The final stage is to set up an iterative scheme where you use the new wave functions determined via the coefficients  $C_{p\alpha}$  to solve iteratively the Hartree-Fock equations till a given self-consistency is reached. A typical way of doing this is to compare the single-particle energies from the previous iteration with those obtained from the new diagonalization. If the total difference is smaller than a prefixed value, the iterative process is stopped.

Compare these results with those you obtained with the full diagonalization. Discuss your results.

1j) This exercise is optional but gives an additional score of 40% if performed. The aim here is to repeat first exercises 1h) and 1i) by writing a program for doing Hartree-Fock calculations. The choice of programming language is optional.

The first check is to write a program that reproduces the results obtained in 1h) and 1i) for two particles with only three oscillator shells using the matrix elements in the table below (see also the file matrixlements.dat). The next steps are:

- Extend the single-particle basis from three shells to eight-ten major shells. Set up the basis and the expectation values of  $\langle i|h_o|j\rangle$ .
- Compute thereafter the Coulomb matrix elements using the expressions in the appendix and the code example (coulomb.cpp on the webpage of the course is an example of a program in c++) and set up a table of anti-symmetric matrix elements. Store these in a table.
- Perform thereafter the Hartree-Fock calculations (focus on one spin value only, the Hartree-Fock energies are independent of spin)) for this enlarged basis for two and six electrons and compare your results with those from 1h) and 1i).
- Study the convergence of the Hartree-Fock energies as functions of the number of shells involved. Comment your results.

# Additional material, table of matrix elements and expressions for the expectation value of the two-body matrix elements

#### A. Expressions for the Coulomb matrix elements

The expression for the Coulomb matrix elements in the article of E. Anisimovas and A. Matulis, J. Phys.: Condens. Matter 10, 601 (1998). At the webpage of the course (see under the midterm link) we provide a file called coulomb.cpp which computes the Coulomb matrix element  $\langle 12|V|34 \rangle$  where the 1,2,3 and 4 are four single-particle state indices. Each state  $|p(=1,2,3,4)\rangle$  can be rewritten in terms of its quantum numbers. In two dimensions, it reads  $|p\rangle = |n_p m_p s_p\rangle$ . For simplicity the angular momentum projection quantum number  $m_l$  will just be written as m in the following equations. The function coulomb(n1,m1,n2,m2,n3,m3,n4,m4) computes thus the integral. Calling this function and paying attention to the spin values, the computation of the direct term is given by direct =  $\delta(ms1, ms3)\delta(ms2, ms4) \times$ coulomb(n1,m1,n2,m2,n4,m4,n3,m3). Pay attention to the explanation text in the file coulomb.cpp. The expression for the Coulomb integral can be written as

$$V_{1234} = \delta_{m_1 + m_2, m_3 + m_4} \sqrt{\left[\prod_{i=1}^{4} \frac{n_i!}{(n_i + |m_i|!)}\right]} \times \sum_{\substack{j_1 = 0, \dots, j_4 = 0}}^{n_1, \dots, n_4} \left[\frac{(-1)^{j_1 + j_2 + j_3 + j_4}}{j_1! j_2! j_3! j_4!} \left[\prod_{k=1}^{4} \binom{n_k + |m_k|}{k - j_k}\right] \frac{1}{2^{\frac{G+1}{2}}} \times \sum_{\substack{\gamma_1 = 0, \dots, \gamma_4 = 0\\l_1 = 0, \dots, l_4 = 0}}^{\gamma_1 = 0, \dots, \gamma_4 = 0} \left(\delta_{l_1, l_2} \,\delta_{l_3, l_4} \,(-1)^{\gamma_2 + \gamma_3 - l_2 - l_3} \left[\prod_{t=1}^{4} \binom{\gamma_t}{l_t}\right] \,\Gamma\left(1 + \frac{\Lambda}{2}\right) \,\Gamma\left(\frac{G - \Lambda + 1}{2}\right)\right)\right]$$
(3)

where

$$\begin{split} \gamma_1 &= j_1 + j_4 + \frac{|m_1| + m_1}{2} + \frac{|m_4| - m_4}{2} \\ \gamma_2 &= j_2 + j_3 + \frac{|m_2| + m_2}{2} + \frac{|m_3| - m_3}{2} \\ \gamma_3 &= j_3 + j_2 + \frac{|m_3| + m_3}{2} + \frac{|m_2| - m_2}{2} \\ \gamma_4 &= j_4 + j_1 + \frac{|m_4| + m_4}{2} + \frac{|m_1| - m_1}{2} \\ G &= \gamma_1 + \gamma_2 + \gamma_3 + \gamma_4 \\ \Lambda &= l_1 + l_2 + l_3 + l_4, \end{split}$$

when the basis set is built upon the single harmonic oscillator orbitals.

The implementation of the function coulomb(...) includes the following subfunctions:

- minusPower(int k) which computes  $(-1)^k$
- LogFac(int n) which computes  $log_e(n!)$
- LogRatio1(int  $j_1$ , int  $j_2$ , int  $j_3$ , int  $j_4$ ) which computes the  $log_e$  of  $\frac{1}{j_1!j_2!j_3!j_4!}$
- LogRatio2(int G) which computes the  $log_e$  of  $\frac{1}{2\frac{G+1}{2}}$
- Product1 (int  $n_1$ , int  $m_1$ , int  $n_2$ , int  $n_3$ , int  $n_3$ , int  $n_4$ , int  $m_4$ ) which computes the explicit (not the  $log_e$ ) product  $\sqrt{\left[\prod_{i=1}^4 \frac{n_i!}{(n_i+|m_i|!)}\right]}$
- LogProduct2(int  $n_1$ , int  $m_1$ , int  $n_2$ , int  $m_2$ , int  $n_3$ , int  $m_3$ , int  $n_4$ , int  $m_4$ , int  $j_1$ , int  $j_2$ , int  $j_3$ , int  $j_4$ ) which computes the  $log_e$  of  $\prod_{k=1}^4 \binom{n_k + |m_k|}{n_k j_k}$
- LogProduct3(int  $l_1$ , int  $l_2$ , int  $l_3$ , int  $l_4$ , int  $\gamma_1$ , int  $\gamma_2$ , int  $\gamma_3$ , int  $\gamma_4$ ) which computes the  $log_e$  of  $\prod_{t=1}^4 {\gamma_t \choose l_t}$
- lgamma(double x) which computes the  $log_e[\Gamma(x)]$

#### Explicit values for the two-body matrix elements for $\hbar\omega = 1$ a.u.

The expectation values for the two-body matrix elements are computed using the closed-form expression tabulated in the article of E. Anisimovas and A. Matulis, J. Phys.: Condens. Matter **10**, 601 (1998).

Note that the integrals below do not include spin. The nomenclature is  $1 = (n = 0, m_l = 0)$ ,  $2 = (n = 0, m_l = -1)$ ,  $3 = (n = 0, m_l = +1)$ ,  $4 = (n = 0, m_l = -2)$ ,  $5 = (n = 1, m_l = 0)$ , and  $6 = (n = 0, m_l = +2)$  with no spin degrees of freedom. Only the integrals are listed, you need to add the spin values and compute the final antisymmetric matrix element. This table can also be found at the webpage of the course, see the file matrixelements.dat listed under the midterm link. Only the non-zero matrix elements are listed.

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5	1	1	1	0.3133285343
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5 5	1 1	2 3	3 2	-0.07833213358 -0.07833213358
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5		2	4	-0.1523202528
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