① Hreintóna sveifill með ástönd $|n\rangle$ og $E_n = \hbar\omega(n+\frac{1}{2})$ ①

er truflaður með $\lambda H' = \lambda \hbar\omega \left(\frac{x}{a}\right)^4$.

Finnum orku grunnástandsins með λ^2 leiðréttingu.

$$\epsilon_0 = E_0 + \langle 0|\lambda H'|0\rangle + \lambda^2 \sum_{n=1}^{\infty} \frac{|\langle n|H'|0\rangle|^2}{E_0 - E_n}$$

Í síðasta skammti fékkst

$$E_0 + \langle 0|\lambda H'|0\rangle = \hbar\omega\left\{\frac{1}{2} + \frac{3\lambda}{4}\right\}$$

Munum að

$$x = \frac{a}{\sqrt{2}}(a_+ + a_-)$$

$$p = \frac{i\hbar}{\sqrt{2}a}(a_+ - a_-)$$

$$a_-|n\rangle = \sqrt{n}\,|n-1\rangle$$

$$a_+|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

$$\langle n|H'|0\rangle = \hbar\omega \langle n|\left(\frac{x}{a}\right)^4|0\rangle$$

$$= \frac{\hbar\omega}{4}\langle n|(a_+ + a_-)^4|0\rangle$$

$$= \frac{\hbar\omega}{4}\left\{ \delta_{n,4}\cdot\sqrt{24} + \delta_{n,0} + \delta_{n,0}\sqrt{4} + \delta_{n,2}\left(\sqrt{18}+\sqrt{8}+\sqrt{2}\right)\right\}$$

$\cdots|a_+a_+a_+a_+|\cdots$ $\quad$ $\cdots|a_-a_+a_-a_+|\cdots$ $\quad$ $\cdots|a_-a_-a_+a_+|\cdots$ $\quad$ $\cdots|a_-a_+a_+a_+|\cdots\sqrt{18}$

$\cdots|a_+a_-a_+a_+|\cdots\sqrt{8}$

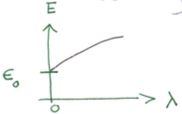
$\cdots|a_+a_+a_-a_+|\cdots\sqrt{2}$

$$= \frac{\hbar\omega}{4}\left\{ \delta_{n,4}\cdot\sqrt{24} + \delta_{n,0}\left(1+\sqrt{4}\right) + \delta_{n,2}\left(\sqrt{18}+\sqrt{8}+\sqrt{2}\right)\right\}$$

$$\epsilon_0 = \hbar\omega\left[\frac{1}{2}+\frac{3\lambda}{4}\right] + \lambda^2\left(\frac{\hbar\omega}{4}\right)^2\left\{\frac{24}{E_0-E_4} + \frac{72}{E_0-E_2}\right\}$$

$$= \hbar\omega\left\{\frac{1}{2}+\frac{3\lambda}{4}\right\} + \lambda^2\frac{\hbar\omega}{16}\left\{\frac{24}{-4} + \frac{72}{-2}\right\}$$

$$= \hbar\omega\left[\frac{1}{2} + \lambda\frac{3}{4} - \lambda^2\frac{21}{8} \cdots\cdots\right]$$



Brillouin-Wigner

2b

$$\epsilon_0 = \hbar\omega\left\{\frac{1}{2} + \frac{3\lambda}{4}\right\} + \lambda^2\left(\frac{\hbar\omega}{4}\right)^2\left\{\frac{24}{\epsilon_0 - \hbar\omega(4+\frac{1}{2})} + \frac{72}{\epsilon_0 - \hbar\omega(2+\frac{1}{2})}\right\}$$

$$\frac{\epsilon_0}{\hbar\omega} = \left\{\frac{1}{2} + \frac{3\lambda}{4}\right\} + \left(\frac{\lambda}{4}\right)^2\left\{\frac{24}{\frac{\epsilon_0}{\hbar\omega} - \frac{9}{2}} + \frac{72}{\frac{\epsilon_0}{\hbar\omega} - \frac{5}{2}}\right\}$$

Reynum lausn á ~~þessari~~ jöfnu fyr- gefin gildi á λ

Ekki ~~beðið~~ um í dæmi, en til gamans

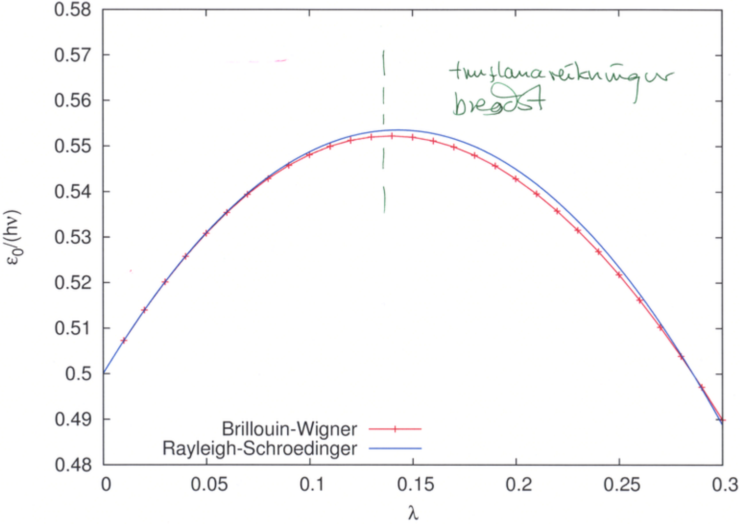
Plús leysa $H_0 + \lambda H'$ í grunni 128 lægstu ástanda notandi

$$\langle n|\frac{x}{a}|m\rangle = \frac{1}{2}\sqrt{n+m+1}\,\delta_{|n-m|,1}$$

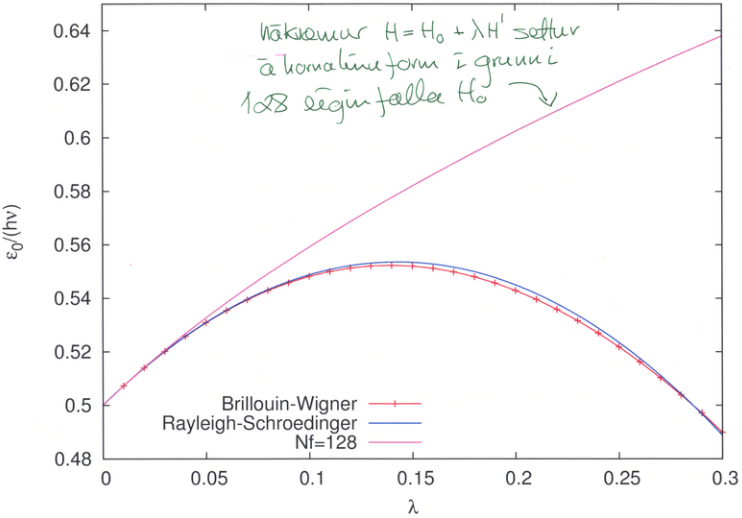
og

$$\langle n|\frac{x^4}{a^4}|m\rangle = \sum_{lpq}\langle n|\frac{x}{a}|l\rangle\langle l|\frac{x}{a}|p\rangle\langle p|\frac{x}{a}|q\rangle\langle q|\frac{x}{a}|m\rangle$$

2C

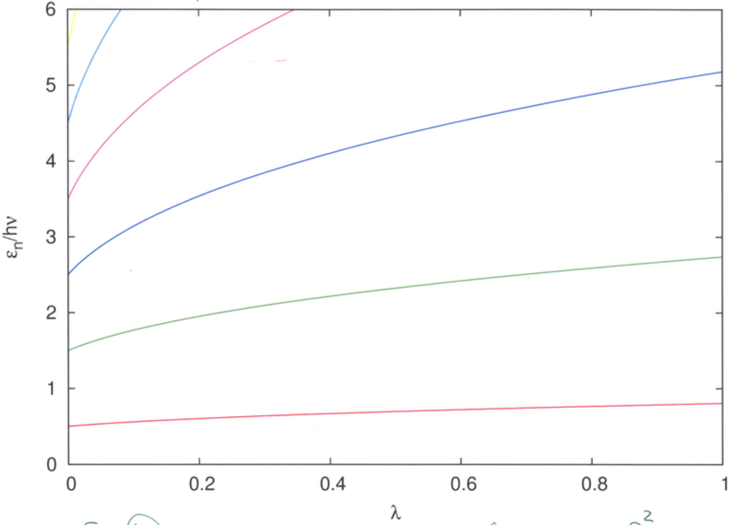

0.58
0.57
0.56
0.55
0.54
0.53
0.52
0.51
0.5
0.49
0.48
0
0.05
0.1
0.15
0.2
0.25
0.3
$\varepsilon_0/(h\nu)$
λ
Brillouin-Wigner
Rayleigh-Schroedinger
truflanareikningur bregðast

2d



Nákvæmur $H = H_0 + \lambda H'$ settur á hornalínuform í grunni 128 eiginfalla H_0
$\varepsilon_0/(h\nu)$
λ
Brillouin-Wigner
Rayleigh-Schroedinger
Nf=128
0.64
0.62
0.6
0.58
0.56
0.54
0.52
0.5
0.48
0
0.05
0.1
0.15
0.2
0.25
0.3

Orkuróf $H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 + \lambda \hbar\omega \left(\frac{x}{a}\right)^4$ 2f



Fundið í grunni 128 eiginfalla $H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$

2) H-atóm lokað inni í kúlu með geisla $a >> a_B$

Hvernig er hægt að reikna $\Delta E = E_{2S} - E_{1S}$?

Kúlan hefur mætti

$$V_{sp}(r) = \begin{cases} 0 & \text{ef} \quad r < a \\ \infty & \text{ef} \quad r > a \end{cases}$$

V_{sp} er aldrei lítil truflun, verðum að snúa við dæminu: Hugsum okkur rafeind í kúlu sem er trufluð með

$$V_{coul}(r) = -\frac{e^2}{4\pi\epsilon_0 r}$$

$$a_B = \frac{4\pi\epsilon_0 \hbar^2}{me^2} \quad \to \quad V_{coul}(r) = -\frac{e^2}{4\pi\epsilon_0}\,\frac{a}{r}\,\frac{me^2}{4\pi\epsilon_0 \hbar^2}$$

$$V_{coul}(r) = -2R_y \cdot \left(\frac{a}{r}\right), \quad R_y = \frac{me^4}{32\pi^2\epsilon_0^2\hbar^2}$$

Ef við byrjum með kúlu

$$\psi_{1s}(\bar{r}) = A_{10}\, j_0\left(\frac{\pi r}{a}\right) Y_{00}(\theta,\varphi)$$

$$j_0(x) = \frac{\sin(x)}{x}$$

og

$$\psi_{2s}(\bar{r}) = A_{20}\, j_0\left(\frac{2\pi r}{a}\right) Y_{00}(\theta,\varphi)$$

$$E_{1s} = E_1 \pi^2$$

$$E_{2s} = E_1 (2\pi)^2$$

Normierung

$$1 = \int_0^a r^2 dr \left| j_0\left(\frac{\pi r}{a}\right)\right|^2 |A_{10}|^2 = \int_0^a r^2 dr \, \frac{\sin^2\left(\frac{\pi r}{a}\right)}{\left(\frac{\pi r}{a}\right)^2} |A_{10}|^2$$

$$\left(\frac{a}{\pi}\right)^3 |A_{10}|^2 \int_0^\pi du \, \sin^2 u = \left(\frac{a}{\pi}\right)^3 |A_{10}|^2 \frac{\pi}{2}$$

$$\rightarrow \quad A_{10} = \sqrt{\frac{2\pi^2}{a^3}}$$

$$1 = \int_0^a r^2 dr \left| j_0\left(\frac{2\pi r}{a}\right)\right|^2 |A_{20}|^2 = \int_0^a r^2 dr \, \frac{\sin^2\left(\frac{2\pi r}{a}\right)}{\left(\frac{2\pi r}{a}\right)^2} |A_{20}|^2$$

$$= \left(\frac{a}{2\pi}\right)^3 |A_{20}|^2 \int_0^{2\pi} du \, \sin^2 u = \left(\frac{a}{2\pi}\right)^3 |A_{20}|^2 \pi$$

$$\rightarrow \quad A_{20} = \sqrt{\frac{8\pi^2}{a^3}}$$

Reynum

$$\langle 1s | V_{Coul} | 1s \rangle = -\frac{2\pi^2}{a^3} \cdot 2R_y \cdot \int_0^a r^2 dr \, \frac{\sin^2\left(\frac{\pi r}{a}\right)}{\left(\frac{\pi r}{a}\right)^2} \, \frac{a}{r}$$

$$= -4R_y \int_0^a \left(\frac{\pi r}{a}\right) d\left(\frac{\pi r}{a}\right) \frac{\sin^2\left(\frac{\pi r}{a}\right)}{\left(\frac{\pi r}{a}\right)^2}$$

$$= \int_0^\pi du \, \frac{\sin^2 u}{u} \qquad = -4R_y \cdot \frac{1}{2}\left[-Ci(2\pi) + \gamma + \ln(2\pi)\right]$$

$$\simeq -4R_y \cdot 1.21883$$

$$\langle 2s | V_{coul} | 2s \rangle = - \frac{8\pi^2}{a^3} 2R_y \cdot \int_0^a r^2 dr \frac{\sin^2\left(\frac{2\pi r}{a}\right)}{\left(\frac{2\pi r}{a}\right)^2} \frac{a}{r}$$

$$= -4R_y \cdot \int_0^a \left(\frac{2\pi r}{a}\right) d\left(\frac{2\pi r}{a}\right) \frac{\sin^2\left(\frac{2\pi r}{a}\right)}{\left(\frac{2\pi r}{a}\right)}$$

$$= -4R_y \int_0^{2\pi} du \frac{\sin^2(u)}{u} \approx -4R_y \cdot 1{,}55718$$

$$\rightarrow \quad \epsilon_{1s} = E_1 \pi^2 - 4R_y \cdot 1{,}21883$$

$$\epsilon_{2s} = E_1 (2\pi)^2 - 4R_y \cdot 1{,}55718$$

$$\left.\begin{aligned} E_1 &= \frac{\hbar^2}{2ma^2} \\ R_y &= \frac{\hbar^2}{2ma_B^2} \end{aligned}\right\} \longrightarrow \begin{aligned} \epsilon_{1s} &= E_1\left\{\pi^2 - 4\frac{R_y}{E_1}\,1.21883\right\} \\ \epsilon_{2s} &= E_1\left\{(2\pi)^2 - 4\frac{R_y}{E_1}\,1.55718\right\} \end{aligned}$$

$$\frac{R_y}{E_1} = \frac{a^2}{a_B^2}$$

$$\rightarrow \quad \epsilon_{1s} = E_1\left\{\pi^2 - 4\left(\frac{a^2}{a_B^2}\right)1.21883\right\}$$

$$\epsilon_{2s} = E_1\left\{(2\pi)^2 - 4\left(\frac{a^2}{a_B^2}\right)1.55718\right\}$$

$$\Delta E^\circ = E_{2s} - E_{1s} = E_1 \left\{ (2\pi)^2 - \pi^2 \right\} = E_1 \pi^2 \cdot 3$$

$$\Delta E \approx \epsilon_{2s} - \epsilon_{1s} = \Delta E^\circ - E_1 4 \left(\frac{a}{a_B}\right)^2 0.3384$$

$$= E_1 \pi^2 \cdot 3 - E_1 4 \left(\frac{a}{a_B}\right)^2 0.3384$$

$$= 3 E_1 \pi^2 \left\{ 1 - \left(\frac{a}{a_B}\right)^2 \frac{4 \cdot 0.3384}{3\pi^2} \right\}$$

$$\approx 3 E_1 \pi^2 \left\{ 1 - 0.0457 \left(\frac{a}{a_B}\right)^2 \right\}$$