ATOM VODÍKU

p^+e^-: $H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V_{el}(|\vec{r}_1 - \vec{r}_2|)$ (laboratorní soustava)

$\Downarrow$

$H = \frac{1}{2}\frac{P_T^2}{M} + \frac{1}{2}\frac{p_R^2}{m_R} + V_{el}(|\vec{r}_{12}|)$ (těžišťová soustava) $M = m_1 + m_2$ celk. hm.

$m_R = \frac{m_1 m_2}{m_1 + m_2}$ redukovaná hmotnost

pohyb těžiště odseparujeme

$$\boxed{H = \frac{p^2}{2m} + V(|\vec{r}|)} \qquad m_R = \frac{m_1 m_2}{m_1 + m_2} \overset{\text{pro } m_1 \ll m_2}{\approx} m_1 \equiv m$$

$\downarrow$

přičemž Coulomb: $V(|\vec{r}|) = V(r) = e\varphi(r) = -\frac{Ze^2}{4\pi r} = -\frac{Z\alpha}{r}$ $\varepsilon_0 = \hbar = c = 1$ v přirozených jednotkách

$\alpha = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{\hbar c} = \frac{e^2}{4\pi}$ = konstanta jemné struktury

SI natural ($\varepsilon_0 = \hbar = c = 1$) $\alpha^{-1} \doteq 137{,}036$

$\Rightarrow$ $H = \frac{p^2}{2m} - \frac{Ze^2}{4\pi r}$

$\downarrow$ přechod k atomovým jednotkám $\hbar = m_e = e = \frac{1}{4\pi\varepsilon_0} = 1$

$\vec{r} = \lambda\vec{r}'$, $\vec{p} = \lambda^{-1}\vec{p}'$ $\lambda = \frac{1}{Z\alpha m}$

$\vec{r} = \frac{\vec{r}'}{Z\alpha m}$ $\vec{p} = Z\alpha m\,\vec{p}'$

$\downarrow$

$$\boxed{H = \frac{p^2}{2} - \frac{1}{r}}$$

$\frac{p^2}{2} = -\frac{\nabla^2}{2} = -\frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{(\nabla^{\vartheta})^2}{r^2}\right) =$

$= \frac{1}{2}\left(p_r^2 + \frac{\hat{L}^2}{r^2}\right)$ $p_r = -i\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$ radiální hybnost

$p_r^2 = -\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)$

$$\boxed{H = \frac{1}{2}\left(p_r^2 + \frac{L^2}{r^2}\right) - \frac{1}{r}}$$

$H|\psi_n\rangle = E_n|\psi_n\rangle$ → energie $\boxed{E_n = -\frac{1}{2n^2}}$ [Ha] = Hartree $E_{SI} = m(Z\alpha)^2 E_{HA}$

→ hladiny degenerované v l, m

⇒ hrubá struktura

→ vlnové funkce $\Psi = \underbrace{R_{nl}(r)}_{\text{radiální fce}}\,\underbrace{Y_{lm}(\vartheta,\varphi)}_{\text{kulové funkce}}$

Laguerrovy polynomy

$R_{10}(r) = 2e^{-r}$

$R_{20}(r) = 2\left(\frac{1}{2}\right)^{3/2}\left(1 - \frac{r}{2}\right)e^{-\frac{r}{2}}$

$R_{21}(r) = \frac{1}{\sqrt{3}}\left(\frac{1}{2}\right)^{3/2} r\, e^{-\frac{r}{2}}$

$Y_{00}(\vartheta,\varphi) = \frac{1}{\sqrt{4\pi}}$

$Y_{10}(\vartheta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\vartheta$

$Y_{1,\pm1}(\vartheta,\varphi) = \mp\sqrt{\frac{3}{8\pi}}\sin\vartheta\, e^{\pm i\varphi}$ } chemické orb. jsou LK

nejsou vl. fce L^2, L_z

I) $\underline{[H, L^2]} = [\frac{p^2}{2} - \frac{1}{r}, L^2] =$

$= [\frac{1}{2}(p_r^2 + \frac{L^2}{r^2}) - \frac{1}{r}, L^2] =$

$= \frac{1}{2}\underset{0}{\underset{\shortparallel}{[p_r^2, L^2]}} + \frac{1}{2}\underset{0}{\underset{\shortparallel}{[\frac{L^2}{r^2}, L^2]}} - \underset{0}{\underset{\shortparallel}{[\frac{1}{r}, L^2]}} = \underline{0}$ $\quad L^2 = -(D^\mu)^2$ – pouze úhlové derivace

$\underline{[H, L_z]} = \frac{1}{2}\underset{0}{\underset{\shortparallel}{[p_r^2, L_z]}} + \frac{1}{2}\underset{[L^2, L_z]=0}{[\frac{L^2}{r^2}, L_z]} - \underset{0}{\underset{\shortparallel}{[\frac{1}{r}, L_z]}} = \underline{0}$ $\quad L_z = i\varepsilon_{zjk} n_j D^\mu_k$

$\{H, L^2, L_z\}$ ÚMKO $\Rightarrow$ můžeme volit společnou bázi

$\Rightarrow$ (vodíkové) vl. fce ψ_{nlm}: $\quad \hat{H}\psi_{nlm} = \underbrace{\frac{-1}{2n^2}}_{E_n}\psi_{nlm}$

$\hat{L}^2\psi_{nlm} = l(l+1)\psi_{nlm}$

$L_z\psi_{nlm} = m\psi_{nlm}$

II) $\overset{\text{eV}}{E_{NAT}} = m_R(Z\alpha)^2 E_{AU} = m_e \frac{m_R}{m_e}(Z\alpha)^2 E_{AU} = \underset{\substack{\text{jako}\\ \text{jediný má}\\ \text{rozměr}}}{m_e} \underbrace{\frac{1}{1+\frac{m_e}{m_j}}}_{\text{opravný faktor}} (Z\alpha)^2 E_{AU}$

$E_{SI} = c^2 E_{NAT} = m_e c^2 \frac{1}{1+\frac{m_e}{m_j}}(Z\alpha)^2 E_{AU} \quad [J]$

$\nu(Hz) = \frac{E_{SI}}{h} = \frac{E_{SI}}{2\pi\hbar} = \frac{m_e c^2}{2\pi\hbar}\frac{m_R}{m_e}(Z\alpha)^2 E_{AU} = \underbrace{\frac{m_e c\alpha^2}{4\pi\hbar}}_{R_\infty \text{ Rydberg constant}} c\frac{m_R}{m_e} 2Z^2 E_{AU}$

$E_{NAT}(eV) \to \nu(Hz)$: $\quad m_e \to \frac{2R_\infty c}{\alpha^2}$

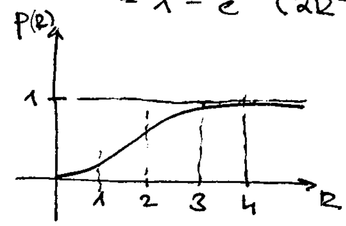
IV) pst. výskytu e^- ve vzdálenosti $(0, R)$ od jádra

$\psi_{1s} = R_{10}(r)\, Y_{00}(\vartheta, \varphi)$ $\quad \hookrightarrow$ radiální pst. výskytu

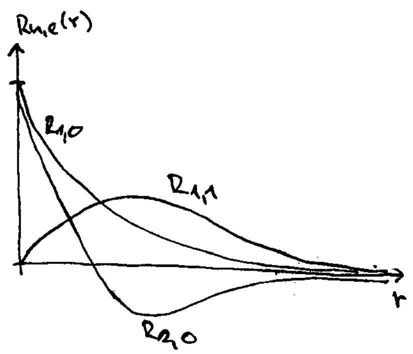
$P(R) = \int_0^R R_{10}^*(r) R_{10}(r)\, r^2 dr = \int_0^R 4e^{-2r} r^2 dr = e^{-2R}(e^{2R} - 2R^2 - 2R - 1) =$

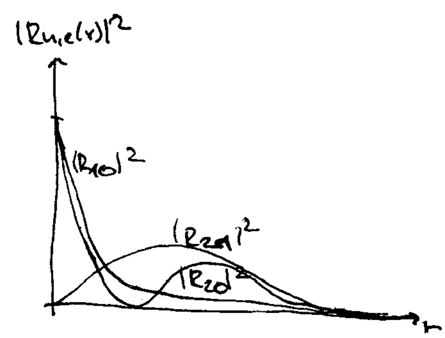
$= 1 - e^{-2R}(2R^2 + 2R + 1)$

Pst (0, R=0,5):	0,0803	8%
pst (0, R=1):	0,3233	32%
pst (0, R=2):	0,7619	76%
pst (0, R=3):	0,9380	94%
pst (0, R=4):	0,9862	99%

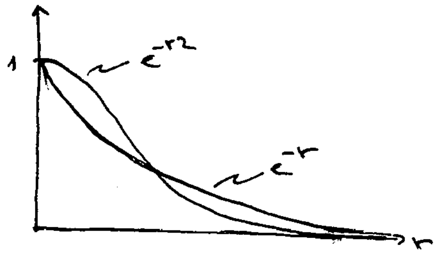


V)





(V) porovnání e^{-r} a e^{-r^2}



→ funkce se podobají

⇒ v praxi při běžných QM výpočtech můžeme zpravidla nahradit vodíkové orbitaly $\sim e^{-r}$ gaussiány $\sim e^{-r^2}$

⇒ ušetří to mnoho výpočetního času

! ale ztrácíme přesnost

⇒ e^{-r^2} klesá rychleji $x \to \infty$

⇒ e^{-r^2} a e^{-r} mají odlišné chování pro $x \to 0$

↳ problém při velmi přesných výpočtech

↳ ani LK gaussiánů nezachytíme chování e^{-r} zcela přesně

(VI) $\varphi_\alpha(r) = N e^{-\alpha r^2}$

$$\langle \varphi_\alpha | \varphi_\alpha \rangle = \int_V \varphi_\alpha^*(r)\, \varphi_\alpha(r)\, d^3\vec{r} =$$

$$= \int_0^\infty \int_0^{2\pi} \int_0^\pi N^2 e^{-2\alpha r^2} r^2 dr \sin\Theta\, d\Theta\, d\varphi =$$

$$= 4\pi N^2 \int_0^\infty e^{-2\alpha r^2} r^2 dr =$$

$$\int_0^\infty x^2 e^{-Ax^2} dx = \frac{1}{4A}\sqrt{\frac{\pi}{A}}$$

$$= 4\pi N^2 \frac{1}{4\cdot 2\alpha}\sqrt{\frac{\pi}{2\alpha}} \stackrel{!}{=} 1 \Rightarrow \underline{N = \left(\frac{2\alpha}{\pi}\right)^{3/4}}$$

$$\Rightarrow \boxed{\varphi_\alpha(r) = \left(\frac{2\alpha}{\pi}\right)^{3/4} e^{-\alpha r^2}}$$

(VII) pst výskytu e ve vzdálenosti $(0,R)$ od jádra

$$P(R) = 4\pi \int_0^R \varphi_\alpha^*(r)\, \varphi_\alpha(r)\, r^2 dr =$$

$$= 4\pi \sqrt{\frac{2\alpha}{\pi}} \cdot \frac{2\alpha}{\pi} \int_0^R e^{-2\alpha r^2} r^2 dr =$$

$$\int_0^R x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}\, \mathrm{erf}(R\sqrt{a})}{4 a^{3/2}} - \frac{R e^{-R^2 a}}{2a}$$

(VIII) $T = -\frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)$

$$T|\varphi_\alpha\rangle = -\frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) N e^{-\alpha r^2} = -\frac{1}{2} N \left[2\alpha(2\alpha r^2 - 1) e^{-\alpha r^2} + \frac{2}{r}(-2\alpha r e^{-\alpha r^2})\right] = \underline{\underline{N\alpha(3 - 2\alpha r^2)\, e^{-\alpha r^2}}}$$

$$\boxed{\langle \varphi_\alpha | T | \varphi_\alpha \rangle} = 4\pi \int_0^\infty dr\, r^2\, N e^{-\alpha r^2}\, N\alpha (3 - 2\alpha r^2)\, e^{-\alpha r^2}$$

$$= 4\pi N^2 \alpha \int_0^\infty dr\, r^2 (3 - 2\alpha r^2)\, e^{-2\alpha r^2} =$$

$$= 4\pi \left(\frac{2\alpha}{\pi}\right)^{3/2} \alpha \left[3\sqrt{\frac{\pi}{2\alpha}}\frac{1}{8\alpha} - 2\alpha\sqrt{\frac{\pi}{2\alpha}}\frac{1}{8\alpha}\frac{3}{4\alpha}\right] =$$

$$\int_0^\infty x^2 e^{-Ax^2} dx = \frac{1}{4A}\sqrt{\frac{\pi}{A}}$$

$$\int_0^\infty x^4 e^{-Ax^2} dx = \frac{3}{2A}\frac{1}{4A}\sqrt{\frac{\pi}{A}}$$

$$= 4\pi \left(\frac{2\alpha}{\pi}\right) \frac{1}{8\alpha} \alpha \left(3 - \frac{3}{2}\right) =$$

$$\boxed{= \frac{3}{2}\alpha}$$

IX $\langle\psi_\alpha|\hat{V}|\psi_\alpha\rangle = \int \psi_\alpha^*\left(-\frac{1}{r}\right)\psi_\alpha \, d^3\vec{r} =$

$$= 4\pi\int_0^\infty dr\, r^2\, N e^{-\alpha r^2}\cdot\frac{-1}{r}\, N e^{-\alpha r^2} =$$

$$= -4\pi N^2 \int_0^\infty dr\, r\, e^{-2\alpha r^2} =$$

$$= -4\pi \left(\frac{2\alpha}{\pi}\right)^{3/2}\frac{1}{4\alpha} =$$

$$\boxed{= -2\sqrt{\frac{2\alpha}{\pi}} = \langle\psi_\alpha|\hat{V}|\psi_\alpha\rangle}$$

$$\int_0^\infty x\, e^{-ax^2}dx = \frac{1}{2a}$$

⇒ celkově pro energii

$$E(\alpha) = \langle T\rangle_\alpha + \langle V\rangle_\alpha = \frac{3}{2}\alpha - 2\sqrt{\frac{2\alpha}{\pi}}$$

$$= \frac{3}{2}x^2 - 2\sqrt{\frac{2}{\pi}}\,x$$

X $\frac{dE(x)}{dx} = 3x - 2\sqrt{\frac{2}{\pi}} \overset{!}{=} 0 \Rightarrow x = \frac{2\sqrt{2}}{3\sqrt{\pi}} = \sqrt{\alpha_0} \Rightarrow \alpha_0 = \frac{8}{9\pi} \approx \underline{\underline{0{,}2829}}$

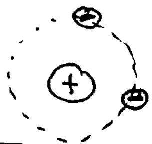
$$E(\alpha_0) = \frac{3}{2}\cdot\frac{8}{9\pi} - 2\sqrt{\frac{2\cdot\frac{8}{9\pi}}{\pi}} = \frac{4}{3\pi} - 2\,\frac{4}{3\pi} = \boxed{-\frac{4}{3\pi} \approx 0{,}4244\ Ha = E_{opt}}$$

XI přesná energie $E_1 = \frac{-1}{2n^2} = \underline{\underline{-\frac{1}{2}\,Ha}}$ $(=-1\,Ry)$

→ variační metoda dává vždy horní odhad $E_{var} \geq E_{exact}$

ATOM HÉLIA

$p^+ \; 2e^-$



$$\boxed{\hat H = \underbrace{\frac{\hat p_1^2}{2} - \frac{1}{r_1}}_{\text{první } e^-} + \underbrace{\frac{\hat p_2^2}{2} - \frac{1}{r_2}}_{\text{druhý } e^-} + \underbrace{\frac{1}{r_{12}}}_{\text{interakce dvou } e^-}} \quad (\text{v AU})$$

kinetická energie + Coulomb s jádrem ⟵ dva neinteragující e^-

→ jak vzít vlnovou fci?

⇒ celkově musí být antisymetrická

= při záměně všech souřadnic (prostor + spin) lib. dvou částic (fermionů, zde elektronů) musíme dostat tu samou vln. fci – až na znaménko ⊖

$$\Psi(x_1,x_2) = -\Psi(x_2,x_1) \qquad x_i = (\vec r_i, \text{spin})$$

→ prostorová × spinová část

$$\Psi(x) = \psi(\vec r)\cdot S$$

pro zákl. stav sym. ⇒ spinová část musí být antisym

$$\psi_{1s}(\vec r)\,\psi_{1s}(\vec r) \qquad \alpha(1)\beta(2) - \beta(1)\alpha(2)$$

↑ ↓ ↓ ↑

⇒ zde součin vodíkových fcí:

$$\Psi(\vec r_1,\vec r_2) = \psi_{1s}(\vec r_1)\,\psi_{1s}(\vec r_2) \qquad \psi_{1s}(\vec r) = \sqrt{\frac{Z'^3}{\pi}}\, e^{-Z' r}$$

$$= \frac{Z'^3}{\pi} e^{-Z'(r_1+r_2)}$$

XI normalizace

$$\underline{\underline{\langle\Psi|\Psi\rangle}} = \iint d^3\vec r_1\, d^3\vec r_2 \left(\frac{Z'^3}{\pi}\right)^2 e^{-Z'(r_1+r_2)}\, e^{-Z'(r_1+r_2)}$$

$$= \left(\frac{Z'^3}{\pi}\right)^2 (4\pi)^2 \underbrace{\int_0^\infty dr_1\, r_1^2 e^{-Z'2r_1}}_{\frac{1}{4Z'^3}} \underbrace{\int_0^\infty dr_2\, r_2^2 e^{-Z'2r_2}}_{\frac{1}{4Z'^3}}$$

$$\underline{\underline{= 1}} \quad \square$$

$$\boxed{\text{viriálový teorém} \quad 2\langle T\rangle_\psi = \langle \vec r\cdot\nabla V(\vec r)\rangle_\psi}$$

$$E_{nlm} = \langle H\rangle_{nlm} = \langle T\rangle_{nlm} + \langle V\rangle_{nlm}$$

$$\nabla V = \frac{\partial}{\partial x_i}\left(\frac{Z}{r}\right) = -\frac{Z}{2}(x_jx_j)^{-\frac32}\left(\overbrace{\frac{\partial x_j}{\partial x_i}}^{\delta_{ij}} x_j + x_j \overbrace{\frac{\partial x_j}{\partial x_i}}^{\delta_{ij}}\right) = -Zx_i\,(x_kx_k)^{-\frac32}$$

$$r = \sqrt{x^2+y^2+z^2} = \sqrt{x_jx_j} = (x_jx_j)^{+\frac12}$$

$$\langle \Psi(\vec r_1,\vec r_2)|T_1|\Psi(\vec r_1,\vec r_2)\rangle = \langle \psi_{1s}(r_1)|T_1|\psi_{1s}(r_1)\rangle\langle\psi_{1s}(r_2)|\psi_{1s}(r_2)\rangle =$$

$$= (4\pi)^2 N^4 \int_0^\infty dr_1 r_1^2\, e^{-z'r_1}\left(-\frac{1}{2}\right)\left(\frac{\partial^2}{\partial r_1^2}+\frac{2}{r_1}\frac{\partial}{\partial r_1}\right)e^{-z'r_1}\int_0^\infty dr_2 r_2^2\, e^{-z'r_2}e^{-z'r_2} =$$

<u>interakce dvou elektronů</u>

IV $$W_{ee}[z'] = \langle\Psi(\vec r_1,\vec r_2)|\frac{1}{|\vec r_1-\vec r_2|}|\Psi(\vec r_1,\vec r_2)\rangle =$$

$$= \int d^3\vec r_1\int d^3\vec r_2\, \frac{z'^3}{\pi}e^{-z'(\vec r_1+r_2)}\frac{1}{r_{12}}\frac{z'^3}{\pi}e^{-z'(r_1+r_2)} =$$

$$= \frac{1}{2}\int d^3\vec r_1 \underbrace{\frac{\sqrt{2}z'^3}{\pi}e^{-z'2r_1}}_{\rho(\vec r_1)}\int d^3\vec r_2\underbrace{\frac{\sqrt{2}z'^3}{\pi}e^{-z'2r_2}}_{\rho(\vec r_2)}\frac{1}{r_{12}}$$

$$= \frac{1}{2}\int d^3\vec r_1\int d^3\vec r_2\,\frac{\rho(\vec r_1)\rho(\vec r_2)}{r_{12}}$$

$\rho(\vec r) \rightsquigarrow$ intenzita el. pole $\vec{\mathcal{E}}(\vec r) \rightsquigarrow$ potenciál $\varphi(\vec r)$

$$\vec\nabla\cdot\vec{\mathcal{E}} = \frac{\rho}{\varepsilon_0} \xrightarrow{\text{v AU}} \vec\nabla\cdot\vec{\mathcal{E}} = 4\pi\rho$$

potenciál sféricky symetrický

$\Rightarrow$ ve sférických souřadnicích:

$$\vec\nabla\cdot\vec E = \underbrace{\frac{1}{r^2}\frac{\partial}{\partial r}(r^2E_r)}_{\text{vzhledem k symetrii uvažujeme jen tuto část}} + \frac{1}{r\sin\Theta}\frac{\partial}{\partial\Theta}(\sin\Theta\, E_\Theta) + \frac{1}{r\sin\Theta}\frac{\partial}{\partial\phi}E_\phi$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\,\mathcal{E}(r)) = 4\pi\rho(r)$$

$$\frac{1}{r_1^2}\frac{d}{dr_1}\left(r_1^2\mathcal{E}(r_1)\right) = 4\pi\rho(r_1)$$

$$d\left(r_1^2\mathcal{E}(r_1)\right) = 4\pi\rho(r_1)\,r_1^2\,dr_1 \qquad \Big/ \int_0^{r_2}$$

$$r_2^2\,\mathcal{E}(r_2) = 4\pi\int_0^{r_2} r_1^2\rho(r_1)\,dr_1$$

← elektrické pole v bodě r_2 způsobené nab. hustotou $\rho(r_1)$

$$\mathcal{E}(r_2) = -\frac{d\varphi(r_2)}{dr_2}$$

$$r_2^2\,\mathcal{E}(r_2) = -r_2^2\frac{d\varphi(r_2)}{dr_2} = 4\pi\int_0^{r_2} r_1^2\rho(r_1)\,dr_1$$

$$\frac{d\varphi(r_2)}{dr_2} = -\frac{4\pi}{r_2^2}\int_0^{r_2} r_1^2\rho(r_1)\,dr_1$$

$$d\varphi(r_2) = -\frac{4\pi}{r_2^2}\int_0^{r_2} r_1^2\rho(r_1)\,dr_1\,dr_2 \qquad \Big/ \int_r^{\infty}$$

$$\varphi(\infty) - \varphi(r) = -4\pi\int_r^{\infty}\frac{1}{r_2^2}\int_0^{r} r_1^2\rho(r_1)\,dr_1\,dr_2$$

$\lim_{r\to\infty}\varphi(r) = 0$ ← požadujeme, aby v nekonečnu vymizel

$$\Rightarrow \boxed{\varphi(r) = 4\pi\int_r^{\infty}\frac{1}{r_2^2}\int_0^{r_2} r_1^2\rho(r_1)\,dr_1\,dr_2}$$

← potenciál v bodě r

$$f'(r_2) = \frac{1}{r_2^2} \Rightarrow f(r_2) = \frac{-1}{r_2}$$

$$g(r_2) = \int_0^{r_2} r_1^2\rho(r_1)\,dr_1 \Rightarrow g'(r_2) = r_2^2\rho(r_2)$$

per partes $\int f'g = \int f\cdot g - \int f\cdot g'$

$$\underline{\underline{\varphi(r)}} = 4\pi\int_r^{\infty}\frac{1}{r_2^2}\int_0^{r} r_1^2\rho(r_1)\,dr_1\,dr_2 = 4\pi\int_r^{\infty} f'(r_2)\,g(r_2)\,dr_2 =$$

$$= 4\pi\left[-\frac{1}{r_2}g(r_2)\right]_r^{\infty} - 4\pi\left[-\frac{1}{r_2}r_2^2\rho(r_2)\right]_r^{\infty}$$

$$\underline{\underline{= 4\pi\,\frac{1}{r}\int_0^{r} r_1^2\rho(r_1)\,dr_1 + 4\pi\int_r^{\infty} r_2\rho(r_2)\,dr_2}}$$

$$W_{ee}[Z'] = \frac{1}{2}\int\varphi(\vec r)\rho(\vec r)\,d^3\vec r =$$

$$= 2\pi\int_0^{\infty} r^2\rho(r)\varphi(r)\,dr =$$

$$= 2\pi\int_0^{\infty} r^2\,\rho(r)\;\underbrace{\times 4\pi\left[\frac{1}{r}\int_0^{r} r_1^2\rho(r_1)\,dr_1 + \int_r^{\infty} r_2\rho(r_2)\,dr_2\right]}_{\varphi(r)} dr =$$

$$= 2\pi\int_0^{\infty} r^2\,\frac{\sqrt{2}Z'^3}{\pi}e^{-Z'2r}\,4\pi\left[\frac{1}{r}\int_0^{r} r_1^2\frac{\sqrt{2}Z'^3}{\pi}e^{-Z'2r_1}\,dr_1 + \int_r^{\infty} r_1\frac{\sqrt{2}Z'^3}{\pi}e^{-Z'2r_1}\,dr_1\right]dr =$$

$$= 8\pi^2\left(\frac{\sqrt{2}Z'^3}{\pi}\right)^2\left\{\int_0^{\infty} r\,e^{-Z'2r}\int_0^{r} r_1^2 e^{-Z'2r_1}\,dr_1\,dr + \int_0^{\infty} r^2 e^{-Z'2r}\int_r^{\infty} r_1 e^{-Z'2r_1}\,dr_1\,dr\right\} =$$

$$= 16Z'^6\left\{\int_0^{\infty} r\,e^{-Z'2r}\left(\frac{1 - (2Z'^2r^2 + 2Z'r + 1)e^{-2Z'r}}{4Z'^3}\right)dr + \int_0^{\infty} r^2 e^{-Z'2r}\left(\frac{(2Z'r+1)e^{-2Z'r}}{4Z'^2}\right)dr\right.$$

$$= 16Z'^6\cdot\frac{5}{128Z'^5} = \boxed{\frac{5}{8}Z'}$$