68 „Teningslagaður" óendanlegur brunnur er truflaður með

$$H' = a^3 V_0 \, \delta(x - \tfrac{a}{4}) \, \delta(y - \tfrac{a}{2}) \, \delta(z - \tfrac{3a}{4})$$

finnum fyrsta stigs nálgun á orku grunnástandsins og lægsta örvaða ástandinu

$$E^0_{n_x n_y n_z} = E_1 \cdot \left\{ n_x^2 + n_y^2 + n_z^2 \right\}, \quad E_1 = \frac{\pi^2 \hbar^2}{2ma^2}$$

$$\psi_{n_x n_y n_z}(x) = \left(\frac{2}{a}\right)^{\frac{3}{2}} \sin\left(n_x \pi \frac{x}{a}\right) \sin\left(n_y \pi \frac{y}{a}\right) \sin\left(n_z \pi \frac{z}{a}\right)$$

Grunnástandið er einfalt $|111\rangle = |g\rangle$

$$E^1_{111} = E^0_{111} + \langle g | V | g \rangle$$

$$\langle g|V|g\rangle = a^3\left(\frac{2}{a}\right)^3 V_0 \int_0^a dx\,dy\,dz\, \sin^2\!\left(\pi\frac{x}{a}\right)\sin^2\!\left(\pi\frac{y}{a}\right)\sin^2\!\left(\pi\frac{z}{a}\right) \cdot \delta\!\left(x-\frac{a}{4}\right)\delta\!\left(y-\frac{a}{2}\right)\delta\!\left(z-\frac{3a}{4}\right)$$

$$= 8V_0 \sin^2\!\left(\frac{\pi}{4}\right)\sin^2\!\left(\frac{\pi}{2}\right)\sin^2\!\left(\frac{3\pi}{4}\right)$$

$$= \frac{8V_0}{4} = 2V_0$$

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fyrsta örvaða ástandið er 3-falt, hlutrúm spannað af $\{|112\rangle, |121\rangle, |211\rangle\}$ því þarf að reikna fylkja stökin fyrir öll þessi ástönd

köllum
$$|112\rangle = |a\rangle$$
$$|121\rangle = |b\rangle$$
$$|211\rangle = |c\rangle$$

byrjum á kornalínu

$$V_{aa} = \langle 112|V|112\rangle = a^3\left(\frac{2}{a}\right)^3 V_0 \int_0^a dxdydz \sin^2\left(\pi\frac{x}{a}\right)\sin^2\left(\pi\frac{y}{a}\right)\cdot$$

$$\sin^2\left(2\pi\frac{z}{a}\right)\delta\left(x-\frac{a}{4}\right)\delta\left(y-\frac{a}{2}\right)\delta\left(z-\frac{3a}{4}\right)$$

$$= 8V_0 \sin^2\left(\frac{\pi}{4}\right)\sin^2\left(\frac{\pi}{2}\right)\sin^2\left(\frac{6\pi}{4}\right) = 8V_0\,\frac{1}{2} = 4V_0$$

$$V_{bb} = \langle 121|V|121\rangle = 8V_0 \sin^2\left(\frac{\pi}{4}\right)\sin^2(\pi)\sin^2\left(\frac{3\pi}{4}\right) = 0$$

$$V_{cc} = \langle 211|V|211\rangle = 8V_0 \sin^2\left(\frac{\pi}{2}\right)\sin^2\left(\frac{\pi}{2}\right)\sin^2\left(\frac{3\pi}{4}\right) = 8V_0\cdot\frac{1}{2} = 4V_0$$

Utan komaliner

$$V_{ab} = \langle 112|V|121\rangle = 8V_0 \sin^2\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{2}\right)\sin(\pi)\sin\left(\frac{3\pi}{4}\right)$$
$$\cdot \sin\left(\frac{6\pi}{4}\right) = 0$$

$$V_{ac} = \langle 112|V|211\rangle = 8V_0 \sin\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{2}\right)\sin^2\left(\frac{\pi}{2}\right)$$
$$\sin\left(\frac{3\pi}{4}\right)\sin\left(\frac{6\pi}{4}\right) = 8V_0\cdot\left(\frac{1}{-2}\right)$$
$$= -4V_0$$

$$V_{bc} = \langle 121|V|211\rangle = 8V_0 \sin\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{2}\right)\sin\left(\frac{\pi}{2}\right)\underline{\sin(\pi)}$$
$$\cdot\sin^2\left(\frac{3\pi}{4}\right) = 0$$

fylkjastökin eru raungild því þurfum við ekki að reikna fleiri

$$V = 4V_0 \begin{array}{c} \begin{array}{ccc} a & b & c \end{array} \\ \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \end{array}$$

röð valin í fylki

Ein lína (eða dálkur með 0) með 0 og hinar tvær eru háðar. Eru eins ef önnur er margfölduð með -1 → aðeins eitt ástand hreyfist til í orku

Finnum eigingildi

þau eru

$8V_0$ einfalt

0 tvöfalt

$$\rightarrow E_e^0 = E_1 \cdot 6 + \begin{cases} 8V_0 & \text{eitt} \\ 0 & \text{tvö} \end{cases}$$

og áður

$$E_g^0 = E_1 \cdot 3 + 2V_0$$

Var hægt að sjá þetta fyrir?

$\delta(y-\frac{a}{2})$ -> engin áhrif á líkur ö rvum í y-átt

$\delta(x-\frac{a}{4})$ - $\delta(z-\frac{3a}{4})$ -> sama gildi en öfugt formerki fyrir líkur örvum í x-og z-átt

-> Aðeins eitt ástand hreyfist til í orku vegna truflanamættisins V

6.17

Fyrir leiðréttinguna vegna afstæðiskenningar höfum við

$$(*) \qquad E_r^1 = -\frac{(E_n^0)^2}{2mc^2}\left\{\frac{4n}{l+\frac{1}{2}} - 3\right\} \qquad E_n^0 = -\frac{R_y}{n^2}$$

fyrir spuna-brautar víxlverkun

$$(**) \qquad E_{so}^1 = \frac{(E_n^0)^2}{mc^2}\left\{\frac{n\left(j(j+1) - l(l+1) - \frac{3}{4}\right)}{l(l+\frac{1}{2})(l+1)}\right\}$$

Sýnum að saman gefi þær

$$E_{fs}^1 = \frac{(E_n^0)^2}{mc^2}\left\{3 - \frac{4n}{j+\frac{1}{2}}\right\}$$

Við höfum $j = l \pm 1/2$ í vetnis atóminu, látum svarið er í j, reiknum því $l = j \pm 1/2$

$l = j + \frac{1}{2}$

$$E_r^1 + E_{so}^1 = \frac{(E_n^0)^2}{mc^2}\left\{\left[-\frac{2n}{j+1} + \frac{3}{2} + \frac{n\left[j(j+1) - (j+\frac{1}{2})(j+\frac{3}{2}) - \frac{3}{4}\right]}{(j+\frac{1}{2})(j+1)(j+\frac{3}{2})}\right]\right\}$$

$$= \frac{(E_n^0)^2}{mc^2}\left\{\left[-\frac{2n}{j+1} + \frac{3}{2} - \frac{n(j+\frac{3}{2})}{(j+\frac{1}{2})(j+1)(j+\frac{3}{2})}\right]\right\}$$

$$= \frac{(E_n^0)^2}{mc^2}\left\{\left[-\frac{2n}{j+1} + \frac{3}{2} - \frac{n}{(j+\frac{1}{2})(j+1)}\right]\right\}$$

$$= \frac{(E_n^0)^2}{mc^2}\left\{\frac{3}{2} - \frac{2n(j+\frac{1}{2}) + n}{(j+1)(j+\frac{1}{2})}\right\} = \frac{(E_n^0)^2}{2mc^2}\left\{3 - \frac{4n}{j+\frac{1}{2}}\right\}$$

$l = j - \frac{1}{2}$

$$E_r^1 + E_{sd}^1 = \frac{(E_n^0)^2}{mc^2}\left\{-\frac{2n}{j} + \frac{3}{2} + \frac{n\left[j(j+1) - (j-\frac{1}{2})(j+\frac{1}{2}) - \frac{3}{4}\right]}{(j-\frac{1}{2})\,j\,(j+\frac{1}{2})}\right\}$$

$$= \frac{(E_n^0)^2}{mc^2}\left\{\frac{3}{2} - \frac{2n}{j} + \frac{n\left[j^2 + j - j^2 + \frac{1}{4} - \frac{3}{4}\right]}{(j-\frac{1}{2})\,j\,(j+\frac{1}{2})}\right\}$$

$$= \frac{(E_n^0)^2}{mc^2}\left\{\frac{3}{2} - \frac{2n}{j} + \frac{n(j-\frac{1}{2})}{(j-\frac{1}{2})\,j\,(j+\frac{1}{2})}\right\}$$

$$= \frac{(E_n^0)^2}{mc^2}\left[\frac{3}{2} - \frac{2n}{j} + \frac{n}{j(j+\frac{1}{2})}\right]$$

$$= \frac{(E_n^0)^2}{mc^2}\left\{\frac{3}{2} + \frac{-2n(j+\frac{1}{2})+n}{j(j+\frac{1}{2})}\right\}$$

$$= \frac{(E_n^0)^2}{mc^2}\left\{\frac{3}{2} - \frac{2n}{(j+\frac{1}{2})}\right\}$$

$$= \frac{(E_n^0)^2}{2mc^2}\left\{3 - \frac{4n}{j+\frac{1}{2}}\right\}$$