Corrigé TD 2

Exo 1

$$\frac{\partial^2}{\partial\rho^2}\left(e^{-\rho}\rho^{l+1}v(\rho)\right) = \frac{\partial}{\partial\rho}\left(-e^{-\rho}\rho^{l+1}v(\rho) + e^{-\rho}(l+1)\rho^{l}v(\rho) + e^{-\rho}\rho^{l+1}\frac{\partial v}{\partial\rho}\right)$$

$$= e^{-\rho}\rho^{l+1}v(\rho) - e^{-\rho}(l+1)\rho^{l}v(\rho) - e^{-\rho}\rho^{l+1}\frac{\partial v}{\partial\rho}$$

$$- e^{-\rho}(l+1)\rho^{l}v(\rho) + e^{-\rho}l(l+1)\rho^{l-1}v(\rho) + e^{-\rho}(l+1)\rho^{l}\frac{\partial v}{\partial\rho}$$

$$- e^{-\rho}\rho^{l+1}\frac{\partial v}{\partial\rho} + e^{-\rho}(l+1)\rho^{l}\frac{\partial v}{\partial\rho} + e^{-\rho}\rho^{l+1}\frac{\partial^2 v}{\partial\rho^2}$$

$$= e^{-\rho}\rho^{l+1}\left(v(\rho) - \frac{l+1}{\rho}v(\rho) - \frac{\partial v}{\partial\rho} - \frac{(l+1)}{\rho}v(\rho) + \frac{l(l+1)}{\rho^2}v(\rho) + \frac{l+1}{\rho}\frac{\partial v}{\partial\rho}\right.$$

$$\left. - \frac{\partial v}{\partial\rho} + \frac{(l+1)}{l}\frac{\partial v}{\partial\rho} + \frac{\partial^2 v}{\partial\rho^2}\right)$$

$$= e^{-\rho}\rho^{l+1}\left(\left(1 - \frac{2(l+1)}{\rho} + \frac{l(l+1)}{\rho^2}\right)v(\rho) + 2\left(\frac{l+1}{\rho} - 1\right)\frac{\partial v}{\partial\rho} + \frac{\partial^2 v}{\partial\rho^2}\right)$$ CQFD

$$0 = \left(\frac{\partial^2}{\partial\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{\rho_0}{\rho} - 1\right)\left(e^{-\rho}\rho^{l+1}v(\rho)\right)$$

$$= e^{-\rho}\rho^{l+1}\left(\left(1 - \frac{2(l+1)}{\rho} + \frac{l(l+1)}{\rho^2}\right)v(\rho) + 2\left(\frac{l+1}{\rho} - 1\right)\frac{\partial v}{\partial\rho} + \frac{\partial^2 v}{\partial\rho^2} - \frac{l(l+1)}{\rho^2}v(\rho) + \frac{\rho_0}{\rho}v(\rho) - v(\rho)\right)$$

$$= e^{-\rho}\rho^{l+1}\left(-\frac{2(l+1)}{\rho}v(\rho) + 2\left(\frac{l+1}{\rho} - 1\right)\frac{\partial v}{\partial\rho} + \frac{\partial^2 v}{\partial\rho^2} + \frac{\rho_0}{\rho}v(\rho)\right)$$

$$= e^{-\rho}\rho^{l}\left(-2(l+1) + \rho_0 + 2(l+1-\rho)\frac{\partial}{\partial\rho} + \rho\frac{\partial^2}{\partial\rho^2}\right)v(\rho)$$

$$\Rightarrow \boxed{\left(\rho_0 - 2(l+1) + 2(l+1-\rho)\frac{\partial}{\partial\rho} + \rho\frac{\partial^2}{\partial\rho^2}\right)v(\rho) = 0}$$

Exo 3

(a) $$\vec{L}^2\,\psi_{Elm} = \hbar^2 l(l+1)\,\psi_{Elm}$$

$$\Rightarrow \left(-\frac{\hbar^2}{2m_e}\left(\frac{2}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2}\right) + \frac{\hbar^2 l(l+1)}{2m_e r^2} - \frac{e^2}{r}\right)R_{El} = E\,R_{El} \qquad (*)$$

2(a)

$$h_l u_{El} = \left(\frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2} + \frac{2}{a_0 r}\right) r R_{El}$$

$$\left(2\frac{\partial}{\partial r} + r\frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r} + \frac{2}{a_0}\right) R_{El}$$

$$\Rightarrow -\frac{\hbar^2}{2m_e r} h_l u_{El} = \left(-\frac{\hbar^2}{2m_e}\left(\frac{2}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2}\right) + \frac{\hbar^2 l(l+1)}{2m_e r^2} - \frac{e^2}{r}\right) R_{El} \overset{(*)}{=} E R_{El} = \frac{1}{r} E u_{El}$$

$$\Rightarrow \boxed{h_l u_{El} = \underbrace{\left(-\frac{2m_e}{\hbar^2} E\right)}_{\epsilon} u_{El}}$$

(b)

$$\int_0^\infty \left(\left(\underbrace{-\frac{\partial}{\partial r} + \frac{l}{r} - \frac{1}{a_0 l}}_{a_l^+}\right) f\right)(r)^* g(r)\, dr$$

$$= \int_0^\infty \left(-\frac{\partial f^*}{\partial r} + \frac{l f^*(r)}{r} - \frac{f^*(r)}{a_0 l}\right) g(r)\, dr$$

$$= \underbrace{-\int_0^\infty \frac{\partial f^*}{\partial r} g(r)\, dr}_{} + l \int_0^\infty \frac{f^*(r)}{r} g(r)\, dr - \frac{1}{a_0 l}\int_0^\infty f^*(r) g(r)\, dr$$

intégration par parties: $f(0) = g(0) = 0$ par hypothèse,
$\lim_{r\to\infty} f(r) = \lim_{r\to\infty} g(r) = 0$ car $\int^\infty |f|^2$ et $\int^\infty |g|^2 < \infty$

$$\Rightarrow -\int_0^\infty \frac{\partial f^*}{\partial r} g(r) dr = + \int_0^\infty f^*(r) \frac{\partial g}{\partial r} dr$$

$$= \int_0^\infty f^*(r)\left(\frac{\partial g}{\partial r} + \frac{l g(r)}{r} - \frac{g(r)}{a_0 l}\right) dr$$

$$= \int_0^\infty f^*(r) \underbrace{\left(\frac{\partial}{\partial r} + \frac{l}{r} - \frac{1}{a_0 l}\right)}_{a_l} g(r)\, dr \qquad \text{CQFD}$$

$$[a_l, a_l^+] = \left[\frac{\partial}{\partial r} + \frac{l}{r}, -\frac{\partial}{\partial r} + \frac{l}{r}\right] = \left[\frac{\partial}{\partial r}, \frac{l}{r}\right] - \left[\frac{l}{r}, \frac{\partial}{\partial r}\right]$$

$$= 2\left[\frac{\partial}{\partial r}, \frac{l}{r}\right]$$ se calcule par l'action sur une fonction test

$$\psi(r): \left[\frac{\partial}{\partial r}, \frac{l}{r}\right]\psi(r) = \frac{\partial}{\partial r}\left(\frac{l}{r}\psi(r)\right) - \frac{l}{r}\frac{\partial \psi}{\partial r} = -\frac{l}{r^2}\psi(r) + \underbrace{\frac{l}{r}\frac{\partial \psi}{\partial r} - \frac{l}{r}\frac{\partial \psi}{\partial r}}_{0}$$

$$\Rightarrow \boxed{[a_l, a_l^+] = -\frac{2l}{r^2}}$$

(c)
$$-a_l^+ a_l + \frac{1}{a_0^2 l^2} = -\left(-\frac{\partial}{\partial r} + \frac{l}{r} - \frac{1}{a_0 l}\right)\left(\frac{\partial}{\partial r} + \frac{l}{r} - \frac{1}{a_0 l}\right) + \frac{1}{a_0^2 l^2}$$

$$= \frac{\partial^2}{\partial r^2} - \frac{l}{r^2} + \frac{l}{r}\frac{\partial}{\partial r} - \frac{1}{a_0 l}\frac{\partial}{\partial r} - \frac{l}{r}\frac{\partial}{\partial r} - \frac{l^2}{r^2} + \frac{1}{a_0 r} + \frac{1}{a_0 l}\frac{\partial}{\partial r} + \frac{1}{a_0 r} - \frac{1}{a_0^2 l^2} + \frac{1}{a_0^2 l^2}$$

$$= \frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2} + \frac{2}{a_0 r} = h_l$$

$$a_{l+1} a_{l+1}^+ = a_{l+1}^+ a_{l+1} + \left[a_{l+1}, a_{l+1}^+\right] = a_{l+1}^+ a_{l+1} - \frac{2(l+1)}{r^2}$$

$$\Rightarrow -a_{l+1} a_{l+1}^+ + \frac{1}{a_0^2 (l+1)^2} = \frac{2(l+1)}{r^2} \underbrace{- a_{l+1}^+ a_{l+1} + \frac{1}{a_0^2(l+1)^2}}_{= h_{l+1} = \frac{\partial^2}{\partial r^2} - \frac{(l+1)(l+2)}{r^2} + \frac{2}{a_0 r}}$$

$$= \frac{\partial^2}{\partial r^2} - \frac{l^2 + 3l + 2 - 2l - 2}{r^2} + \frac{2}{a_0 r}$$

$$= \frac{\partial^2}{\partial r^2} - \frac{l(l+1)}{r^2} + \frac{2}{a_0 r} = h_l$$

(d)
$$h_{l+1}\left(a_{l+1}^+ u_{\epsilon l}\right) = \overbrace{\left(-a_{l+1}^+ a_{l+1} + \frac{1}{a_0^2(l+1)^2}\right)}^{h_{l+1} \text{ selon (c)}} a_{l+1}^+ u_{\epsilon l}$$

$$= a_{l+1}^+ \underbrace{\left(-a_{l+1} a_{l+1}^+ + \frac{1}{a_0^2(l+1)^2}\right)}_{h_l \text{ selon (c)}} u_{\epsilon l} = a_{l+1}^+ \epsilon u_{\epsilon l} = \epsilon \left(a_{l+1}^+ u_{\epsilon l}\right)$$

(e)
$$0 \leq \langle a_{l+1}^+ u_{\epsilon l} | a_{l+1}^+ u_{\epsilon l}\rangle = \langle u_{\epsilon l} | a_{l+1} a_{l+1}^+ u_{\epsilon l}\rangle = \langle u_{\epsilon l} | -h_l + \frac{1}{a_0^2 (l+1)^2} | u_{\epsilon l}\rangle$$

$$= \frac{1}{a_0^2 (l+1)^2} - \epsilon_l$$

$$\Rightarrow \epsilon_l \leq \frac{1}{a_0^2(l+1)^2} \quad \text{et} \quad \epsilon_{\hat{l}} = \frac{1}{a_0^2(\hat{l}+1)^2} \text{ si } a_{\hat{l}+1}^+ u_{\epsilon \hat{l}} = 0$$

$$\Rightarrow E_{\hat{l}+1} = -\frac{\hbar^2}{2m_e}\epsilon_{\hat{l}} = -\frac{\hbar^2}{2m_e}\left(\frac{m_e e^2}{\hbar^2}\right)^2 \frac{1}{(\hat{l}+1)^2} = -\frac{m_e e^4}{2\hbar^2(\hat{l}+1)^2}$$

$$\hat{l} \in \mathbb{N}$$

(f) $$\left(-\frac{\partial}{\partial r} + \frac{\hat{l}+1}{r} - \frac{1}{a_0(\hat{l}+1)}\right) u_{\varepsilon\hat{l}} = 0$$

Soit l'EDO $f'(x) = g(x) f(x)$, alors $f(x) = A \exp\left(\int^x g(x')\,dx'\right)$ avec A = cte,

Ici:
$$u_{\varepsilon\hat{l}} = A \exp\left(\int^r \left(\frac{\hat{l}+1}{r'} - \frac{1}{a_0(\hat{l}+1)}\right) dr'\right) = A \exp\left((\hat{l}+1)\ln r - \frac{r}{a_0(\hat{l}+1)}\right)$$
$$= A\, r^{\hat{l}+1} e^{-\frac{r}{a_0(\hat{l}+1)}}$$
normalisable car exponentiellement décroissante à ∞