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MACC EXERCISE 01 SS 2022

19.4.22
Lambert Theisen

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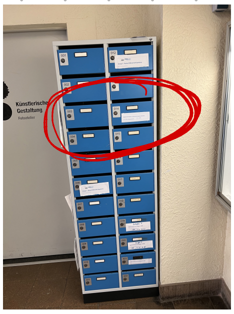
- Me
- RWTHOnline : All exercise

#2 03.05 CHW2



Homeworks (5-6 sheets)

→ 2 weeks time

→ Submit into the blue box in Rogowski

→ Complementary to lecture (some new material, exam relevant)

→ Upload some days before exercise ⇒ Questions a-priori via mail

→ Any other questions? Dates ok?

E 1 Hydrogen Schrödinger EVP

Eigenvalue (Energy)

Find (Φ, E) s.t. $\mathcal{H}\Phi = E\Phi$ (EVP)

with $\mathcal{H} := -\Delta + \frac{1}{|x|}$ $\quad x \in \mathbb{R}^3$

Eigenfunction (Wave function)

Ansatz: Spherical Coords : $\Phi := \Phi\begin{pmatrix} r \\ \theta \\ \varphi \end{pmatrix}$ with $r \in (0,\infty)$, $\theta \in [0,\pi]$, $\varphi \in [0,2\pi]$

⇝ Insert & transform Diff-Ops:

$$-\frac{1}{\partial r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\Phi\right) - \frac{1}{\partial r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\Phi\right) - \frac{1}{\partial r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\Phi - \frac{\Phi}{r} = E\Phi$$

Ansatz: Separation of Variables: $\Phi\begin{pmatrix} r \\ \theta \\ \varphi \end{pmatrix} := R(r)\cdot Y(\theta,\varphi)$

⇝ Insert & separate :

I) $\frac{1}{R(r)}\frac{d}{dr}\left(r^2\frac{d}{dr}R(r)\right) + 2r(1+Er) = \lambda$

II) $\frac{1}{Y\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}Y\right) + \frac{1}{Y\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}Y - \lambda = 0$

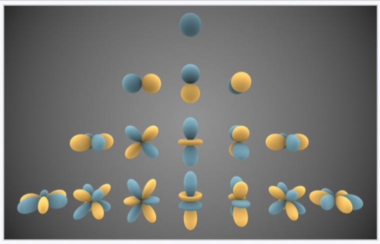
Spherical Harmonics

→ Solution to II)

$$Y_l^m(\theta,\varphi) = \begin{cases} (-1)^{|m|} N_l^{|m|} P_l^{|m|}(\cos\theta)\sin(|m|\theta) & m<0 \\ N_l^{|m|} P_l^{0}(\cos\theta) & m=0 \\ (-1)^{|m|} N_l^{m} P_l^{m}(\cos\theta)\sin(m\theta) & m>0 \end{cases}$$

$$\boxed{\begin{array}{l} l \in \mathbb{N}_0 := \{0,1,\dots\} \\ -l \leq m \leq l \end{array}}$$

- P_l^m are assoc. Legendre Polynomials of degree l & order m.
- Coeffs $N_l^m := \begin{cases} \sqrt{\frac{2l+1}{4\pi}} & m=0 \\ \sqrt{2}\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-m)!}{(l+m)!}} & m>0 \end{cases}$
- Value for λ for Y_l^m is $l\cdot(l+1)$ ✓



Visual representations of the first few real spherical harmonics. Blue portions represent regions where the function is positive, and yellow portions represent where it is negative. The distance of the surface from the origin indicates the absolute value of $Y_\ell^m(\theta,\phi)$ in angular direction (θ,ϕ).

Radial Part:

- Use $R(r) = \frac{g(r)}{r}$ & $E = -\frac{\mu^2}{2} < 0$, I) can be reduced to:

$$g''(r) + \left(-\mu^2 + \frac{2}{r} - \frac{l(l+1)}{r^2}\right) g(r) = 0$$

Since: $r^2 \frac{d}{dr} R(r) = -\frac{r^2 g(r)}{r^2} + \frac{g'(r)\cdot r^2}{r}$ $\quad r^2 \frac{d}{dr} R(r) = \frac{d}{dr}\left(\frac{1}{r}\right)\cdot g(r) r^2 + \left(\frac{r^2}{r}\right)\cdot \frac{d}{dr}(g(r))$

$$\Rightarrow \frac{d}{dr}\left(r^2 \frac{d}{dr} R(r)\right) = -g'(r) + g''(r)\cdot r + g'(r) = g''(r)\cdot r$$

$$\Rightarrow \frac{1}{R(r)} \frac{d}{dr}\left(r^2 \frac{d}{dr} R(r)\right) + 2r(1 + Er) - \underbrace{\lambda}_{l(l+1)} = 0$$

$$\Leftrightarrow \quad g''(r)\cdot r + 2\, g(r)\left(1 + \frac{\mu^2}{2} r - \frac{l(l+1)}{2r}\right) = 0 \qquad \Big| : r$$

$$g''(r) + g(r)\left(\frac{2}{r} - \mu^2 - \frac{l(l+1)}{r^2}\right) = 0 \qquad (7)$$

Far-Field Asymptotic Limit ($r \to \infty$)

- For $r \to \infty$, (7) reduces to $g_\infty''(r) - g_\infty(r)\mu^2 = 0$

$$\Rightarrow \quad g_\infty(r) = C_1 e^{-\mu\cdot r}$$

a): Change-of-Variables $(x := 2\mu r)$

$\to$ Then $g(r) = g\left(\frac{x}{2\mu}\right) =: \tilde{g}(x)$

$\to$ Chain rule: $\frac{d}{dx}\tilde{g}(x) = g'(r) \cdot \frac{1}{2\mu} \iff \tilde{g}'(x)\, 2\mu = g'(r)$

$$\frac{d}{dx}\tilde{g}'(x) = \frac{1}{2\mu}\frac{d}{dx}g'(r) = \frac{1}{2\mu}\frac{d}{dx}g'\left(\frac{x}{2\mu}\right) = \frac{1}{(2\mu)^2}g''(r) \iff \tilde{g}''(x)\cdot 4\mu^2 = g''(r)$$

Insert into (7): $4\mu^2\tilde{g}''(x) + \tilde{g}(x)\left(\frac{2}{\left(\frac{x}{2\mu}\right)} - \mu^2 - \frac{\ell(\ell+1)}{\left(\frac{x}{2\mu}\right)^2}\right) = 0$

$$4\mu^2\tilde{g}'' + \tilde{g}\left(\frac{4\mu}{x} - \mu^2 - \frac{\ell(\ell+1)\,4\mu^2}{x^2}\right) = 0 \quad \Big| : 4\mu^2$$

$$\tilde{g}'' + \tilde{g}\left(\frac{1}{\mu x} - \frac{1}{4} - \frac{\ell(\ell+1)}{x^2}\right) = 0 \quad \checkmark$$

Relabel: g'' g

b) c),d),e) $\rightsquigarrow$ HW b) Euler?

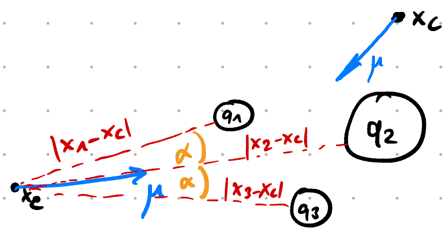
[2] Electronic Density

$$\rho(x,t) := N \cdot \int_{\mathbb{R}^{3(N-1)}} |\Psi(x, x_2, \dots, x_N)|^2\, dx_2 \cdots dx_N$$

Probability to find any electron at position $x \in \mathbb{R}^3$ at time $t \in \mathbb{R}^+$

$\rightsquigarrow$ Use that Ψ is anti-symmetric: $\Psi(x_1, \dots, x_i, \dots, x_j, \dots, x_N) = -\Psi(x_1, \dots, x_j, \dots, x_i, \dots, x_N)$

[3] Dipole Operator



$$\vec{\mu} = \sum_{i=1}^{N} q_i(x_i - x_c)$$

Quantum Dipole operator: $P: L^2(\mathbb{R}^{3N}) \to L^2(\mathbb{R}^{3N})$ of N electrons with charge -1

$$P := P(x_1, \dots, x_N) = -\sum_{i=1}^{N}(x_i - x_c)$$

To show: Mean-Value of dipole measurement for a state $|\Psi\rangle$:

$$\langle \psi | \mathcal{P} \psi \rangle := \int_{\mathbb{R}^{3N}} \psi^*(x_1 \dots x_N)\, \mathcal{P}\, \psi(x_1 \dots x_N)\, dx_1 \cdots dx_N$$

$$= -\int_{\mathbb{R}^{3N}} \psi^* \left(\sum_{i=1}^{N} (x_i - x_c) \right) \psi \quad dx_1 \cdots dx_N \Big) \, dx_i$$

$|\psi|^2$ ①

...

$\rightarrow \rho(x,t)$ erkennen....

$$\int_{\mathbb{R}^3} \left[\int_{\mathbb{R}^{3(N-1)}} \psi^* \psi \quad dx_1 .. dx_5 dx_7 d_0 \right] d\, x_i$$

[4] Poisson Brackets:

$\rightarrow$ N particles in 1D with position q_i, momentum p_i

$\rightarrow$ collect in $\mathbb{R}^{2N} \ni x = \begin{pmatrix} q \\ p \end{pmatrix} = \begin{bmatrix} q_1 \\ \vdots \\ q_N \\ p_1 \\ \vdots \\ p_N \end{bmatrix}$

Poisson Bracket: Let $\phi_1, \phi_2 \in C_0^\infty(\mathbb{R}^{2N})$ (compactly supported test functions).

$$\{\phi_1, \phi_2\}(x) := (\nabla_x \phi_1(x))^T J \nabla_x \phi_2(x) \quad \text{with} \quad J = \begin{bmatrix} 0 & 1_N \\ -1_N & 0 \end{bmatrix} = \left[\begin{array}{c|c} 0 & \begin{smallmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{smallmatrix} \\ \hline \begin{smallmatrix} -1 & & 0 \\ & \ddots & \\ 0 & & -1 \end{smallmatrix} & 0 \end{array}\right]$$

$1_N \in \mathbb{R}^{N \times N}$

a) i) Linearity: $\{\varphi_1, \alpha\varphi_2 + \beta\varphi_3\} \overset{!}{=} \alpha\{\varphi_1, \varphi_2\} + \beta\{\varphi_1, \varphi_3\} \; \forall \alpha, \beta \in \mathbb{R}$

$\rightsquigarrow$ Just insert

linear $\beta \cdot \bullet$ linear

$$\{\varphi_1, \alpha\varphi_2 + \beta\varphi_3\} = [\nabla_x \varphi_1(x)]^T \left[\begin{array}{c|c} 0 & 1_N \\ \hline -1_N & 0 \end{array}\right] [\alpha \nabla_x \varphi_2(x) + \beta \nabla_x \varphi_3(x)]$$

$$= \alpha \begin{bmatrix} \nabla_q \varphi_1(x) \\ \nabla_p \varphi_1(x) \end{bmatrix}^T \left[\begin{array}{c|c} 0 & 1_N \\ \hline -1_N & 0 \end{array}\right] \begin{bmatrix} \nabla_q \varphi_2(x) \\ \nabla_p \varphi_2(x) \end{bmatrix} + \beta \begin{bmatrix} \nabla_q \varphi_1(x) \\ \nabla_p \varphi_1(x) \end{bmatrix}^T \left[\begin{array}{c|c} 0 & 1_N \\ \hline -1_N & 0 \end{array}\right] \begin{bmatrix} \nabla_q \varphi_3(x) \\ \nabla_p \varphi_3(x) \end{bmatrix}$$

// unnötiger Schritt

$$= \alpha \begin{bmatrix} \nabla_q \varphi_1(x) \\ \nabla_p \varphi_1(x) \end{bmatrix}^T \begin{bmatrix} \nabla_p \varphi_2(x) \\ \nabla_q \varphi_2(x) \end{bmatrix} + \beta \begin{bmatrix} \nabla_q \varphi_1(x) \\ \nabla_p \varphi_1(x) \end{bmatrix}^T \begin{bmatrix} \nabla_p \varphi_3(x) \\ \nabla_q \varphi_3(x) \end{bmatrix}$$

$$= \alpha \{\varphi_1, \varphi_2\}(x) + \beta \{\varphi_1, \varphi_3\}(x) \; \checkmark \quad \forall \alpha, \beta \in \mathbb{R}$$

ii) - v) $\rightsquigarrow$ HW

b) $\{q_i, q_j\} = [\nabla_x q_i]^T J \nabla_x q_j = \begin{bmatrix} \nabla_q \begin{pmatrix} 0 \\ \vdots \\ q_i \\ \vdots \\ 0 \\ \vdots \\ 0 \end{pmatrix} \end{bmatrix}^T J \; \nabla_q \begin{pmatrix} 0 \\ \vdots \\ q_j \\ \vdots \\ 0 \\ \vdots \\ 0 \end{pmatrix} = e_i^T J e_j = e_i^T(-e_{j+N}) = 0$

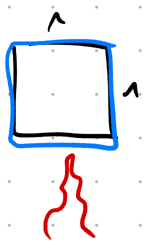
...

c) To show: $\{H, H\}(x)$ $\rightsquigarrow$ Insert & use separability of $H(x) = V(q) + T(p)$

d) Define whole momentum $P(x) := \frac{1}{N} \sum_{i=1}^{N} p_i$ & calc. $\{P, H\}(x) = \dots = 0 \; \checkmark$

Separation of Variables

$-\Delta u = 1$
$u = 0$



$$-\partial_{xx} u - \partial_{yy} u = 1 \iff -X''(x)\cdot Y(y) - X(x)\,Y''(y) = 0$$

$$\iff -X''\cdot Y = X\cdot Y'' \quad \Big|\cdot \frac{1}{X\cdot Y}$$

SV: $u = X(x)\,Y(y)$

$$f(x) = -\frac{X''(x)}{X(x)} = \frac{Y''(y)}{Y(y)} = g(y)$$

When x varies, $f(x) = \text{const}$ because $g(y)$

Extract 2 ODEs

I) $-\frac{X''}{X} = \lambda^2$ ⤳ $\lambda = ?$

II) $\frac{Y''}{Y} = \lambda^2$

I) $\Rightarrow$ $X(x) = \overset{\text{BC}}{A}\cdot \sin(\pi x) + \overset{\text{BC}}{B}\cos(\pi x)$

$X''(x) = -\pi^2 \cdot X$

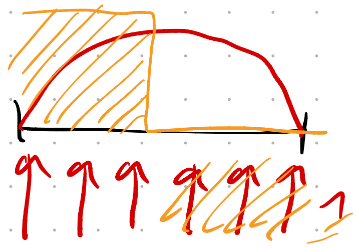
$u = 0 \Rightarrow B = 0$

Weak Solutions

Find $T \in C^2$

$-\partial_{xx} T = 1$ on $\forall x \in (0,1) = \Omega$

$T = 0$ on $\partial\Omega$



$T = \sin(\pi x)$

$$-\partial_{xx4} T = \begin{cases} 1 & \text{on } x \leq 0.5 \\ 0 & \end{cases}$$

$$\int_0^1 -\partial_{xx} T \cdot \varphi = \int_0^1 \begin{Bmatrix} 1 \\ 0 \end{Bmatrix} \cdot \varphi \qquad \forall \varphi \in C_c^\infty$$