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Advanced Quantum Mechanics

Exercise Series 3

Problem 7

For every $\lambda \in \mathbb{R}^+$ we define a function $n_\lambda : \mathbb{R}^3 \setminus \{0\} \to \mathbb{R}^+$ such that

$$n_\lambda(x) := A_\lambda \frac{\lambda^{3/2}}{\|x\|^{3/2}} \exp\left(- \frac{\sqrt{\|x\|}}{\sqrt{\lambda}} \right) \quad \text{for } x \in \mathbb{R}^3 \setminus \{0\}$$

$\{n_\lambda \mid \lambda \in \mathbb{R}^+\}$ defines the family of test functions, we are using for the electron density. In that case we can find another function

$$\tilde{n}_\lambda : \mathbb{R}^+ \longrightarrow \mathbb{R}^+, \quad \tilde{n}_\lambda(r) = A \frac{\lambda^{3/2}}{r^{3/2}} \exp\left(- \frac{\sqrt{r}}{\sqrt{\lambda}} \right)$$

$$\Longrightarrow \quad \tilde{n}_\lambda(\|x\|) = n_\lambda(x) \quad \text{for all } x \in \mathbb{R}^3 \setminus \{0\}, \ \lambda \in \mathbb{R}^+$$

(we define $A_\lambda \in \mathbb{R}$ to be a constant and choose $\lambda \in \mathbb{R}^+$)

From normalization we know: $\int_{\mathbb{R}^3} n_\lambda(x) \, d^3x = N \in \mathbb{N}$

$$\Longrightarrow \int_{\mathbb{R}^3} n_\lambda(x) \, d^3x = \int_{\mathbb{R}^3} \tilde{n}_\lambda(\|x\|) \, d^3x = 4\pi \int_0^\infty \tilde{n}_\lambda(r) \, r^2 \, dr$$

$$= 4\pi A_\lambda \lambda^{3/2} \int_0^\infty \sqrt{r} \exp\left(- \frac{\sqrt{r}}{\sqrt{\lambda}} \right) dr$$

$$\varphi : \mathbb{R}^+ \longrightarrow \mathbb{R}^+, \quad \varphi(r) := \sqrt{r} / \sqrt{\lambda}$$

$$= 4\pi A_\lambda \lambda^{3/2} \int_0^\infty \frac{2\sqrt{\lambda} \cdot \sqrt{r}}{2\sqrt{\lambda} \cdot \sqrt{r}} \cdot \sqrt{r} \exp\left(- \frac{\sqrt{r}}{\sqrt{\lambda}} \right) dr$$

$$\Longrightarrow \varphi'(r) = \frac{1}{2\sqrt{\lambda}} \cdot \frac{1}{\sqrt{r}}$$

$$= 4\pi A_\lambda \lambda^{3/2} \int_0^\infty 2 \lambda^{3/2} \varphi^2(r) \exp\left(- \varphi(r) \right) \cdot \varphi'(r) \, dr$$

$$\Longrightarrow r = \lambda \varphi^2(r)$$

$$= 8\pi A_\lambda \lambda^3 \int_{\varphi(0)}^{\varphi(\infty)} s^2 e^{-s} \, ds = 8\pi A \lambda^3 \left[\underbrace{- s^2 e^{-s} \Big|_0^\infty}_{=0} + 2 \int_0^\infty s e^{-s} \, ds \right]$$

$$= 16\pi A_\lambda \lambda^3 \left[- s e^{-s} \Big|_0^\infty + \int_0^\infty e^{-s} \, ds \right] = 16\pi A_\lambda \lambda^3 = N$$

$$\Longrightarrow \quad A_\lambda = \frac{N}{16\pi\lambda^3} \quad \Longrightarrow \quad \tilde{n}_\lambda(r) = \frac{N}{16\pi\lambda^{3/2}} \cdot r^{-3/2} \exp\left(-\frac{\sqrt{r}}{\sqrt{\lambda}}\right), \ r \in \mathbb{R}^+$$

The energy of the atom is given for every $\lambda \in \mathbb{R}^+$ by

$$E(\lambda) = \frac{3\gamma}{5} \int_{\mathbb{R}^3} n_\lambda^{5/3}(x)\, d^3x \;-\; Ze^2 \int_{\mathbb{R}^3} \frac{n_\lambda(x)}{\|x\|}\, d^3x$$

$$+ \frac{e^2}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{n_\lambda(x)\, n_\lambda(y)}{\|x-y\|}\, d^3y\, d^3x \qquad \text{with } Z \in \mathbb{N}$$

We compute the integrals:

$$\int_{\mathbb{R}^3} n_\lambda^{5/3}(x)\, d^3x = \int_{\mathbb{R}^3} \tilde{n}_\lambda^{5/3}(\|x\|)\, d^3x = 4\pi \int_0^\infty \tilde{n}_\lambda(r)\, r^2\, dr$$

$$= \frac{N}{4\lambda^{5/2}} \int_0^\infty \frac{1}{\sqrt{r}} \exp\left(-\frac{5\sqrt{r}}{3\sqrt{\lambda}}\right) dr$$

$$= \frac{N}{4\lambda^{5/2}} \int_0^\infty \frac{6\sqrt{\lambda}}{5} \varphi'(r) \exp\left(-\varphi(r)\right) dr$$

$$= \frac{3N}{10\lambda^2} \int_{\varphi(0)}^{\varphi(\infty)} e^{-s}\, ds = \frac{3N}{10\lambda^2}$$

$$\Longrightarrow \quad \frac{3\gamma}{5} \int_{\mathbb{R}^3} n_\lambda^{5/3}(x)\, d^3x = \frac{9}{50} \frac{\gamma N}{\lambda^2}$$

$\varphi : \mathbb{R}^+ \longrightarrow \mathbb{R}^+$

$\varphi(r) := \dfrac{5\sqrt{r}}{3\sqrt{\lambda}}, \ r \in \mathbb{R}^+$

$\Longrightarrow \varphi'(r) = \dfrac{5}{6\sqrt{\lambda}} \cdot \dfrac{1}{\sqrt{r}}$

$\Longrightarrow r = \dfrac{9}{25} \lambda \varphi^2(r)$

$$\int_{\mathbb{R}^3} \frac{n_\lambda(x)}{\|x\|}\, d^3x = \int_{\mathbb{R}^3} \frac{\tilde{n}_\lambda(\|x\|)}{\|x\|}\, d^3x = 4\pi \int_0^\infty \tilde{n}_\lambda(r)\, r\, dr$$

$$= \frac{N}{4\lambda^{3/2}} \int_0^\infty \frac{1}{\sqrt{r}} \exp\left(-\frac{\sqrt{r}}{\sqrt{\lambda}}\right) dr$$

$$= \frac{N}{2\lambda} \int_0^\infty \varphi'(r) \cdot \exp\left(-\varphi(r)\right) dr$$

$$= \frac{N}{2\lambda} \int_{\varphi(0)}^{\varphi(\infty)} e^{-s}\, dr = \frac{N}{2\lambda}$$

$\varphi : \mathbb{R}^+ \longrightarrow \mathbb{R}^+$

$\varphi(r) := \dfrac{\sqrt{r}}{\sqrt{\lambda}}, \ r \in \mathbb{R}^+$

$\Longrightarrow \varphi'(r) = \dfrac{1}{2\sqrt{\lambda}} \cdot \dfrac{1}{\sqrt{r}}$

$\Longrightarrow r = \lambda \varphi^2(r)$

$$\Rightarrow \quad Ze^2 \int_{\mathbb{R}^3} \frac{n_\lambda(x)}{\|x\|} \, d^3x = \frac{Ze^2 N}{2\lambda}$$

From the note we know:

$$\frac{e^2}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{n_\lambda(x)\, n_\lambda(y)}{\|x-y\|} \, d^3y \, d^3x = -\frac{e}{2} \int \varphi_\lambda(x)\, n_\lambda(x) \, d^3x$$

with a potential $\varphi_\lambda : \mathbb{R}^3 \setminus \{0\} \to \mathbb{R}$ such that for all $x \in \mathbb{R}^3 \setminus \{0\}$

$\varphi_\lambda(x) = f\left(\frac{\sqrt{\|x\|}}{\sqrt{\lambda}}\right)$ for a function $f : \mathbb{R}^+ \to \mathbb{R}$ and a constant $\mu \in \mathbb{R}$ such that $f(y) := \frac{\mu}{y^2}\left[1 - (1+y)e^{-y}\right]$

for all $y \in \mathbb{R}^+$. But we have to show the differential equation.

$$\Rightarrow \quad f'(y) = \frac{-2\mu}{y^3}\left[1-(1+y)e^{-y}\right] - \frac{\mu}{y^2}\left[e^{-y} - (1+y)e^{-y}\right]$$

$$= -\frac{2f(y)}{y} + \frac{\mu e^{-y}}{y}$$

$$\Rightarrow \quad f''(y) = -2\left[\frac{f'(y)y - f(y)}{y^2}\right] - \mu \frac{(1+y)e^{-y}}{y^2}$$

$$\Rightarrow \quad y f''(y) + 3f'(y) = f'(y) + \frac{2f(y)}{y} - \mu \frac{1+y}{y} e^{-y}$$

$$= -\frac{2f(y)}{y} + \frac{\mu e^{-y}}{y} + \frac{2f(y)}{y} - \frac{\mu(1+y)e^{-y}}{y} = -\mu e^{-y}$$

$$\Rightarrow \quad \frac{1}{4\lambda^2 y^3}\left(y f''(y) + 3f'(y)\right) = -\frac{\mu}{4\lambda^2} \frac{e^{-y}}{y^3} = -4\pi e A \frac{e^{-y}}{y^3}$$

with $\frac{\mu}{4\lambda^2} = 4\pi e A = \frac{Ne}{4\lambda^3} \Rightarrow \mu = \frac{Ne}{\lambda}$

Therefore f fullfills with $\mu = \frac{Ne}{\lambda}$ the given differential equation.

$$\Rightarrow \quad \varphi_\lambda(x) = f\left(\frac{\sqrt{\|x\|}}{\sqrt{\lambda}}\right) = \frac{Ne}{\|x\|}\left[1 - \left(1 + \frac{\sqrt{\|x\|}}{\sqrt{\lambda}}\right) \exp\left(-\frac{\sqrt{\|x\|}}{\sqrt{\lambda}}\right)\right]$$

$$\Rightarrow \int_{\mathbb{R}^3} \varphi_\lambda(x)\, n_\lambda(x)\, d^3x = \int_{\mathbb{R}^3} f\left(\frac{\sqrt{\|x\|}}{\sqrt{\lambda}}\right) \tilde{n}_\lambda(\|x\|)\, d^3x$$

$$= 4\pi \int_0^\infty f\left(\frac{\sqrt{r}}{\sqrt{\lambda}}\right) \tilde{n}_\lambda(r)\, r^2\, dr$$

$$= 4\pi \cdot Ne \cdot \frac{N}{16\pi \lambda^{3/2}} \int_0^\infty \frac{1}{r}\left[1 - \left(1 + \frac{\sqrt{r}}{\sqrt{\lambda}}\right) \exp\left(-\frac{\sqrt{r}}{\sqrt{\lambda}}\right)\right] \frac{1}{r^{3/2}} \exp\left(-\frac{\sqrt{r}}{\sqrt{\lambda}}\right) r^2\, dr$$

$$= \frac{N^2 e}{4\lambda^{3/2}} \int_0^\infty \left[\frac{1}{\sqrt{r}} \exp\left(-\frac{\sqrt{r}}{\sqrt{\lambda}}\right) - \frac{1}{\sqrt{r}} \exp\left(-\frac{2\sqrt{r}}{\sqrt{\lambda}}\right) - \frac{1}{\sqrt{\lambda}} \exp\left(-\frac{2\sqrt{r}}{\sqrt{\lambda}}\right)\right] dr$$

(note: $\int_0^\infty \frac{1}{\sqrt{r}} \exp\left(-\frac{\sqrt{r}}{\sqrt{\lambda}}\right) dr = 2\sqrt{\lambda} \int_0^\infty e^{-s}\, ds = 2\sqrt{\lambda}$

$$\Rightarrow \int_0^\infty \frac{1}{\sqrt{r}} \exp\left(-\frac{2\sqrt{r}}{\sqrt{\lambda}}\right) dr = \sqrt{\lambda}$$

$$\int_0^\infty \frac{1}{\sqrt{\lambda}} \exp\left(-\frac{2\sqrt{r}}{\sqrt{\lambda}}\right) dr = \int_0^\infty \frac{\sqrt{r}}{\sqrt{\lambda r}} \exp\left(-\frac{2\sqrt{r}}{\sqrt{\lambda}}\right) dr = \frac{\sqrt{\lambda}}{2} \int_0^\infty s\, e^{-s}\, ds$$

$$= \frac{\sqrt{\lambda}}{2} \quad)$$

$$= \frac{N^2 e}{4\lambda^{3/2}} \cdot \frac{\sqrt{\lambda}}{2} = \frac{N^2 e}{8\lambda} \quad \Rightarrow -\frac{e}{2} \int_{\mathbb{R}^3} \varphi_\lambda(x)\, n_\lambda(x)\, d^3x = -\frac{N^2 e^2}{16\lambda}$$

$$\Rightarrow E(\lambda) = \frac{9}{50} \frac{\gamma N}{\lambda^2} - \frac{ZNe^2}{2\lambda} - \frac{N^2 e^2}{16\lambda}$$

$$= \frac{\alpha}{\lambda^2} - \frac{\beta}{\lambda} \quad \text{with } \alpha := \frac{9}{50}\gamma N, \ \beta := \frac{Ne^2}{2}\left(Z - \frac{N}{8}\right)$$

$$\Rightarrow \left.\frac{dE(\tilde{\lambda})}{d\tilde{\lambda}}\right|_\lambda = \frac{-2\alpha}{\lambda^3} + \frac{\beta}{\lambda^2}$$

Now we want to find $\lambda_{min} \in \mathbb{R}^+$ such that $\left.\frac{dE(\tilde{\lambda})}{d\tilde{\lambda}}\right|_{\lambda_{min}} = 0$

$$\Rightarrow \frac{-2\alpha}{\lambda_{min}^3} + \frac{\beta}{\lambda_{min}^2} = 0 \Rightarrow \lambda_{min} = \frac{2\alpha}{\beta}$$

$$\Rightarrow \quad \lambda_{min} = \frac{9}{50} \frac{\gamma}{e^2\left(z - \frac{N}{8}\right)}$$

$$E(N,z) := E(\lambda_{min}) = \frac{\beta^2}{4\alpha} - \frac{\beta^2}{2\alpha} = -\frac{\beta^2}{4\alpha}$$

$$= -\frac{50}{18} \frac{e^4}{\gamma} N \left(z - \frac{N}{8}\right)^2$$

case $\quad z = N: \qquad E(N,N) = -\frac{50 \cdot 49}{18 \cdot 64} \frac{N^2 e^4}{\gamma}$