

First project fall 2015 FYS-KJM4480/9480

Date given: Thursday October 8, 2015.

Date revised: Monday October 19, 2015. Deadline: Monday November 2 at 12pm (noon). It counts 30% of the final mark.

Introduction and background

This project contains 3 exercises.

A *quantum dot* is a system of electrons confined in semiconducting heterostructures. Such systems 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 such diverse applications as quantum computers, optimized solar cells, laser technology and medical imaging, to name a few. On the other hand, strongly confined electrons offer a wide variety of complex and subtle phenomena which pose severe challenges to existing many-body methods.

We study a model called *the parabolic quantum dot*: A system of electrons confined in two dimensions by a harmonic oscillator potential. Our Hamiltonian for N electrons takes the following form

$$\hat{H} = \sum_{i=1}^N \left(\frac{-\hbar^2}{2m_e} \nabla_i^2 \right) + \sum_{i=1}^N \frac{1}{2} m_e \omega^2 r_i^2 + \sum_{i<j}^N \frac{ke^2}{r_{ij}} = \hat{H}_0 + \hat{W}, \quad (1)$$

with

$$\hat{H}_0 = \sum_{i=1}^N \hat{h}(\vec{r}_i), \quad \hat{h}(\vec{r}) = -\frac{\hbar^2}{2m_e} \nabla^2 + \frac{1}{2} m_e \omega^2 r^2. \quad (2)$$

Here, $r \equiv |\vec{r}|$, $r_i \equiv |\vec{r}_i|$, and $r_{ij} \equiv |\vec{r}_i - \vec{r}_j|$.

We will consider a system of $N = 2$ and $N = 6$ electrons. These represent so-called closed shell systems for the parabolic quantum dot. The next “magic numbers” for the parabolic quantum dot is $N = 12$, $N = 20$, $N = 30$, $N = 42$, and these electron numbers are analogous to noble gas electron numbers in atoms and closed-shell structures in atomic nuclei.

As single-particle basis functions for our calculations we will use spin-orbitals made from the harmonic oscillator eigenfunctions $\psi_{nm}(r, \theta)$ in polar coordinates,

$$\hat{h}(\vec{r})\psi_{nm}(r, \theta) = e_{nm}\psi_{nm}(r, \theta) \quad (3)$$

with

$$e_{nm} = \frac{1}{2} \hbar \omega (2n + |m| + 1). \quad (4)$$

and (with $a = \sqrt{m_e \omega / \hbar}$),

$$\psi_{nm}(r, \theta) = a e^{im\theta} \sqrt{\frac{n!}{\pi(n+|m|)!}} (ar)^{|m|} L_n^{|m|}(a^2 r^2) \exp(-a^2 r^2/2). \quad (5)$$

Here, $L_n^{|m|}$ are the so-called associated Laguerre polynomials, the first few of which are

$$L_0^{|m|}(x) = 1, \quad (6)$$

$$L_1^{|m|}(x) = -x + 1 + |m|. \quad (7)$$

The quantum number n is the number of nodes in the radial part, while $\hbar m$ is the orbital angular momentum, the eigenvalue of the operator

$$\hat{L}_z(\vec{r}) = -i\hbar \frac{\partial}{\partial \theta}. \quad (8)$$

You will not need to use all the details of the form of ψ_{nm} in this project.

The spin-orbitals become

$$\phi_p(x) = \psi_{nm}(r, \theta) \chi_\alpha(\sigma), \quad p = p(nm\alpha), \quad (9)$$

where $\alpha = \pm 1/2$ is the quantum number for the z -projection of the electron spin, and χ_α is the corresponding spinor basis function, $\langle \chi_\alpha | \chi_\beta \rangle = \delta_{\alpha\beta}$. Thus p counts the spin-orbitals, and can be considered as an invertible function of the quantum numbers $nm\alpha$.

(We sometimes write n_p , m_p , and α_p for the quantum numbers belonging to a given spin-orbital index p .)

The spin-projection operator can be written in terms of its action on the spin-orbital basis,

$$\hat{s}_z |\phi_p\rangle = \hbar \alpha_p |\phi_p\rangle. \quad (10)$$

The orbital angular momentum operator is, on first-quantized form,

$$\hat{L}_z = \sum_{i=1}^N \hat{L}_z(i), \quad (11)$$

while the spin-projection operator is

$$\hat{S}_z = \sum_{i=1}^N \hat{s}_z(i). \quad (12)$$

Note that each eigenvalue e_{nm} of the harmonic-oscillator \hat{h} is now doubly degenerate due to spin. The one-particle operator \hat{h} is now diagonal in the spin-orbital basis. Writing $p = p(\alpha nm)$ and $p' = p'(\alpha' n' m')$, we get

$$\langle \phi_p | \hat{h}(\vec{r}) | \phi_{p'} \rangle = \langle \chi_\alpha | \chi_{\alpha'} \rangle \langle \psi_{nm} | \hat{h} | \psi_{n'm'} \rangle = \delta_{\alpha, \alpha'} \delta_{n, n'} \delta_{m, m'} e_{nm} = \delta_{p, p'} e_{nm}. \quad (13)$$

Note that

$$\delta_{p, p'} = \delta_{\alpha, \alpha'} \delta_{n, n'} \delta_{m, m'} \quad (14)$$

since $p = p'$ if and only if $\alpha = \alpha'$, $n = n'$, and $m = m'$.

The matrix elements of the Coulomb interaction \hat{W} in the spin-orbital basis can be written in terms of the integrals

$$\begin{aligned} & (\psi_{n_1 m_1} \psi_{n_2 m_2} | \hat{W} | \psi_{n_3 m_3} \psi_{n_4 m_4}) = \\ & \iint r_1 dr_1 d\theta_1 r_2 dr_2 d\theta_2 \psi_{n_1 m_1}^*(r_1, \theta_1) \psi_{n_2 m_2}^*(r_2, \theta_2) \frac{ke^2}{r_{12}} \psi_{n_3 m_3}(r_1, \theta_1) \psi_{n_4 m_4}(r_2, \theta_2). \end{aligned} \quad (15)$$

The explicit values for these matrix elements for $ke^2 = 1$ are found in the appendix of this project. Note well that these matrix elements do not include spin. When setting up, say, the matrix elements $\langle \phi_{p_1} \phi_{p_2} | \hat{W} | \phi_{p_3} \phi_{p_4} \rangle$, you need to consider the spin degrees of freedom as well.

Our computational Hilbert space will be defined by the three lowest harmonic oscillator single-particle energy levels. In total, when we add spin, we have $L = 12$ single-particle states. Thus, we have 6 orbitals and 12 spin-orbitals. These are illustrated in Fig. 1.

Exercise 1 (10 points)

1a) Let c_p^\dagger and c_p be creation and annihilation operators for the spin-orbitals ϕ_p .

Define the second-quantized forms of \hat{L}_z and \hat{S}_z . Using that the spin-orbitals are eigenfunctions, simplify the expressions as much as possible.

1b) Show that any Slater determinant $|p_1 \cdots p_N\rangle$ (built from the spin-orbitals ϕ_p) is an eigenfunction for \hat{L}_z with eigenvalue $\hbar M = \hbar \sum_i m_i$, where $m_i = m_{p_i}$. Show that the Slater determinant is also an eigenfunction for \hat{S}_z with eigenvalue $\hbar S_z = \hbar \sum_i \alpha_i$, where $\alpha_i = \alpha_{p_i}$.

1c) Show that

$$[\hat{S}_z, \hat{L}_z] = 0, \quad (16)$$

by computing the action of each commutator on an arbitrary Slater determinant.

From 1c) and the fact that $[\hat{H}, \hat{L}_z] = [\hat{H}, \hat{S}_z] = 0$ (you do not have to show this) we obtain that the ground-state wavefunction of \hat{H} can be chosen to be an eigenfunction of both \hat{S}_z and \hat{L}_z . We will in the rest of the exercise consider only the case $M = 0$ and $S_z = 0$. From 1c) we then obtain that the ground-state wavefunction can be constructed as a linear combination of those Slater determinants that have $M = S_z = 0$ only: all the m_i 's sum to zero and all the α_i 's sum to zero for these determinants. All other Slater determinants are eliminated *a priori*.

Exercise 2 (20 points)

We can transform the Hamiltonian to dimensionless form by introducing a suitable set of units. We will compute in a set of units where

$$\hbar = m_e = k e^2 = 1. \quad (17)$$

leaving ω as the last independent parameter, controlling the strength of the confinement potential. In the rest of the project, we use these units for simplicity.

We also limit ourselves to the case

$$\omega = 1. \quad (18)$$

2a) We start with the two-electron system and define our single-particle Hilbert space to consist of the orbitals $(n = 0, m = 0)$, $(n = 1, m = 0)$, $(n = 0, m = \pm 1)$ and $(n = 0, m = \pm 2)$, with their corresponding spin degeneracies, see Fig. 1 for a schematic picture. Without spin we have thus six single-particle states. Adding the two spin degeneracies, we end up with 12 states. In the figure, the indices $P = P(n, m, \alpha)$ are listed below each spin-orbital.

Set up the $M = S_z = 0$ ground-state of the noninteracting problem (\hat{H}_0) as a reference Slater determinant $|\Phi\rangle$. Use second quantization. Define the Fermi level/energy. Draw a diagram of the reference state, in the same fashion as Fig. 1. (If you use L^AT_EX, such diagrams can be easily made, see the source code for this project.)

Define quasiparticle creation- and annihilation operators for this problem.

Construct thereafter all possible one-particle-one-hole excitations $|\Phi_i^a\rangle$, where i is an index below the Fermi level, and a is an index above the Fermi level. Write the Slater determinants in terms of quasiparticle operators. Ensure that you only write down those states that have $M = m_1 + m_2 = 0$ and $S_z = \alpha_1 + \alpha_2 = 0$. Draw diagrams.

Construct thereafter all possible two-particle-two-hole excitations $|\Phi_{ij}^{ab}\rangle$ in a similar manner. Draw diagrams.

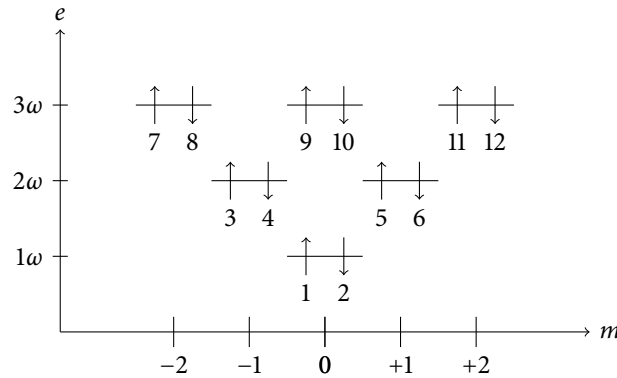


Figure 1: Spin-orbitals for an electron in a two-dimensional oscillator well using a so-called Fock–Darwin representation. Here we show the states and their oscillator energies for three harmonic-oscillator levels. The oscillator energies are given by $e_{nm} = \hbar\omega(2n + |m| + 1)$.

- 2b) Write down the Hamiltonian \hat{H} on second-quantized form. Use Eqns. (13) and (15). Include only nonzero terms in the sums. (Do not separate the sums over spin-orbitals into particles and holes; keep the sums over general spin-orbitals.)

Compute the expectation value

$$\langle \Phi | \hat{H} | \Phi \rangle \quad (19)$$

and obtain a numerical value by using the integral table in the Appendix. Explain why this expectation value can be considered an approximation to the exact ground-state energy.

- 2c) We now limit ourselves to the configuration-interaction with singles (CIS) basis, consisting of $|\Phi\rangle$ and the one-particle-one-hole functions $|\Phi_i^a\rangle$ you found in 2a).

Compute the matrix elements (without inserting the numerical values of the \hat{w} matrix elements) of

$$\langle \Phi | \hat{H} | \Phi_j^b \rangle, \quad \langle \Phi_i^a | \hat{H} | \Phi \rangle,$$

and

$$\langle \Phi_i^a | \hat{H} | \Phi_j^b \rangle.$$

Use Wick's Theorem for quasiparticles.

Insert then the explicit values for the various matrix elements and set up the final CIS Hamiltonian matrix and diagonalize it using your favorite tool, for example Octave, Matlab, Python, C++ or Fortran.

Compare your results from those of exercise 2b) and comment your results. The exact ground-state energy with our Hamiltonian is $E_0 = 3$ for the two-electron quantum dot. "Exact" means in the limit of a complete infinite-dimensional harmonic-oscillator basis.

- 2d) We repeat exercises b) and c) but now for the six electron quantum dot. Define the reference wave-function $|\Phi\rangle$ and limit yourself again to one-particle-one-hole excitations.

Compute the reference energy $\langle \Phi | \hat{H} | \Phi \rangle$, inserting the numerical values for the \hat{w} matrix elements. Thereafter you will need to set up the appropriate Hamiltonian matrix which involves also one-particle-one-hole excitations, also using numerical values for matrix elements. Diagonalize this matrix and compare your eigenvalues with $\langle \Phi | \hat{H} | \Phi \rangle$ and comment the result. The best numerical result

for our Hamiltonian is obtained with Diffusion Monte Carlo calculations, and for $\omega = 1$ the energy for the ground state is $E_0 = 20.1597$ atomic units for the six electron quantum dot, see for example Lohne Pedersen *et al*, Physical Review B **84**, 115302 (2011).

Exercise 3 (35 points)

Having treated the parabolic quantum dot with configuration-interaction, we now turn to a restricted Hartree–Fock (RHF) treatment.

Recall that we have 12 spin-orbitals, but only 6 orbitals. Define an index $P = P(n, m)$ to count the orbitals without spin. Thus, $P = 1, 2, \dots, 6$.

$$P(0, 0) = 1, \quad P(0, -1) = 2, \quad P(0, 1) = 3, \quad P(0, -2) = 4, \quad P(1, 0) = 5, \quad P(0, 4) = 6.$$

This is the numbering used in the Appendix. Note well, that this is for the *spatial orbitals* only, hence the capital “ P ” instead of the lowercase “ p ”.

- 3a) Define the RHF wavefunction $|\Phi_{\text{RHF}}\rangle$ for $N = 2$ and $N = 6$. Use the notation $\tilde{\psi}_I(\vec{r})$, $I = 1, 2, \dots, N/2$, for the unknown spatial orbitals to be found.

Compute, in terms of the spatial matrix elements of \hat{h} and \hat{w} ,

$$E_{\text{RHF}} = \langle \Phi_{\text{RHF}} | \hat{H} | \Phi_{\text{RHF}} \rangle, \quad (20)$$

In what manner does the RHF wavefunction ansatz and energy expression differ from the general Hartree–Fock wavefunction for fermions?

- 3b) In the remainder, we will expand the RHF spatial orbitals in the harmonic oscillator functions $\psi_P(\vec{r})$, $P = 1, \dots, 6$. Define therefore an 6×6 matrix U and write

$$\tilde{\psi}_Q(\vec{r}) = \sum_{P=1}^6 \psi_P(\vec{r}) U_{PQ}. \quad (21)$$

Explain why the matrix U must be a unitary matrix. What part of U corresponds to the occupied RHF orbitals? What part corresponds to the virtual RHF orbitals?

- 3c) Using your result in 3a) and the definition (21), show that the RHF energy of can be written

$$E_{\text{RHF}} = \langle \Phi_{\text{RHF}} | \hat{H} | \Phi_{\text{RHF}} \rangle = 2 \sum_{PQI} U_{QI}^* (\psi_Q | \hat{h} | \psi_P) U_{PI} + \sum_{PQI} U_{QI}^* \left(\sum_{RS} D_{SR} [QR|PS] \right) U_{PI}. \quad (22)$$

The sums over I and J go from 1 to $N/2$, while the sums over P , Q , R , and S go from 1 to $L/2$, and we have defined

$$[QR|PS] \equiv (\psi_Q \psi_R | \hat{w} | \psi_P \psi_S) - \frac{1}{2} (\psi_Q \psi_R | \hat{w} | \psi_S \psi_P). \quad (23)$$

We have also defined the reduced density matrix,

$$D_{SR} = 2 \sum_I U_{SI} U_{RI}^*. \quad (24)$$

Split the \hat{W} -part of E_{RHF} into a direct and an exchange energy. Explain their origin, and compare with standard HF theory formulated in an orthonormal spin-orbital basis.

3d) The RHF equations in the given basis can be written

$$F(D)U = U\epsilon, \quad (\text{Roothan-Hall equation}) \quad (25)$$

(you do not have to show this), where $F(D)$ is the Fock matrix,

$$F_{QP}(D) = (\psi_Q|\hat{h}|\psi_P) + \sum_{RS} D_{SR}[QR|PS], \quad (26)$$

and where $\epsilon = \text{diag}(\epsilon_1, \dots, \epsilon_{L/2})$ is a diagonal matrix of eigenvalues.

Explain in what way the Roothan-Hall equation differs from an ordinary matrix eigenvalue problem.

3e) Show that the RHF energy can be written

$$E_{\text{RHF}} = 2 \sum_I \epsilon_I - \sum_{IPQ} U_{QI}^* \left(\sum_{SR} D_{SR}[QR|PS] \right) U_{PI}. \quad (27)$$

Hint: Multiply The Roothan-Hall equation with U^H from the left, and compare with Eq. (22).

3f) We are now going to solve the Roothan-Hall equation numerically. Use your favorite programming language and environment. Use comments to document your code and make it readable.

You will need to read the integrals $(\psi_P\psi_Q|\hat{w}|\psi_R\psi_S)$ from a text file `coulomb.dat` downloadable from the course web page. This file is listed in the Appendix. You can then tabulate $[PQ|RS]$.

Write first a subroutine/function/module that, given a reduced density matrix D_0 , computes the corresponding Fock matrix $F(D_0)$, and then diagonalizes it.

Thus, your subroutine should solve the standard eigenvalue problem $F(D_0)U = U\epsilon$ and return U and the diagonal elements of ϵ .

(A useful check on the sanity of your implementation is that F is Hermitian, $F_{PQ} = F_{QP}^*$.)

Make sure the eigenvalues are sorted in increasing order (the eigenvectors also need to be in corresponding order). Hint: if you use LAPACK library calls, it can be useful to eliminate some numerical noise that can cause LAPACK to call a non-symmetric eigenvalue solver. For example, you can explicitly symmetrize the matrix by diagonalizing $(F + F^H)/2$.

3g) Write a program that performs SCF iterations,

$$F(U^{(k-1)})U^{(k)} = U^{(k)}\epsilon^{(k)}, \quad (28)$$

with $U^{(0)} = I$, the identity matrix.

You will need approximately 15 iterations for convergence. Measure the convergence via

$$\delta_k = \max_P \{ |\epsilon_P^{(k)} - \epsilon_P^{(k-1)}| \}. \quad (29)$$

Plot δ_k versus k , with δ_k on a log-axis.

At each iteration $k = 1, 2, \dots$, compute E_{RHF} . Discuss the convergence properties.

Compare the converged RHF energy with the results obtained for CIS, and with the numerically exact values listed elsewhere in this project.

Make sure your program handles both $N = 2$ and $N = 6$, and that you discuss both cases.

Appendix: Table of matrix elements and expressions for the expectation value of the two-body matrix elements

Explicit values for the two-body matrix elements

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

Each line in the table below is on the form

P Q R S ($\psi_P \psi_Q | w | \psi_R \psi_S$).

Only the non-zero matrix elements are listed. Note that the integrals below do not include spin. The indices P, Q , etc, are related to the quantum numbers (n, m) as $1 = (n = 0, m = 0)$, $2 = (n = 0, m = -1)$, $3 = (n = 0, m = +1)$, $4 = (n = 0, m = -2)$, $5 = (n = 1, m = 0)$, and $6 = (n = 0, m = +2)$ with no spin degrees of freedom. This table can also be found in text format at the webpage of the course, see the file `coulomb.dat` available from the course page.

1	1	1	1	1.253314137
1	1	1	5	0.3133285343
1	1	2	3	0.3133285343
1	1	3	2	0.3133285343
1	1	4	6	0.1174982004
1	1	5	1	0.3133285343
1	1	5	5	0.2349964007
1	1	6	4	0.1174982004
1	2	1	2	0.939985603
1	2	2	1	0.3133285343
1	2	2	5	-0.07833213358
1	2	3	4	0.2769459142
1	2	4	3	0.1661675485
1	2	5	2	0.07833213358
1	3	1	3	0.939985603
1	3	2	6	0.2769459142
1	3	3	1	0.3133285343
1	3	3	5	-0.07833213358
1	3	5	3	0.07833213358
1	3	6	2	0.1661675485
1	4	1	4	0.744155269
1	4	2	2	0.2769459142
1	4	4	1	0.1174982004
1	4	4	5	-0.08812365028
1	4	5	4	-0.009791516698
1	5	1	1	0.3133285343
1	5	1	5	0.8616534694
1	5	2	3	-0.07833213358
1	5	3	2	-0.07833213358
1	5	4	6	-0.08812365028
1	5	5	1	0.2349964007
1	5	5	5	0.1370812338
1	5	6	4	-0.08812365028

1 6 1 6	0.744155269
1 6 3 3	0.2769459142
1 6 5 6	-0.009791516698
1 6 6 1	0.1174982004
1 6 6 5	-0.08812365028
2 1 1 2	0.3133285343
2 1 2 1	0.939985603
2 1 2 5	0.07833213358
2 1 3 4	0.1661675485
2 1 4 3	0.2769459142
2 1 5 2	-0.07833213358
2 2 1 4	0.2769459142
2 2 2 2	0.8616534694
2 2 4 1	0.2769459142
2 2 4 5	-0.1523202528
2 2 5 4	-0.1523202528
2 3 1 1	0.3133285343
2 3 1 5	-0.07833213358
2 3 2 3	0.8616534694
2 3 3 2	0.2349964007
2 3 4 6	0.3035370176
2 3 5 1	-0.07833213358
2 3 5 5	0.1370812338
2 3 6 4	0.1468727505
2 4 2 4	0.7539467857
2 4 4 2	0.3035370176
2 5 1 2	-0.07833213358
2 5 2 1	0.07833213358
2 5 2 5	0.7245722356
2 5 3 4	-0.1246256614
2 5 4 3	-0.1523202528
2 5 5 2	0.1370812338
2 6 1 3	0.2769459142
2 6 2 6	0.7539467857
2 6 3 1	0.1661675485
2 6 3 5	-0.1246256614
2 6 5 3	-0.1523202528
2 6 6 2	0.1468727505
3 1 1 3	0.3133285343
3 1 2 6	0.1661675485
3 1 3 1	0.939985603
3 1 3 5	0.07833213358
3 1 5 3	-0.07833213358
3 1 6 2	0.2769459142
3 2 1 1	0.3133285343
3 2 1 5	-0.07833213358
3 2 2 3	0.2349964007
3 2 3 2	0.8616534694
3 2 4 6	0.1468727505

3 2 5 1	-0.07833213358
3 2 5 5	0.1370812338
3 2 6 4	0.3035370176
3 3 1 6	0.2769459142
3 3 3 3	0.8616534694
3 3 5 6	-0.1523202528
3 3 6 1	0.2769459142
3 3 6 5	-0.1523202528
3 4 1 2	0.2769459142
3 4 2 1	0.1661675485
3 4 2 5	-0.1246256614
3 4 3 4	0.7539467857
3 4 4 3	0.1468727505
3 4 5 2	-0.1523202528
3 5 1 3	-0.07833213358
3 5 2 6	-0.1246256614
3 5 3 1	0.07833213358
3 5 3 5	0.7245722356
3 5 5 3	0.1370812338
3 5 6 2	-0.1523202528
3 6 3 6	0.7539467857
3 6 6 3	0.3035370176
4 1 1 4	0.1174982004
4 1 2 2	0.2769459142
4 1 4 1	0.744155269
4 1 4 5	-0.009791516698
4 1 5 4	-0.08812365028
4 2 2 4	0.3035370176
4 2 4 2	0.7539467857
4 3 1 2	0.1661675485
4 3 2 1	0.2769459142
4 3 2 5	-0.1523202528
4 3 3 4	0.1468727505
4 3 4 3	0.7539467857
4 3 5 2	-0.1246256614
4 4 4 4	0.7160046585
4 5 1 4	-0.08812365028
4 5 2 2	-0.1523202528
4 5 4 1	-0.009791516698
4 5 4 5	0.6682710146
4 5 5 4	0.1395291129
4 6 1 1	0.1174982004
4 6 1 5	-0.08812365028
4 6 2 3	0.3035370176
4 6 3 2	0.1468727505
4 6 4 6	0.7160046585
4 6 5 1	-0.08812365028
4 6 5 5	0.1395291129
4 6 6 4	0.1285136567

5 1 1 1	0.3133285343
5 1 1 5	0.2349964007
5 1 2 3	-0.07833213358
5 1 3 2	-0.07833213358
5 1 4 6	-0.08812365028
5 1 5 1	0.8616534694
5 1 5 5	0.1370812338
5 1 6 4	-0.08812365028
5 2 1 2	0.07833213358
5 2 2 1	-0.07833213358
5 2 2 5	0.1370812338
5 2 3 4	-0.1523202528
5 2 4 3	-0.1246256614
5 2 5 2	0.7245722356
5 3 1 3	0.07833213358
5 3 2 6	-0.1523202528
5 3 3 1	-0.07833213358
5 3 3 5	0.1370812338
5 3 5 3	0.7245722356
5 3 6 2	-0.1246256614
5 4 1 4	-0.009791516698
5 4 2 2	-0.1523202528
5 4 4 1	-0.08812365028
5 4 4 5	0.1395291129
5 4 5 4	0.6682710146
5 5 1 1	0.2349964007
5 5 1 5	0.1370812338
5 5 2 3	0.1370812338
5 5 3 2	0.1370812338
5 5 4 6	0.1395291129
5 5 5 1	0.1370812338
5 5 5 5	0.7490510274
5 5 6 4	0.1395291129
5 6 1 6	-0.009791516698
5 6 3 3	-0.1523202528
5 6 5 6	0.6682710146
5 6 6 1	-0.08812365028
5 6 6 5	0.1395291129
6 1 1 6	0.1174982004
6 1 3 3	0.2769459142
6 1 5 6	-0.08812365028
6 1 6 1	0.744155269
6 1 6 5	-0.009791516698
6 2 1 3	0.1661675485
6 2 2 6	0.1468727505
6 2 3 1	0.2769459142
6 2 3 5	-0.1523202528
6 2 5 3	-0.1246256614
6 2 6 2	0.7539467857

6 3 3 6	0.3035370176
6 3 6 3	0.7539467857
6 4 1 1	0.1174982004
6 4 1 5	-0.08812365028
6 4 2 3	0.1468727505
6 4 3 2	0.3035370176
6 4 4 6	0.1285136567
6 4 5 1	-0.08812365028
6 4 5 5	0.1395291129
6 4 6 4	0.7160046585
6 5 1 6	-0.08812365028
6 5 3 3	-0.1523202528
6 5 5 6	0.1395291129
6 5 6 1	-0.009791516698
6 5 6 5	0.6682710146
6 6 6 6	0.7160046585