INTRODUCTION TO THE HARTREE-FOCK METHOD FOR QUANTUM DOTS AND PREPARATIONS FOR VARIATIONAL MONTE-CARLO.

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http://github.com/kingoslo/flintstones

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ABSTRACT

This is a report submission for the first project of «Computational physics 2» at the Institute of Physics, University of Oslo, autumn 2016.

INTRODUCTION

In this project we completed a variety of tasks to prepare ourselves for the final term project. We set up basis for compact subsets of $\mathbb{R}^2$ using quantum harmonic oscillator state functions. We did this by making a $\alpha \mapsto (n_x, n_y)$ bijection from the set of natural numbers to the two-tuples of harmonic oscillator principal quantum numbers on $\mathbb{R}^2$. In the class we included method to evaluate any given state basis function at the point $x \in \mathbb{R}^2$ and a method to return single Hermite polynomials. The latter was useful when we went ahead to build a Gaussian-quadrature Hermite integrator. The intent was that we would use this integrator to compute Coulomb interaction matrix elements, $\langle\alpha\beta|V|\gamma\delta\rangle$, for the quantum dot variety of the Hartree-Fock method. However, halfway through the project period, the course administration decided to supply a function which calculated the matrix elements in polar coordinates. The Hermite integrator was therefore never implemented further than for the integration of polynomials. Finally we wrote a program to solve the induced Hartree-Fock equations. Suppose μ is the Fermi level of some quantum dot. We wanted to find a $N \times N$-matrix C and an N-tuple $(\varepsilon_1, \cdots, \varepsilon_N)$ such that

$$\sum_{\beta=1}^{N} F_{\alpha\beta} C_{\beta\gamma} = \varepsilon_\gamma C_{\gamma\alpha} \qquad \text{for} \qquad F_{\alpha\beta} = \varepsilon_\alpha \delta_{\alpha\beta} + \sum_{j=1}^{\mu} \sum_{\gamma=1}^{N} \sum_{\delta=1}^{N} C^*_{j\gamma} C_{j\delta} \Big(\langle\alpha\gamma|V|\beta\delta\rangle - \langle\alpha\gamma|V|\delta\beta\rangle \Big). \quad (1)$$

We will call these equations the Hartree-Fock equations.

The report is structured by «introduction»-, «methods»-, «results and discussion»- and finally a «conclusion and perspectives»-sections.

METHODS

As we noted, the project required the completion of a variety of tasks. At the time of writing, it was unclear that there was any overarching methods. We will therefore use this section to present how the tasks were completed.

We set up the harmonic oscillator is several steps. First we used the energy function

$$E(n_x, n_y) = \hbar\omega\left(n_x + n_y + 1\right) \qquad \text{(Sakurai 2011, p. 92)(Griffiths 2005, p. 190)}$$

Clearly, this uniquely determines a hierarchy of groups of states ordered by energy. Assuming the particles were fermions we allowed exactly two spin projections for all combinations of n_x and n_y. As you may recall, we were not satisfied by a group hierarchy: From this we constructed a bijection $\alpha \mapsto (n_x, n_y)$ from the set of natural numbers using a dictionary type ordering (Munkres 2000, p. 26) on $\mathbb{N} \times \mathbb{N}$. We present a table in the results. We will also present the assignment rule for the bijection in the case of polar coordinates.

As explained, it was natural to implement the Hermite polynomials into the class. We know that the Hermite polynomials are of the form $H_n(x) = \sum_{m=0}^{n} a_m (2x)^m$. Under this hypothesis, insertion in the recurrence relation $H_{n+1}(x) = 2xH_n(x) - 2nH_n(x)$ straightforwardly reduces to

$$H_n(x) = n! \sum_{m=0}^{\lfloor n/2 \rfloor} \frac{(-1)^m}{m!(n-2m)!}(2x)^{n-2m},$$

in the case we treat n as being even and odd separately. Here we mean that $\lfloor \cdot \rfloor$ denotes the floor function on $\mathbb{R}$. Due to separation of variables, and according to Sakurai 2011, p. 93, the harmonic oscillator state functions are

$$\psi_{n_x,n_y}(x, y) = \psi_{n_x}(x)\psi_{n_y}(y), \qquad \psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{H_n((m\omega/\hbar)^{1/2}x)}{(2^n n!)^{1/2}} \exp\left(-m\omega/(2\hbar)x^2\right).$$

Having deduced an expression for H_n, implementing this into any harmonic basis for quantum dots is straightforward.

The next task which was initiated was to implement a Gaussian quadrature algorithm.

THEOREM 1 (Gaussian quadrature)**.** *Suppose $A \subseteq \mathbb{R}$ and there exist an orthogonal basis $\{H_n\}_{n=0}^{\infty}$ of polynomials for the set of square integrable functions on A with respect to the inner product*

$$\langle f, g \rangle = \int_A (Wfg)(x)\,\mathrm{d}x.$$

Suppose also that H_n is a degree n-polynomial and $|\langle H_n, H_n \rangle| = c_n$. If $f : \mathbb{R} \to \mathbb{R}$ is integrable on A and there exist and $N \in \mathbb{N}$ such that $f(x) = (WP_{2N-1})(x)$, then

$$\int_A f(x)\,\mathrm{d}x = c_0 \sum_{i=1}^{N} (H^{-1})_{0n} P_{2N-1}(x_n),$$

where $\{x_n\}_{n=1}^{N}$ are the zeros of H_N and $(H^{-1})_{0n}$ is the inverse of the matrix with elements $H_{nk} = H_k(x_n)$.

Proof of the theorem is contained in the appendix. This method was implemented according to the theorem. In particular, as the course administration decided to switch to polar coordinates, an analytical expression was supplied, and the integrator was therefore only used to integrate holomorphic functions on $\mathbb{R}$, where according to Stein and Shakarchi 2003, pp. 9,18 and 2, the integrator is stable. However, since the integrand of $\langle \alpha\beta | V | \gamma\delta \rangle$ is not holomorphic, I am not able to argue that the integrator is suitable to compute $\langle \alpha\beta | V | \gamma\delta \rangle$. Lastly, we were encouraged to work out the expression for $\langle \alpha\beta | V | \gamma\delta \rangle$. Suppose the principal quantum numbers of two-electron state indexed by t are n_t, m_t, $V(r) = -e^2/(4\pi^2\varepsilon_0 r)$ denote

the Coloumb potential, $\alpha, \beta, \gamma, \delta \in \{1, 2, \cdots\}$ and let $A = \{\alpha, \beta, \gamma, \delta\}$, $B = \{(1, \alpha), (2, \beta), (1, \delta), (2, \gamma)\}$ then a parameterisation of the matrix element $\langle \alpha\beta | V | \gamma\delta \rangle$ is

$$\begin{aligned}
\langle \alpha\beta | V | \gamma\delta \rangle &= \iiiint_{\mathbb{R}^4} \psi_\alpha^*(\mathbf{r}_1)\psi_\beta^*(\mathbf{r}_2)V(\|\mathbf{r}_1 - \mathbf{r}_2\|)\psi_\delta^*(\mathbf{r}_1)\psi_\gamma^*(\mathbf{r}_2)\,\mathrm{d}\mathbf{r}_1\,\mathrm{d}\mathbf{r}_2 \\
&= -C \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \prod_{(k,t)\in B} H_{n_t}(u_k)H_{m_t}(v_k) \frac{\exp\left(\sum_{i=1}^{2} u_i^2 + v_i^2\right)\mathrm{d}u_1\mathrm{d}v_1\mathrm{d}u_2\mathrm{d}v_2}{([u_1 - u_2]^2 + [v_1 - v_2]^2)^{1/2}},
\end{aligned}$$

$$\text{for normalization factor} \quad C = \frac{\omega^{1/2}e^2}{4\pi^3\varepsilon_0}\left(2^{\sum_{i\in A} n_i + m_i} \prod_{j\in A} n_j!m_j!\right)^{-1/2}.$$

$$n(\alpha) = \frac{1}{2}\left[\left(\frac{E}{\hbar\omega}\right)(\alpha) - |m(\alpha)| - 1\right]$$

$$m(\alpha) = -\left|\left(\frac{E}{\hbar\omega}\right)(\alpha) - 1\right| + 2\lfloor\frac{1}{2}\left[\alpha - 1 - \left(\left(\frac{E}{\hbar\omega}\right)(\alpha) - 1\right)\left(\frac{E}{\hbar\omega}\right)(\alpha)\right]\rfloor$$

$$\left(\frac{E}{\hbar\omega}\right)(\alpha) = \lceil\frac{1}{2}(1 + 4\alpha)^{1/2} - \frac{1}{2}\rceil$$

$$A(m, l) = \lceil\left(\frac{m + l}{2}\right)\left(\frac{m + l}{2} - 1\right)\rceil + (m + l) - \max(m, l)$$

Lastly, we solved the Hartree-Fock equations 1 by iteration. All $\langle \alpha\beta | V | \gamma\delta \rangle$ were pre calculated. It is easy to see that if one let

$$V_{\alpha\beta\gamma\delta} = \langle \alpha\beta | V | \gamma\delta \rangle - \langle \alpha\beta | V | \delta\gamma \rangle,$$

Then $V_{\alpha\beta\gamma\delta}$ is anti-symmetric in its two first and last indecies:

$$V_{\alpha\beta\gamma\delta} = -V_{\beta\alpha\gamma\delta} = -V_{\alpha\beta\delta\gamma} = V_{\beta\alpha\delta\gamma} = V_{\beta\alpha\delta\gamma},$$

Moreover since ψ_n can be made real

$$V_{\alpha\beta\gamma\delta} = V_{\gamma\delta\alpha\beta}.$$

In addition, we can show that $V_{\alpha\beta\gamma\delta} = 0$ whenever the total spin of $|\alpha\beta\rangle$ is different from the total spin of $|\gamma\delta\rangle$. Similarly $V_{\alpha\beta\gamma\delta} = 0$ whenever the total angular momentum of $|\alpha\beta\rangle$ is different from the total spin of $|\gamma\delta\rangle$. For some choices of μ and N, this reduced the number of stored matrix by a few orders of magnitudes, since we could compute only a few elements, and let the algorithm use the symmetries still determine the correct matrix elements. In this notation, the Hartree-Fock equations become:

$$\sum_{\beta=1}^{N} F_{\alpha\beta}C_{\beta\gamma} = \varepsilon_\gamma C_{\gamma\alpha} \qquad \text{for} \qquad F_{\alpha\beta} = \varepsilon_\alpha\delta_{\alpha\beta} + \sum_{\gamma=1}^{N}\sum_{\delta=1}^{N}\sum_{j=1}^{\mu}\left(C_{j\gamma}^* C_{j\delta}\right)V_{\alpha\gamma\beta\delta}$$

As we explained, the equations were solved iteritatively. We let the value of $C_{\alpha\beta} = \mathrm{diag}(1, 1, \cdots 1, 0, 0, \cdots, 0)$, where the number of one-elements were exactly μ. Using this candidate for $C_{\alpha\beta}$, $F_{\alpha\beta}$ was determined for each iteration. Thereafter, the matrix F was diagonalized $F = CDC^{-1}$, where $D = \mathrm{diag}(\varepsilon_1, \cdots, \varepsilon_N)$. Such a decomposition exists since F has exactly N eigenvalues and ε_j are the single state energies since the columns of C are eigenvectors of F by The Diagonalization theorem of linear algebra (Lay 2012, p. 282). Clearly then, the algorithm is implemented by a 5-dimensional loop. One for each index $\alpha, \beta, \gamma, \delta$, and one loop until the desired precision is obtained. For brevity, the please see the github-page for the implementation: `http://github.com/kingoslo/flintstones`.

Much effort was made to ensure that the code ran correctly. As we will see in the results, the code produced the correct energies for a number of values of μ an N.

RESULTS AND DISCUSSION

We introduce the results in the order they appeared in the project description.

`(nx,ny,spin,energy)`:

```
(0,0,0,1),(0,0,1,1),
(0,1,0,2),(0,1,1,2),(1,0,0,2),(1,0,1,2),
(0,2,0,3),(0,2,1,3),(1,1,0,3),(1,1,1,3),(2,0,0,3),(2,0,1,3),
(0,3,0,4),(0,3,1,4),(1,2,0,4),(1,2,1,4),(2,1,0,4),(2,1,1,4),(3,0,0,4),(3,0,1,4),
```

Find the energy for 6,12,20,30 elektroner `(nx,ny,spin,energy)`:

```
(0,0,0,1),(0,0,1,1),
(0,1,0,2),(0,1,1,2),(1,0,0,2),(1,0,1,2),
(0,2,0,3),(0,2,1,3),(1,1,0,3),(1,1,1,3),(2,0,0,3),(2,0,1,3),
(0,3,0,4),(0,3,1,4),(1,2,0,4),(1,2,1,4),(2,1,0,4),(2,1,1,4),(3,0,0,4),(3,0,1,4),
```

Integrator. Which quantum numbers are conserved? what are the possible total spin values?

PROPOSITION 1. *The Hartree-Fock basis is orthonormal.*

Proof. It is easy to see that the two dimensional Harmonic oscillator functions are orthonormal. To see this, just write up $\langle\psi_\alpha|\psi_\beta\rangle$ and factor each state function into a product of 1 dimensional state functions. Therefore

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi_\alpha^*(x,y)\psi_\beta(x,y)\,\mathrm{d}x\,\mathrm{d}y = \delta_{\alpha\beta} = \iint_{\mathbb{R}^2}\psi_\alpha^*\psi_\beta\,\mathrm{d}\sigma = \langle\alpha|\beta\rangle = \delta_{\alpha\beta} \tag{2}$$

Moreover, since the matrix elements C are unitary,

$$\sum_{\alpha=1}^{\infty}(C^\dagger)_{\alpha p}C_{q\alpha} = \delta_{pq} \tag{3}$$

$$\begin{aligned}
\langle\psi_p|\psi_q\rangle &= \iint_{\mathbb{R}^2}\psi_p^*\psi_q\,\mathrm{d}\sigma = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi_p^*(x,y)\psi_q(x,y)\,\mathrm{d}x\,\mathrm{d}y \\
&= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Big[\sum_{\alpha=1}^{\infty}C_{p\alpha}\psi_\alpha(x,y)\Big]^*\Big[\sum_{\beta=1}^{\infty}C_{q\beta}\psi_\beta(x,y)\Big]\,\mathrm{d}x\,\mathrm{d}y \\
&= \sum_{\alpha=1}^{\infty}\sum_{\beta=1}^{\infty}C_{p\alpha}^*C_{q\beta}\underbrace{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\psi_\alpha^*(x,y)\psi_\beta(x,y)\,\mathrm{d}x\,\mathrm{d}y}_{=\delta_{\alpha\beta}\quad(2)} \overset{(2)}{=} \sum_{\alpha=1}^{\infty}\sum_{\beta=1}^{\infty}C_{p\alpha}^*C_{q\beta}\delta_{\alpha\beta} \\
&= \sum_{\alpha=1}^{\infty}C_{p\alpha}^*C_{q\alpha} = \sum_{\alpha=1}^{\infty}(\underbrace{C_{p\alpha}}_{=C^{\mathsf{T}}{}_{\alpha p}})^*C_{q\alpha} = \sum_{\alpha=1}^{\infty}(C^{\mathsf{T}}{}_{\alpha p})^*C_{q\alpha} = \sum_{\alpha=1}^{\infty}(C^\dagger)_{\alpha p}C_{q\alpha} \overset{(3)}{=} \delta_{pq},
\end{aligned}$$

which proves that the Hartree-Fock basis is orthonormal ■

PROPOSITION 2. *Let $\psi_{p_1\cdots p_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)$ and $\psi_{\beta_1\cdots\beta_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)$ denote the Hartree-Fock and harmonic oscillator slater determintants respectively, then:*

$$\psi_{p_1\cdots p_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n) = \det(C)\psi_{\beta_1\cdots\beta_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)$$

Proof. Let's agree to write $\psi_{p_i}(x_j, y_j) = \psi_{p_i}(\mathbf{r}_j) = \psi_{p_i j}$. Now suppose A and B are matrices. Then we know that $\det(AB) = \det(A)\det(B)$ (†) by the multiplicative determinant theorem (Lay 2012, p. 173). Therefore it clearly follows that $\psi_{p_1\cdots p_n}(\mathbf{r}_1, \cdots, \mathbf{r}_n) = \det(C)\psi_{\alpha_1\cdots\alpha_n}(\mathbf{r}_1, \cdots, \mathbf{r}_n)$. To see this write

$$\begin{aligned}
\psi_{p_1\cdots p_n}(\mathbf{r}_1, \cdots, \mathbf{r}_n) &= \frac{1}{(n!)^{1/2}} \begin{vmatrix} \psi_{p_1 1} & \psi_{p_1 2} & \cdots & \psi_{p_1 n} \\ \psi_{p_2 1} & \psi_{p_2 2} & \cdots & \psi_{p_2 n} \\ \vdots & \ddots & & \vdots \\ \psi_{p_n 1} & \psi_{p_n 2} & \cdots & \psi_{p_n n} \end{vmatrix} \\
&= \frac{1}{(n!)^{1/2}} \begin{vmatrix} \sum_{\beta_1=1}^{\infty} C_{p_1\beta_1}\psi_{\beta_1 1} & \sum_{\beta_1=1}^{\infty} C_{p_1\beta_1}\psi_{\beta_1 2} & \cdots & \sum_{\beta_1=1}^{\infty} C_{p_1\beta_1}\psi_{\beta_1 n} \\ \sum_{\beta_2=1}^{\infty} C_{p_2\beta_2}\psi_{\beta_2 1} & \sum_{\beta_2=1}^{\infty} C_{p_2\beta_2}\psi_{\beta_2 2} & \cdots & \sum_{\beta_2=1}^{\infty} C_{p_2\beta_2}\psi_{\beta_2 n} \\ \vdots & \ddots & & \vdots \\ \sum_{\beta_n=1}^{\infty} C_{p_n\beta_n}\psi_{\beta_n 1} & \sum_{\beta_1=1}^{\infty} C_{p_n\beta_n}\psi_{\beta_n 2} & \cdots & \sum_{\beta_n=1}^{\infty} C_{p_n\beta_n}\psi_{\beta_n n} \end{vmatrix} \\
&= \frac{1}{(n!)^{1/2}} \begin{vmatrix} (C\psi)_{\beta_1 1} & (C\psi)_{\beta_1 2} & \cdots & (C\psi)_{\beta_1 n} \\ (C\psi)_{\beta_2 1} & (C\psi)_{\beta_2 2} & \cdots & (C\psi)_{\beta_2 n} \\ \vdots & \ddots & & \vdots \\ (C\psi)_{\beta_n 1} & (C\psi)_{\beta_n 2} & \cdots & (C\psi)_{\beta_n n} \end{vmatrix} \overset{(\dagger)}{=} \det(C)\psi_{\beta_1\cdots\beta_n}(\mathbf{r}_1, \cdots, \mathbf{r}_n),
\end{aligned}$$

which proves the proposition. ■

Lets show two corollaries of this proposition. We first show a little lemma

LEMMA 1. *Suppose C is unitary over $\mathbb{C}$. Then there exist a $\theta \in (-\pi, \pi]$ such that* $\det(C) = e^{i\theta}$.

Proof. Since by the Leibniz formula, $\det(C) \in \mathbb{C}$ and hence there exist $\theta \in (-\pi, \pi]$ and $r > 0$ such that $\det C = re^{i\theta}$. Therefore $r = 1$ if and only if $|\det(C)| = 1$. Since we know that for any matrix $\det A = \det A^{\mathsf{T}}$ $(*)$ (Lay 2012, p. 172). Moreover as a corollary of the Leibniz formula, $\det(A^*) = (\det A)^*$ $(**)$. We know that the determinant of the identity is 1, so we can write

$$\begin{aligned}
1 = \det(I) = \det(C^\dagger C) &\overset{(\dagger)}{=} \det(C^\dagger)\det(C) = \det\left((C^*)^{\mathsf{T}}\right)\det(C) \\
&\overset{(*)}{=} \det\left(C^*\right)\det(C) \overset{(**)}{=} \det(C)^*\det(C) = |\det(C)|^2 \qquad \text{only if} \qquad |\det(C)| = \pm 1, \qquad (4)
\end{aligned}$$

But since we saw that $\det C = re^{i\theta}$, we get

$$0 < r = |r| = |r||e^{i\theta}| = |re^{i\theta}| = |\det(C)| \overset{(4)}{=} \pm 1,$$

and the lemma follows. ■

In particular, the norm of the determinant is 1. To obtain the first corollary is easy now since it is

COROLLARY 1. *Assume $\psi_{p_1\cdots p_n}(\mathbf{r}_1, \cdots, \mathbf{r}_n)$ and $\psi_{\beta_1\cdots\beta_n}(\mathbf{r}_1, \cdots, \mathbf{r}_n)$ denote the Hartree-Fock and harmonic oscillator slater determintants respectively, then there exist an $\alpha \in \mathbb{R}$ such that.*

$$\psi_{p_1\cdots p_n}(\mathbf{r}_1, \cdots, \mathbf{r}_n) = e^{i\theta}\psi_{\beta_1\cdots\beta_n}(\mathbf{r}_1, \cdots, \mathbf{r}_n)$$

Proof. By proposition 2 we have that

$$\psi_{p_1\cdots p_n}(\mathbf{r}_1, \cdots, \mathbf{r}_n) = \det(C)\psi_{\beta_1\cdots\beta_n}(\mathbf{r}_1, \cdots, \mathbf{r}_n)$$

Now since C is unitary we know by lemma 1 that there exist an $\alpha \in \mathbb{R}$ such that $\det C = e^{i\alpha}$. ■

The second corollary is a also very easy,

COROLLARY 2. *Assume $\psi_{p_1\cdots p_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)$ and $\psi_{\beta_1\cdots\beta_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)$ denote the Hartree-Fock and harmonic oscillator slater determintants respectively. Then $\psi_{p_1\cdots p_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)$ is normalized if and only if $\psi_{\beta_1\cdots\beta_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)$ is normalized regardless of the choice of norm.*

Proof. By the corollary we know that

$$\psi_{p_1\cdots p_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n) = e^{i\theta}\psi_{\beta_1\cdots\beta_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)$$

Now suppose that $\|\cdot\|$ is any norm, then $\|a\psi\| = |a|\|\psi\|$ (/) (Lindstrøm 2016, p. 124). Then

$$\|\psi_{p_1\cdots p_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)\| = \|e^{i\theta}\psi_{\beta_1\cdots\beta_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)\| \overset{(/)}{=} |e^{i\theta}|\|\psi_{\beta_1\cdots\beta_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)\| = \|\psi_{\beta_1\cdots\beta_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)\|$$

And hence $\psi_{\beta_1\cdots\beta_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)$ is normalized if and only if $\psi_{p_1\cdots p_n}(\mathbf{r}_1,\cdots,\mathbf{r}_n)$ is normalized. ■

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)
Vis siste avsnitt 1d
Forklar hva de forskjellige termene er

R	N							
	2	4	6	8	12	14	18	20
4	3.1626916	10.747470	20.766927	34.829996	70.673854	92.85253	145.9196	177.9632
5	3.1619219	10.745515	20.748418	34.266168	67.569938	89.21037	139.7442	168.5296
6	3.1619219	10.744865	20.720248	34.184146	67.296902	87.85635	134.8867	161.3397
7	3.1619096	10.744678	20.720123	34.152530	66.934710	87.33664	133.9035	159.9586
9	3.1619143	10.744446	20.719239	34.152248	66.912283	87.13293	132.8712	158.2259
13	-	-	-	-	-	-	-	-

Hvor mange singlepartikkel tilstander trenger vi før hartree fock energien stabiliseres? Kalles Hartree fock limit
Sammenlign hartree fock energi og uforstyrret energi
How much do the single-particle energies change compared to the harmonic oscillator energies?
Are the degeneracies seen in the harmonic oscillator calculations preserved?

CONCLUSION AND PERSPECTIVES

APPENDIX

THEOREM 2 (Gaussian quadrature)**.** *Suppose $A \subseteq \mathbb{R}$ and there exist an orthogonal basis $\{H_n\}_{n=0}^{\infty}$ of polynomials for the set of square integrable functions on A with respect to the inner product*

$$\langle f, g\rangle = \int_A (Wfg)(x)\,\mathrm{d}x.$$

Suppose also that H_n is a degree n-polynomial and $|\langle H_n, H_n\rangle| = c_n$. If $f : \mathbb{R} \to \mathbb{R}$ is integrable on A and there exist and $N \in \mathbb{N}$ such that $f(x) = (WP_{2N-1})(x)$, then

$$\int_A f(x)\,\mathrm{d}x = c_0 \sum_{i=1}^{N} (H^{-1})_{0n} P_{2N-1}(x_n),$$

where $\{x_n\}_{n=1}^{N}$ are the zeros of H_N and $(H^{-1})_{0n}$ is the inverse of the matrix with elements $H_{nk} = H_k(x_n)$.

Proof. Assume that the hypothesis is true, then in particular

$$f(x) = (WP_{2N-1})(x) \tag{5}$$

Since $\{H_n\}_{n=1}^{\infty}$ is a polynomial basis for the space of square integrable $\mathbb{R} \to \mathbb{R}$-functions, there exist polynomials Q_{N-1} and R_{N-1}, such that

$$P_{2N-1}(x) = H_N(x)R_{N-1}(x) + Q_{N-1}(x) = H_N(x)\sum_{k=0}^{N-1} r_n H_k(x) + \sum_{k=0}^{N-1} q_k H_k(x) \tag{6}$$

Moreover, since the basis is orthogornal with respect to the given inner product, there exist normalization c_m such that

$$\langle H_n, H_m \rangle = \int_A W(x)H_n(x)H_m(x)\,\mathrm{d}x = c_m \delta_{mn}. \tag{7}$$

Therefore the integral of interest is

$$\begin{aligned}\int_A f(x)\,\mathrm{d}x &\overset{5}{=} \int_A W(x)P_{2N-1}(x)\,\mathrm{d}x \overset{(6)}{=} \int_A W(x)\left[H_N(x)\sum_{k=0}^{N-1} r_n H_k(x) + \sum_{k=0}^{N-1} q_k H_k(x)\right]\mathrm{d}x \\ &\overset{(7)}{=} 0 + \sum_{k=0}^{N-1}\int_A W(x)q_k H_k(x)\,\mathrm{d}x = \sum_{k=0}^{N-1} q_k \int_A W(x)H_k(x)\cdot \underbrace{1}_{=H_0}\,\mathrm{d}x \overset{(7)}{=} \sum_{k=0}^{N-1} q_k c_k \delta_{k0} \\ &= q_0 c_0 \end{aligned} \tag{8}$$

Since $H_N(x)$ is a degree N polynomial by assumption, H_N has exactly N zeros by the fundamental theorem of algebra (Forster 1991, p. 12). Therefore there exist a set $\{x_k\}_{k=1}^{N}$ such that $H_N(x_k) = 0$ for all $1 \le k \le N$. Define now $c_n = Q_{N-1}(x_n)$ and observe that

$$c_n = Q_{N-1}(x_n) \overset{(6)}{=} \sum_{k=0}^{N-1} q_k H_k(x_n) \equiv \sum_{k=0}^{N-1} q_k H_{nk} \tag{9}$$

Since $\{H_n\}$ is a basis, each element is linearly independent, and therefore the matrix consisting of elements H_{nk} is invertible with inverse $(H^{-1})_{mn}$. By solving for b_k we obtain

$$\sum_{n=0}^{N-1}(H^{-1})_{mn}Q_{N-1}(x_n) = \sum_{n=0}^{N-1}(H^{-1})_{mn}c_n \overset{(9)}{=} \sum_{k=0}^{N-1}\sum_{n=0}^{N-1} q_k (H^{-1})_{mn}H_{nk} = \sum_{k=0}^{N-1} q_k \delta_{mk} = q_m \tag{10}$$

But since $\{x_k\}$ are the zeros (†) of H_N, we see that

$$\begin{aligned} q_m &\overset{(10)}{=} \sum_{n=0}^{N-1}(H^{-1})_{mn}Q_{N-1}(x_n) \overset{(6)}{=} \sum_{n=0}^{N-1}(H^{-1})_{mn}\Big[P_{2N-1}(x_n) - \underbrace{H_N(x_n)}_{=0 \quad (\dagger)} R_{N-1}(x_n)\Big] \\ &\overset{(\dagger)}{=} \sum_{n=0}^{N-1}(H^{-1})_{mn}P_{2N-1}(x_n) \qquad \text{only if} \qquad q_0 = \sum_{n=0}^{N-1}(H^{-1})_{0n}P_{2N-1}(x_n). \end{aligned} \tag{11}$$

By setting (11) equal to (8), the theorem follows. ■

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