6-32

Hamiltonvirki einhvers kerfis er fall af stikanum λ, því köllum við

$$H(\lambda),\ E_n(\lambda) \text{ og } |n(\lambda)\rangle$$

eigingildi og eiginástönd $H(\lambda)$

Feynman-Hellmann setningin er þá

$$\partial_\lambda E_n(\lambda) = \langle n(\lambda)|\partial_\lambda H(\lambda)|n(\lambda)\rangle$$

þ.s. $E_n(\lambda)$ er annaðhvort einfalt eða „góð" samantekt margfaldra ástanda

a) Sýna fram á

$$\frac{\partial}{\partial \lambda} H(\lambda) = \frac{H(\lambda + d\lambda) - H(\lambda)}{d\lambda}$$

$$E_n(\lambda) = \langle n(\lambda) | H(\lambda) | n(\lambda) \rangle \quad \text{nákvæmt}$$

$$E_n(\lambda + d\lambda) = \langle n(\lambda+d\lambda) | H(\lambda+d\lambda) | n(\lambda+d\lambda) \rangle \quad \text{nákvæmt}$$

1. Stigs truflun gefur

$$E_n(\lambda + d\lambda) \simeq \langle n(\lambda) | H(\lambda+d\lambda) | n(\lambda) \rangle + O(\lambda^2)$$

$$dE_n(\lambda) = E_n(\lambda+d\lambda) - E_n(\lambda) \simeq \langle n(\lambda) | \big(H(\lambda+d\lambda) - H(\lambda) \big) | n(\lambda) \rangle$$

$$H(\lambda+d\lambda) - H(\lambda) = \frac{\partial H}{\partial \lambda} d\lambda$$

$$\rightarrow \quad \frac{\partial E_n(\lambda)}{\partial \lambda} = \langle n(\lambda) | \frac{\partial H}{\partial \lambda} | n(\lambda) \rangle$$

nākvamloga, pri pegar $d\lambda \to 0$ verder 1. stig trueflemi nākvom

b) 1D - H.O. nctum , $E_n = \hbar\omega(n+\frac{1}{2})$, $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$

i) Računam $\lambda = \omega$

$$\frac{\partial E_n}{\partial \omega} = \frac{E_n}{\omega} \quad , \quad \langle n | \frac{\partial H}{\partial \omega} | n \rangle = \langle n | m\omega x^2 | n \rangle$$

$$= m\omega \langle n | x^2 | n \rangle$$

$$\rightarrow \langle n | x^2 | n \rangle = \frac{E_n}{m\omega^2} = (n+\tfrac{1}{2})\frac{\hbar}{m\omega} = a^2 (n+\tfrac{1}{2})$$

Sada lika $\langle n | V | n \rangle = \frac{1}{2}m\omega^2 \langle n | x^2 | n \rangle = \frac{1}{2}(n+\frac{1}{2})\hbar\omega = \frac{E_n}{2}$

ii) $\lambda = \hbar \rightarrow \frac{\partial E_n}{\partial \hbar} = \frac{E_n}{\hbar}$, $T = -\frac{\hbar^2}{2m}\partial_x^2$

$$\langle n | \frac{\partial H}{\partial \hbar} | n \rangle = \langle n | \frac{\partial T}{\partial \hbar} | n \rangle = \frac{2}{\hbar} \langle n | T | n \rangle$$

$\rightarrow \langle n | T | n \rangle = \frac{E_n}{2}$, eða $\frac{1}{2m} \langle n | p^2 | n \rangle = \frac{E_n}{2}$

$\rightarrow \langle n | p^2 | n \rangle = E_n \cdot m$

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iii) $\lambda = m$, $\frac{\partial}{\partial m} E_n = 0$

$$\langle n | \frac{\partial H}{\partial m} | n \rangle = \langle n | \left\{ -\frac{T}{m} + \frac{V}{m} \right\} | n \rangle$$

$\rightarrow \langle n | T | n \rangle = \langle n | V | n \rangle$ eins og búið er að koma í ljós í i) og ii)

(5)

6.33 Nota Feynman-Hellmann til þess að reikna $\langle \frac{1}{r} \rangle$ og $\langle \frac{1}{r^2} \rangle$ fyrir Vetni

Virka H fyrir r-hlutann er

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} - \frac{e^2}{4\pi\epsilon_0 r}$$

og eigin gildin

$$E_n = -\underbrace{\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2}}_{R_y}\frac{1}{\underbrace{(j_{max}+l+1)^2}_{n^2}},$$

$E_n = -\frac{R_y}{n^2}$ en þetta form er heppilegt fyrir lið b)

a) Nota $\lambda = e$ til þess að finna $\langle \frac{1}{r} \rangle$

$$\langle \psi | \frac{\partial H}{\partial \lambda} | \psi \rangle = - \frac{2e}{4\pi\epsilon_0} \langle \psi | \frac{1}{r} | \psi \rangle$$

$$\frac{\partial E_n}{\partial e} = - \frac{4me^3}{32\pi^2\epsilon_0^2\hbar^2(j_{max}+l+1)^2} = \frac{4E_n}{e}$$

$$\to \boxed{\frac{4E_n}{e} = - \frac{2e}{4\pi\epsilon_0} \langle \psi | \frac{1}{r} | \psi \rangle} \quad , \quad E_n = -R_y \frac{1}{n^2}$$

Husk at

$$R_y = \frac{\hbar^2}{2ma^2} = \frac{me^4}{\hbar^2 32\pi^2\epsilon_0^2} \quad , \quad a = \frac{4\pi\epsilon_0\hbar^2}{me^2}$$

$$\to \frac{4R_y}{en^2} = \frac{2e}{4\pi\epsilon_0} \left\langle \frac{1}{r} \right\rangle \to \left\langle \frac{1}{r} \right\rangle = \frac{8\pi\epsilon_0 R_y}{e^2 n^2}$$

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{n^2 a}$$ eins og gefið var áður í bók

b) nota $\lambda = l$

$$\frac{\partial E_n}{\partial l} = \frac{2me^4}{32\pi^2\epsilon_0^2\hbar^2\left(j_{max}+l+1\right)^3} = -\frac{2E_n}{n}$$

$$\frac{\partial H}{\partial l} = \frac{\hbar^2(2l+1)}{2mr^2} \quad \rightarrow \quad \frac{\hbar^2(2l+1)}{2m}\left\langle\frac{1}{r^2}\right\rangle = -\frac{2E_n}{n}$$

$$\rightarrow \left\langle\frac{1}{r^2}\right\rangle = -\frac{4mE_n}{\hbar^2(2l+1)\hbar^2\cdot n} = +\frac{4mR_y}{\hbar^2(2l+1)\hbar^2 n^3}$$

$$= \frac{1}{n^3\left(l+\frac{1}{2}\right)a^2}$$

eins og áður