SOME TITLE

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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

A.

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

METHODS

Suppose $\lfloor\cdot\rfloor$ denotes the floor function on $\mathbb{R}$, then we know that the Hermite polynomials are given by

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

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

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(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),
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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, $p, q, r, s \in \{1, 2, \cdots\}$ and let $A = \{p, q, r, s\}$, $B = \{(1, p), (2, q), (1, r), (2, s)\}$ then a parameterization of the matrix element $\langle pq|V|rs\rangle$ is

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

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

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

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

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

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

RESULTS AND DISCUSSION

CONCLUSION AND PERSPECTIVES

APPENDIX

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. Assume that the hypothesis is true, then in particular

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

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

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

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

$$\langle H_n, H_m\rangle = \int_A W(x)H_n(x)H_m(x)\,\mathrm{d}x = c_m\delta_{mn}. \tag{3}$$

Therefore the integral of interest is

$$\begin{aligned}\int_A f(x)\,\mathrm{d}x &\stackrel{1}{=} \int_A W(x)P_{2N-1}(x)\,\mathrm{d}x \stackrel{(2)}{=} \int_A W(x)\left[H_N(x)\sum_{k=0}^{N-1} r_n H_k(x) + \sum_{k=0}^{N-1} q_k H_k(x)\right]\mathrm{d}x \\ &\stackrel{(3)}{=} 0 + \sum_{k=0}^{N-1}\int_A W(x) q_k H_k(x)\,\mathrm{d}x = \sum_{k=0}^{N-1} q_k \int_A W(x)H_k(x)\cdot \underbrace{1}_{=H_0}\,\mathrm{d}x \stackrel{(3)}{=} \sum_{k=0}^{N-1} q_k c_k \delta_{k0} \\ &= q_0 c_0 \end{aligned} \tag{4}$$

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 $1 \leq k \leq N$. Define now $c_n = Q_{N-1}(x_n)$ and observe that

$$c_n = Q_{N-1}(x_n) \overset{(2)}{=} \sum_{k=0}^{N-1} q_k H_k(x_n) \equiv \sum_{k=0}^{N-1} q_k H_{nk} \tag{5}$$

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

$$\sum_{n=0}^{N-1} (H^{-1})_{mn} Q_{N-1}(x_n) = \sum_{n=0}^{N-1} (H^{-1})_{mn} c_n \overset{(5)}{=} \sum_{k=0}^{N-1} \sum_{n=0}^{N-1} q_k (H^{-1})_{mn} H_{nk} = \sum_{k=0}^{N-1} q_k \delta_{mk} = q_m \tag{6}$$

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

$$\begin{aligned} q_m &\overset{(6)}{=} \sum_{n=0}^{N-1} (H^{-1})_{mn} Q_{N-1}(x_n) \overset{(2)}{=} \sum_{n=0}^{N-1} (H^{-1})_{mn} \Big[P_{2N-1}(x_n) - \underbrace{H_N(x_n)}_{=0 \quad (\dagger)} R_{N-1}(x_n) \Big] \\ &\overset{(\dagger)}{=} \sum_{n=0}^{N-1} (H^{-1})_{mn} P_{2N-1}(x_n) \qquad \text{only if} \qquad q_0 = \sum_{n=0}^{N-1} (H^{-1})_{0n} P_{2N-1}(x_n). \end{aligned} \tag{7}$$

By setting (7) equal to (4), the theorem follows. ■

LITERATURE CITED

[1] Otto Forster. *Lectures on Riemann Surfaces*. 1st ed. New York: Springer-Verlag, 1991.