4. zadaća iz kvantne fizike

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Zadatak 1

Hamiltonijan u sustavu s dva stanja ima oblik:

$$H = E_1 |1\rangle\langle 1| + E_2 |2\rangle\langle 2| + V|2\rangle\langle 1| + V^* |1\rangle\langle 2|$$

gdje konstante E_1, E_2 i V imaju dimenziju energije ($E_1, E_2 \in \mathbb{R}$). Odredite svojstvene energije i stanja sustava.

Zapišimo problem u matričnom obliku:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$H \begin{pmatrix} 1 \\ 0 \end{pmatrix} = H|1\rangle = E_1|1\rangle + V|2\rangle = \begin{pmatrix} E_1 \\ V \end{pmatrix}$$

$$H \begin{pmatrix} 0 \\ 1 \end{pmatrix} = H|2\rangle = E_2|2\rangle + V^*|1\rangle = \begin{pmatrix} V^* \\ E_2 \end{pmatrix}$$

$$\Rightarrow \quad H = \begin{pmatrix} E_1 & V^* \\ V & E_2 \end{pmatrix}$$

Svojstvene energije ... $\quad H|\psi\rangle = \varepsilon|\psi\rangle$

$$\det(H - \varepsilon) = 0 = \det \begin{pmatrix} E_1 - \varepsilon & V^* \\ V & E_2 - \varepsilon \end{pmatrix} =$$

$$= (E_1 - \varepsilon)(E_2 - \varepsilon) - |V|^2 = \varepsilon^2 - (E_1 + E_2)\varepsilon + E_1 E_2 - |V|^2 = 0$$

$$\rightsquigarrow \quad \varepsilon_\pm = \frac{1}{2}\left[E_1 + E_2 \pm \sqrt{(E_1+E_2)^2 - 4E_1E_2 + 4|V|^2}\right] =$$

$$= \frac{1}{2}\left[E_1 + E_2 \pm \sqrt{(E_1 - E_2) + 4|V|^2}\right]$$

Svojstvena stanja ...

$$|\psi_\pm\rangle = a_\pm |1\rangle + b_\pm |2\rangle = \begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix}$$

$$H|\psi_\pm\rangle = \varepsilon_\pm |\psi_\pm\rangle$$

$$H|\psi_\pm\rangle = \begin{pmatrix} E_1 a_\pm + V^* b_\pm \\ V a_\pm + E_2 b_\pm \end{pmatrix} = \begin{pmatrix} \varepsilon_\pm a_\pm \\ \varepsilon_\pm b_\pm \end{pmatrix}$$

$$\rightarrow \quad b_\pm = \frac{\varepsilon_\pm - E_1}{V^*} a_\pm$$

Normalizacija ...

$$\langle\psi_\pm|\psi_\pm\rangle = |a_\pm|^2 + |b_\pm|^2 = |a_\pm|^2 \left(1 + \frac{(\varepsilon_\pm - E_1)^2}{|V|^2}\right)$$

$$\rightarrow \quad a_\pm = \left(1 + \frac{(\varepsilon_\pm - E_1)^2}{|V|^2}\right)^{-1/2} =$$

$$\Rightarrow \quad |\psi_\pm\rangle = \left(1 + \frac{(\varepsilon_\pm - E_1)^2}{|V|^2}\right)^{-1/2} \left(|1\rangle + \frac{\varepsilon_\pm - E_1}{V^*} |2\rangle\right)$$

Zadatak 2

Izvedite izraz za korekciju energije i valne funkcije u trećem redu računa smetnje.

Rješavamo svojstveni problem $H|\psi_n\rangle = E_n|\psi_n\rangle$, gdje se hamiltonijan može napisati kao zbroj dva hermitska dijela $H = H_0 + V$. Pretpostavimo da znamo rješenje svojstvenog problema $H_0|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle$ i da je V "malo" u odnosu na H, tj. da ga možemo smatrati za smetnju.

Definirajmo funkciju $H(\lambda) = H_0 + \lambda V$ i pretpostavimo da je kontinuirana na $\lambda \in [0,1]$ te da postoje kontinuirana rješenja svojstvenog problema na tom intervalu λ:

$$H(\lambda)|\psi_n(\lambda)\rangle = E_n(\lambda)|\psi_n(\lambda)\rangle \qquad (1)$$

Naći ćemo aproksimativno rješenje (1) u trećem redu u λ. Rješenje originalnog problema dobijemo stavljajući $\lambda = 1$.

Razvijemo $E_n(\lambda)$ i $|\psi_n(\lambda)\rangle$ u Taylorov red:

$$E_n(\lambda) = \sum_{k=0}^{\infty} \frac{\lambda^k}{k!} \frac{\partial^k E_n}{\partial \lambda^k}\bigg|_0 = E_n(0) + \lambda \frac{\partial E_n}{\partial \lambda}\bigg|_0 + \frac{\lambda^2}{2}\frac{\partial^2 E_n}{\partial \lambda^2}\bigg|_0 + \dots$$

$$|\psi_n(\lambda)\rangle = \sum_{k=0}^{\infty} \frac{\lambda^k}{k!}\left(\frac{\partial^k}{\partial\lambda^k}|\psi_n(\lambda)\rangle\right)\bigg|_0 = |\psi_n(0)\rangle + \lambda\left(\frac{\partial}{\partial\lambda}|\psi_n(\lambda)\rangle\right)\bigg|_0 + \dots$$

Nazovimo koeficijente u Taylorovom razvoju:

$$E_n(0) = E_n^{(0)} \quad , \quad \frac{1}{k!}\left(\frac{\partial^k}{\partial\lambda^k}E_n(\lambda)\right)\bigg|_0 = E_n^{(k)}$$

$$|\psi_n(0)\rangle = |\psi_n^{(0)}\rangle \quad , \quad \frac{1}{k!}\left(\frac{\partial^k}{\partial\lambda^k}|\psi_n(\lambda)\rangle\right)\bigg|_0 = |\psi_n^{(k)}\rangle$$

Pa imamo:

$$E_m(\lambda) = E_m^{(0)} + \lambda E_m^{(1)} + \lambda^2 E_m^{(2)} + \lambda^3 E_m^{(3)} + \dots$$

$$|\psi_m(\lambda)\rangle = |\psi_m^{(0)}\rangle + \lambda|\psi_m^{(1)}\rangle + \lambda^2|\psi_m^{(2)}\rangle + \lambda^3|\psi_m^{(3)}\rangle + \dots \qquad (2)$$

$E_m^{(0)}$ i $|\psi_m^{(0)}\rangle$ su rješenje svojstvenog problema za $H(0)$.

Uvrstimo (2) u $H(\lambda)|\psi_m(\lambda)\rangle = E_m(\lambda)|\psi_m(\lambda)\rangle$:

$$(H_0 + \lambda V)\left(|\psi_m^{(0)}\rangle + \lambda|\psi_m^{(1)}\rangle + \lambda^2|\psi_m^{(2)}\rangle + \lambda^3|\psi_m^{(3)}\rangle + \dots\right) =$$

$$= \left(E_m^{(0)} + \lambda E_m^{(1)} + \lambda^2 E_m^{(2)} + \lambda^3 E_m^{(3)} + \dots\right) \times$$

$$\times \left(|\psi_m^{(0)}\rangle + \lambda|\psi_m^{(1)}\rangle + \lambda^2|\psi_m^{(2)}\rangle + \lambda^3|\psi_m^{(3)}\rangle + \dots\right)$$

Skupimo članove istog reda u λ:

$$\left(H_0|\psi_m^{(0)}\rangle - E_m^{(0)}|\psi_m^{(0)}\rangle\right) +$$

$$+ \lambda\left(H_0|\psi_m^{(1)}\rangle + V|\psi_m^{(0)}\rangle - E_m^{(0)}|\psi_m^{(1)}\rangle - E_m^{(1)}|\psi_m^{(0)}\rangle\right) +$$

$$+ \lambda^2\left(H_0|\psi_m^{(2)}\rangle + V|\psi_m^{(1)}\rangle - E_m^{(0)}|\psi_m^{(2)}\rangle - E_m^{(1)}|\psi_m^{(1)}\rangle - E_m^{(2)}|\psi_m^{(0)}\rangle\right) +$$

$$+ \lambda^3\left(H_0|\psi_m^{(3)}\rangle + V|\psi_m^{(2)}\rangle - E_m^{(0)}|\psi_m^{(3)}\rangle - E_m^{(1)}|\psi_m^{(2)}\rangle -\right.$$

$$\left. - E_m^{(2)}|\psi_m^{(1)}\rangle - E_m^{(3)}|\psi_m^{(0)}\rangle\right) + O(\lambda^4) = 0 \qquad (3)$$

Jednadžba (3) vrijedi $\forall \lambda \in [0,1]$ pa članovi uz različite potencije λ moraju zasebno iščezavati.

Nulti red $(\sim\lambda^0)$:

$$H_0|\psi_m^{(0)}\rangle = E_m^{(0)}|\psi_m^{(0)}\rangle$$

Prvi red $(\sim\lambda)$:

$$H_0|\psi_m^{(1)}\rangle + V|\psi_m^{(0)}\rangle = E_m^{(0)}|\psi_m^{(1)}\rangle + E_m^{(1)}|\psi_m^{(0)}\rangle \qquad (4)$$

Drugi red $(\sim\lambda^2)$:

$$H_0|\psi_m^{(2)}\rangle + V|\psi_m^{(1)}\rangle = E_m^{(0)}|\psi_m^{(2)}\rangle + E_m^{(1)}|\psi_m^{(1)}\rangle + E_m^{(2)}|\psi_m^{(0)}\rangle \qquad (5)$$

Treći red $(\sim\lambda^3)$:

$$H_0|\psi_m^{(3)}\rangle + V|\psi_m^{(2)}\rangle =$$

$$= E_m^{(0)}|\psi_m^{(3)}\rangle + E_m^{(1)}|\psi_m^{(2)}\rangle + E_m^{(2)}|\psi_m^{(1)}\rangle + E_m^{(3)}|\psi_m^{(0)}\rangle \qquad (6)$$

Rješenje nultog reda je po pretpostavci poznato.

Definirajmo pokrate: $V_{ij} = \langle\psi_i^{(0)}|V|\psi_j^{(0)}\rangle$

$$\Delta E_k = E_m^{(0)} - E_k^{(0)}$$

Može se pokazati da imamo slobodu odabrati

$$\langle\psi_m^{(0)}|\psi_m^{(k)}\rangle = 0 \qquad (7)$$

Pretpostavimo da je stanje $|\psi_m^{(0)}\rangle$ nedegenerirano u energiji!

Prvi red:

$$\langle\psi_m^{(0)}|\cdot \;/\; (4)$$

$$\rightarrow \langle\psi_m^{(0)}|H_0|\psi_m^{(1)}\rangle + \langle\psi_m^{(0)}|V|\psi_m^{(0)}\rangle =$$

$$= E_m^{(0)}\cancel{\langle\psi_m^{(0)}|\psi_m^{(1)}\rangle} + E_m^{(1)}\langle\psi_m^{(0)}|\psi_m^{(0)}\rangle$$

$$E_n^{(1)} = E_n^{(0)} \cancel{\langle \psi_n^{(0)} | \psi_n^{(1)} \rangle} + \langle \psi_n^{(0)} | V | \psi_n^{(0)} \rangle$$

$$\Rightarrow \boxed{E_n^{(1)} = V_{nn}}$$

Popravka energije u prvom redu

Rješenje problema $H_0 |\psi_k^{(0)}\rangle = E_k^{(0)} |\psi_k^{(0)}\rangle$ definira potpun skup $\{|\psi_k^{(0)}\rangle\}$. Tako možemo razviti $|\psi_n^{(1)}\rangle$ po svojstvenim stanjima H_0 : (uzmimo u obzir (7))

$$|\psi_n^{(1)}\rangle = \sum_{k \neq n} \langle \psi_k^{(0)} | \psi_n^{(1)} \rangle |\psi_k^{(0)}\rangle$$

Ako odredimo sve koeficijente u razvoju $\langle \psi_k^{(0)} | \psi_n^{(1)} \rangle$ odredili smo $|\psi_n^{(1)}\rangle$.

$$\langle \psi_k^{(0)} | \cdot / (6)$$

$$\rightarrow \langle \psi_k^{(0)} | H_0 | \psi_n^{(1)} \rangle + \langle \psi_k^{(0)} | V | \psi_n^{(0)} \rangle =$$

$$= E_n^{(0)} \langle \psi_k^{(0)} | \psi_n^{(1)} \rangle + E_n^{(1)} \cancel{\langle \psi_k^{(0)} | \psi_n^{(0)} \rangle}$$

$$E_k^{(0)} \langle \psi_k^{(0)} | \psi_n^{(1)} \rangle + \langle \psi_k^{(0)} | V | \psi_n^{(0)} \rangle =$$

$$= E_n^{(0)} \langle \psi_k^{(0)} | \psi_n^{(1)} \rangle$$

$$\Rightarrow \langle \psi_k^{(0)} | \psi_n^{(1)} \rangle = \frac{V_{kn}}{\Delta E_k}$$

$$\Rightarrow \boxed{|\psi_n^{(1)}\rangle = \sum_{k\neq n} \frac{V_{kn}}{\Delta E_k} |\psi_k^{(0)}\rangle}$$

Popravka valne funkcije u prvom redu

Drugi red :

$\langle \psi_n^{(0)}| \cdot \; / \; (5)$

$$\rightarrow \langle \psi_n^{(0)}| H_0 |\psi_n^{(2)}\rangle + \langle \psi_n^{(0)}|V|\psi_n^{(1)}\rangle =$$

$$= E_n^{(0)} \cancel{\langle \psi_n^{(0)}|\psi_n^{(2)}\rangle} + E_n^{(1)} \cancel{\langle \psi_n^{(0)}|\psi_n^{(1)}\rangle} + E_n^{(2)} \langle \psi_n^{(0)}|\psi_n^{(0)}\rangle$$

$$E_n^{(2)} = E_n^{(0)} \cancel{\langle \psi_n^{(0)}|\psi_n^{(2)}\rangle} = \langle \psi_n^{(0)}|V| \sum_{k\neq n} \frac{V_{kn}}{\Delta E_k} |\psi_k^{(0)}\rangle$$

$$\Rightarrow \boxed{E_n^{(2)} = \sum_{k\neq n} \frac{V_{kn} V_{nk}}{\Delta E_k}}$$

Popravka energije u drugom redu

$$|\psi_n^{(2)}\rangle = \sum_{l\neq n} \langle \psi_l^{(0)}|\psi_n^{(2)}\rangle |\psi_l^{(0)}\rangle$$

$\langle \psi_l^{(0)}| \cdot \; / \; (5)$

$$\langle \psi_l^{(0)}| H_0 |\psi_n^{(2)}\rangle + \langle \psi_l^{(0)}|V|\psi_n^{(1)}\rangle =$$

$$= E_n^{(0)} \langle \psi_l^{(0)}|\psi_n^{(2)}\rangle + E_n^{(1)} \langle \psi_l^{(0)}|\psi_n^{(1)}\rangle + E_n^{(0)} \cancel{\langle \psi_l^{(0)}|\psi_n^{(0)}\rangle}$$

$$E_l^{(0)}\langle\psi_l^{(0)}|\psi_m^{(2)}\rangle + \langle\psi_l^{(0)}|V\sum_{k\neq m}\frac{V_{km}}{\Delta E_k}|\psi_k^{(0)}\rangle =$$

$$= E_m^{(0)}\langle\psi_l^{(0)}|\psi_m^{(2)}\rangle + V_{mm}\langle\psi_l^{(0)}|\sum_{k\neq m}\frac{V_{km}}{\Delta E_k}|\psi_k^{(0)}\rangle$$

$$\Rightarrow \quad \langle\psi_l^{(0)}|\psi_m^{(2)}\rangle = \sum_{k\neq m}\frac{V_{lk}V_{km}}{\Delta E_l\,\Delta E_k} - \frac{V_{mm}V_{lm}}{(\Delta E_l)^2}$$

$$\Rightarrow \boxed{|\psi_m^{(2)}\rangle = \sum_{l\neq m}\left(\sum_{k\neq m}\frac{V_{lk}V_{km}}{\Delta E_l\Delta E_k} - \frac{V_{mm}V_{lm}}{(\Delta E_l)^2}\right)|\psi_l^{(0)}\rangle}$$

Popravka valne funkcije u drugom redu

Treći red:

$$\langle\psi_m^{(0)}|\cdot/\ (6)$$

$$\langle\psi_m^{(0)}|H_0|\psi_m^{(3)}\rangle + \langle\psi_m^{(0)}|V|\psi_m^{(2)}\rangle =$$

$$= E_m^{(0)}\cancel{\langle\psi_m^{(0)}|\psi_m^{(3)}\rangle} + E_m^{(1)}\cancel{\langle\psi_m^{(0)}|\psi_m^{(2)}\rangle} +$$

$$+ E_m^{(2)}\cancel{\langle\psi_m^{(0)}|\psi_m^{(1)}\rangle} + E_m^{(3)}\langle\psi_m^{(0)}|\psi_m^{(0)}\rangle$$

$$E_m^{(3)} = E_m^{(0)}\cancel{\langle\psi_m^{(0)}|\psi_m^{(3)}\rangle} +$$

$$+ \langle\psi_m^{(0)}|V\sum_{l\neq m}\left(\sum_{k\neq m}\frac{V_{lk}V_{km}}{\Delta E_l\,\Delta E_k} - \frac{V_{mm}V_{lm}}{(\Delta E_l)^2}\right)|\psi_l^{(0)}\rangle$$

$$\Rightarrow \boxed{E_n^{(3)} = \sum_{\ell \neq n} \left(\sum_{k \neq n} \frac{V_{n\ell} V_{\ell k} V_{kn}}{\Delta E_\ell \Delta E_k} - \frac{V_{nn} V_{n\ell} V_{\ell n}}{(\Delta E_\ell)^2} \right)}$$

Popravka energije u trećem redu

$$|\psi_n^{(3)}\rangle = \sum_{m \neq n} \langle \psi_m^{(0)} | \psi_n^{(3)} \rangle |\psi_m^{(0)}\rangle$$

$$\langle \psi_m^{(0)} | \cdot \ / \ (6)$$

$$\rightarrow \langle \psi_m^{(0)} | H_0 | \psi_n^{(3)} \rangle + \langle \psi_m^{(0)} | V | \psi_n^{(2)} \rangle =$$

$$= E_n^{(0)} \langle \psi_m^{(0)} | \psi_n^{(3)} \rangle + E_n^{(1)} \langle \psi_m^{(0)} | \psi_n^{(2)} \rangle +$$

$$+ E_n^{(2)} \langle \psi_m^{(0)} | \psi_n^{(1)} \rangle + E_n^{(3)} \cancel{\langle \psi_m^{(0)} | \psi_n^{(0)} \rangle}$$

$$E_m^{(0)} \langle \psi_m^{(0)} | \psi_n^{(3)} \rangle + \langle \psi_m^{(0)} | V | \psi_n^{(2)} \rangle =$$

$$= E_n^{(0)} \langle \psi_m^{(0)} | \psi_n^{(3)} \rangle + E_n^{(1)} \langle \psi_m^{(0)} | \psi_n^{(2)} \rangle + E_n^{(2)} \langle \psi_m^{(0)} | \psi_n^{(1)} \rangle$$

$$\rightarrow \langle \psi_m^{(0)} | \psi_n^{(3)} \rangle = \frac{\langle \psi_m^{(0)} | V | \psi_n^{(2)} \rangle}{\Delta E_m} - \frac{E_n^{(1)} \langle \psi_m^{(0)} | \psi_n^{(2)} \rangle}{\Delta E_m} -$$

$$- \frac{E_n^{(2)} \langle \psi_m^{(0)} | \psi_n^{(1)} \rangle}{\Delta E_m} =$$

$$= \frac{\langle \psi_m^{(0)} | V}{\Delta E_m} \sum_{\ell \neq n} \left(\sum_{k \neq n} \frac{V_{\ell k} V_{kn}}{\Delta E_\ell \Delta E_k} - \frac{V_{nn} V_{\ell n}}{(\Delta E_\ell)^2} \right) |\psi_\ell^{(0)}\rangle -$$

$$- \frac{V_{nn}}{\Delta E_m} \left(\sum_{k \neq n} \frac{V_{mk} V_{kn}}{\Delta E_m \Delta E_k} - \frac{V_{nn} V_{mn}}{(\Delta E_m)^2} \right) - \sum_{k \neq n} \frac{V_{kn} V_{nk}}{\Delta E_m \Delta E_k} \frac{V_{mn}}{\Delta E_m}$$

$$\Rightarrow \langle \psi_m^{(0)} | \psi_n^{(3)} \rangle =$$

$$= \sum_{l \neq n} \left(\sum_{k \neq n} \frac{V_{ml} V_{lk} V_{kn}}{\Delta E_m \Delta E_l \Delta E_k} - \frac{V_{nn} V_{ml} V_{ln}}{\Delta E_m (\Delta E_l)^2} \right) -$$

$$- \sum_{k \neq n} \frac{V_{nn} V_{mk} V_{kn}}{(\Delta E_m)^2 \Delta E_k} + \frac{V_{nn}^{\,2} V_{mn}}{(\Delta E_m)^3} - \sum_{k \neq n} \frac{V_{kn} V_{nk} V_{mn}}{(\Delta E_m)^2 \Delta E_k}$$

Uvrstimo gornji rezultat u:

$$|\psi_n^{(3)}\rangle = \sum_{m \neq n} \langle \psi_m^{(0)} | \psi_n^{(3)} \rangle \, | \psi_m^{(0)} \rangle$$

Popravka valne funkcije u trećem redu

Zadatak 3

Jednodimenzionalni harmonički oscilator je pod utjecajem smetnje oblika

$$\delta V(x) = \frac{\lambda}{x^2+a^2}$$

Odredite prvu popravku energije osnovnog stanja harmoničkog oscilatora u slučaju kada je:

(a) $a \ll \sqrt{\frac{\hbar}{m\omega}}$, (b) $a \gg \sqrt{\frac{\hbar}{m\omega}}$

Osnovno stanje harmoničkog oscilatora:

$$\psi(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega x^2}{2\hbar}\right)$$

Prva popravka energije:

$$\Delta E = \langle\psi|\delta V|\psi\rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x)\,\delta V(x)\,\psi(x) =$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} \lambda \int_{-\infty}^{\infty} dx \frac{\exp\left(-\frac{m\omega}{\hbar}x^2\right)}{x^2+a^2} = \left\{ \begin{array}{l} z = \sqrt{\frac{m\omega}{\hbar}}\, x \\ dx = \sqrt{\frac{\hbar}{m\omega}}\, dz \end{array} \right.$$

$$= \frac{\lambda}{\sqrt{\pi}} \int_{-\infty}^{\infty} dz \frac{e^{-z^2}}{\frac{\hbar}{m\omega}z^2 + a^2} =$$

$$= \frac{m\omega}{\hbar}\frac{\lambda}{\sqrt{\pi}} \int_{-\infty}^{\infty} dz \frac{e^{-z^2}}{z^2 + \frac{m\omega}{\hbar}a^2} = \left\{ \alpha = \sqrt{\frac{m\omega}{\hbar}}\, a \right.$$

$$= \frac{m\omega}{\hbar}\frac{\lambda}{\sqrt{\pi}} \int_{-\infty}^{\infty} dz \frac{e^{-z^2}}{z^2+\alpha^2} = \frac{m\omega}{\hbar}\frac{\lambda}{\sqrt{\pi}}\, I$$

$$I = \int_{-\infty}^{\infty} dz \, \frac{e^{-z^2}}{z^2+\alpha^2} = ?$$

Integral I riješit ćemo na dva načina.

1. način

Definiramo: $I(\beta) = \int_{-\infty}^{\infty} dz \, \frac{e^{-\beta z^2}}{z^2+\alpha^2}$, $\beta \geq 0$; $I = I(1)$

$$\frac{dI(\beta)}{d\beta} = -\int_{-\infty}^{\infty} dz \, \frac{z^2 e^{-\beta z^2}}{z^2+\alpha^2}$$

Konstruiramo diferencijalnu jednadžbu za $I(\beta)$:

$$-\frac{dI(\beta)}{d\beta} + \alpha^2 I(\beta) = \int_{-\infty}^{\infty} dz \, \frac{z^2 e^{-\beta z^2}}{z^2+\alpha^2} + \int_{-\infty}^{\infty} dz \, \frac{\alpha^2 e^{-\beta z^2}}{z^2+\alpha^2} =$$

$$= \int_{-\infty}^{\infty} dz \, \frac{\cancel{(z^2+\alpha^2)} \exp(-\beta z^2)}{\cancel{z^2+\alpha^2}} = \int_{-\infty}^{\infty} dz \, e^{-\beta z^2} = \sqrt{\frac{\pi}{\beta}}$$

$$\Rightarrow \quad \frac{dI(\beta)}{d\beta} - \alpha^2 I(\beta) = -\sqrt{\frac{\pi}{\beta}} \quad (*)$$

Jednadžba $(*)$ je prvog reda $\rightarrow$ treba nam jedan rubni uvjet. Znamo odrediti $I(0)$:

$$I(0) = \int_{-\infty}^{\infty} \frac{dz}{z^2+\alpha^2} = \frac{1}{\alpha} \arctan\left(\frac{z}{\alpha}\right)\Big|_{-\infty}^{\infty} = \frac{\pi}{\alpha}$$

$\rightarrow$ $I(0) = \frac{\pi}{\alpha}$ rubni uvjet

Asimptotski, za $\beta \to \infty$ je ⊛ približno:

$$\frac{dI(\beta)}{d\beta} \approx \alpha^2 I(\beta) \implies I(\beta) \sim e^{\beta\alpha^2}$$

Pretpostavimo $I(\beta) = f(\beta)\, e^{\beta\alpha^2}$

$$\frac{dI(\beta)}{d\beta} = \frac{df}{d\beta} e^{\beta\alpha^2} + \alpha^2 I(\beta)$$

Uvrstimo u ⊛:

$$\implies \underline{\frac{df}{d\beta} = -\sqrt{\frac{\pi}{\beta}}\, e^{-\beta\alpha^2}} \quad \Big/ \int_0^\beta$$

$$\int_0^\beta \frac{df}{dw} dw = f(\beta) - f(0) = -\sqrt{\pi} \int_0^\beta dw\, \frac{e^{-\alpha^2 w}}{\sqrt{w}} = \left\{ \begin{array}{l} t = \alpha\sqrt{w} \\ \frac{dw}{\sqrt{w}} = \frac{2}{\alpha} dt \end{array} \right.$$

$$= -\frac{2\sqrt{\pi}}{\alpha} \int_0^{\alpha\sqrt{\beta}} dt\, e^{-t^2} = -\frac{\pi}{\alpha} \operatorname{erf}(\alpha\sqrt{\beta})$$

$$\to f(\beta) = f(0) - \frac{\pi}{\alpha} \operatorname{erf}(\alpha\sqrt{\beta})$$

$$\to I(\beta) = e^{\beta\alpha^2} f(\beta) = e^{\beta\alpha^2} f(0) - \frac{\pi}{\alpha} e^{\beta\alpha^2} \operatorname{erf}(\alpha\sqrt{\beta})$$

Rubni uvjet:

$$I(0) = \frac{\pi}{\alpha} = f(0) - \frac{\pi}{\alpha}\operatorname{erf}(0) = f(0)$$

$$\implies I(\beta) = e^{\beta\alpha^2} \frac{\pi}{\alpha} \left(1 - \operatorname{erf}(\alpha\sqrt{\beta})\right)$$

Pa je traženo rješenje:

$$\underline{I = I(1) = e^{\alpha^2} \frac{\pi}{\alpha} \left(1 - \operatorname{erf}(\alpha)\right)}$$

2. način (zahvaljujući Klajnu)

$$I = \int_{-\infty}^{\infty} dz \, \frac{e^{-z^2}}{z^2+\alpha^2} = ?$$

Primjetimo da je: $\displaystyle\int_{1}^{\infty} d\beta \, e^{-\beta(z^2+\alpha^2)} = \frac{e^{-(z^2+\alpha^2)}}{z^2+\alpha^2}$

$$I = e^{\alpha^2}\int_{-\infty}^{\infty} dz \, \frac{e^{-(z^2+\alpha^2)}}{z^2+\alpha^2} = e^{\alpha^2}\int_{-\infty}^{\infty} dz \int_{1}^{\infty} d\beta \, e^{-\beta(z^2+\alpha^2)} =$$

$$= e^{\alpha^2}\int_{1}^{\infty} d\beta \, e^{-\beta\alpha^2}\int_{-\infty}^{\infty} dz \, e^{-\beta z^2} = e^{\alpha^2}\int_{1}^{\infty} d\beta \, e^{-\beta\alpha^2}\sqrt{\frac{\pi}{\beta}} =$$

$$= \sqrt{\pi}\, e^{\alpha^2}\int_{1}^{\infty} d\beta \, \frac{e^{-\beta\alpha^2}}{\sqrt{\beta}} = \left\{ \begin{array}{l} t = \alpha\sqrt{\beta} \\ \frac{d\beta}{\sqrt{\beta}} = \frac{2}{\alpha}dt \end{array} \right.$$

$$= \frac{2\sqrt{\pi}}{\alpha} e^{\alpha^2}\int_{\alpha}^{\infty} dt \, e^{-t^2} = \frac{2\sqrt{\pi}}{\alpha} e^{\alpha^2}\left(\int_{0}^{\infty} dt\, e^{-t^2} - \int_{0}^{\alpha} dt\, e^{-t^2}\right) =$$

$$= \frac{2\sqrt{\pi}}{\alpha} e^{\alpha^2}\left(\frac{\sqrt{\pi}}{2} - \int_{0}^{\alpha} dt\, e^{-t^2}\right) = \frac{\pi}{\alpha} e^{\alpha^2}\left(1 - \frac{2}{\sqrt{\pi}}\int_{0}^{\alpha} dt\, e^{-t^2}\right) =$$

$$= \underline{\frac{\pi}{\alpha} e^{\alpha^2}\left(1 - \operatorname{erf}(\alpha)\right)}$$

Pa imamo analitički izraz za prvu popravku energije:

$$\Delta E = \underline{\frac{\sqrt{\pi}\, m\omega\lambda}{\hbar}\, \frac{e^{\alpha^2}}{\alpha}\left(1 - \operatorname{erf}(\alpha)\right)} =$$

$$= \underline{\underline{\sqrt{\frac{\pi m\omega}{\hbar}}\, \frac{\lambda}{a}\left[1 - \operatorname{erf}\left(\sqrt{\frac{m\omega}{\hbar}}\, a\right)\right] \exp\left(\frac{m\omega}{\hbar} a^2\right)}}$$

Nađimo sada tražene limese . . .

(a) $a \ll \sqrt{\frac{\hbar}{m\omega}} \longrightarrow \underline{\alpha \ll 1}$

Razvijemo $erf(\alpha)$ u red potencija po α:

$$erf(\alpha) = \frac{2}{\sqrt{\pi}} \int_0^\alpha dw\, e^{-w^2} = \frac{2}{\sqrt{\pi}} \int_0^\alpha dw \sum_{n=0}^{\infty} \frac{(-w^2)^n}{n!} =$$

$$= \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-)^n}{n!} \int_0^\alpha dw\, w^{2n} = \underline{\frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-)^n}{n!} \frac{\alpha^{2n+1}}{2n+1}}$$

$$\longrightarrow \underline{erf(\alpha) \approx \frac{2}{\sqrt{\pi}} \alpha}$$

$$e^{\alpha^2} \approx 1 + \alpha^2$$

$$\Longrightarrow \Delta E \approx \frac{\sqrt{\pi}\, m\omega\lambda}{\hbar} \frac{1}{\alpha} (1+\alpha^2)(1-\alpha) \approx \frac{\sqrt{\pi}\, m\omega\lambda}{\hbar\alpha} =$$

$$= \underline{\underline{\sqrt{\frac{\pi m\omega}{\hbar}} \frac{\lambda}{a}}}$$

(b) $a \gg \sqrt{\frac{\hbar}{m\omega}} \longrightarrow \underline{\alpha \gg 1}$

Razvijemo $e^{\alpha^2}(1-erf(\alpha))$ u asimptotski red:

$$e^{\alpha^2}(1-erf(\alpha)) = e^{\alpha^2}\left(1 - \frac{2}{\sqrt{\pi}} \int_0^\alpha dt\, e^{-t^2}\right) =$$

$$= e^{\alpha^2} \frac{2}{\sqrt{\pi}} \left(\frac{\sqrt{\pi}}{2} - \int_0^\alpha dt\, e^{-t^2}\right) = e^{\alpha^2} \frac{2}{\sqrt{\pi}} \left(\int_0^\infty dt\, e^{-t^2} - \int_0^\alpha dt\, e^{-t^2}\right) =$$

$$= \frac{2}{\sqrt{\pi}} e^{\alpha^2} \int_\alpha^\infty dt\, e^{-t^2} = \frac{2}{\sqrt{\pi}} \int_\alpha^\infty dt\, e^{-(t^2-\alpha^2)} = \left\{ \begin{array}{l} w = t^2 - \alpha^2 \\ dt = \frac{dw}{2\sqrt{w^2+\alpha^2}} \end{array} \right.$$

$$= \frac{1}{\sqrt{\pi}} \int_0^\infty dw \frac{e^{-w}}{\sqrt{w^2+\alpha^2}} = \frac{1}{\alpha\sqrt{\pi}} \int_0^\infty dw \frac{e^{-w}}{\sqrt{1+\frac{w^2}{\alpha^2}}} = \left(\begin{array}{l} \text{u smislu} \\ \text{asimptotskog} \\ \text{razvoja} \end{array} \right)$$

$$= \frac{1}{\alpha\sqrt{\pi}} \int_0^\infty dw\, e^{-w} \sum_{n=0}^\infty \frac{(2n)!}{(2^n n!)^2} \left(\frac{w^2}{\alpha^2}\right)^n =$$

$$= \frac{1}{\alpha\sqrt{\pi}} \sum_{n=0}^\infty \frac{(2n)!}{(2^n n! \alpha^n)^2} \int_0^\infty dw\, e^{-w} w^{2n} =$$

$$= \frac{1}{\alpha\sqrt{\pi}} \sum_{n=0}^\infty \frac{[(2n)!]^2}{[2^n n! \alpha^n]^2} \approx \frac{1}{\alpha\sqrt{\pi}} \quad , \text{ za } \alpha \gg 1$$

$$\Rightarrow \Delta E \approx \frac{m\omega\lambda}{\hbar\alpha^2} = \underline{\underline{\frac{\lambda}{a^2}}}$$

Zadatak 4

Promatramo česticu mase m u potencijalu $V(x)$ koji se može prikazati preko razvoja u red:

$$V(x) = \frac{1}{2} m\omega^2 x^2 + \alpha x^4 + \dots$$

gdje je $\alpha\left(\frac{\hbar}{2m\omega}\right)^2 \ll \hbar\omega$. Odredite popravke energije osnovnog i pobuđenih stanja u prvom i drugom redu računa smetnje koje dolaze od anharmoničkog člana. Nacrtajte (na istom grafu) energijske nivoe harmoničkog oscilatora te popravljene nivoe. Odredite za koja stanja ne vrijedi harmonička aproksimacija.

Za nesmetani hamiltonijan imamo: $H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$

Svojstvene valne funkcije i energije za H_0 su:

$$\psi_n^{(0)}(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) \exp\left(-\frac{m\omega}{2\hbar} x^2\right)$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

Smetnja je $\delta V(x) = \alpha x^4$.

Izrazi za popravke energije n-tog stanja dane su sa:

$$\Delta E_n^{(1)} = \langle \psi_n^{(0)} | \delta V | \psi_n^{(0)} \rangle$$

$$\Delta E_n^{(2)} = \sum_{\substack{k=0 \\ k \neq n}}^{\infty} \frac{\langle \psi_n^{(0)} | \delta V | \psi_k^{(0)} \rangle \langle \psi_k^{(0)} | \delta V | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}}$$

Potrebno je naći matrične elemente:

$$\langle \psi_k^{(0)} | \delta V | \psi_n^{(0)} \rangle = ?$$

$$\langle \psi_k^{(0)} | \delta V | \psi_n^{(0)} \rangle = \int_{-\infty}^{\infty} dx \left(\psi_k^{(0)}(x)\right)^* \delta V(x)\, \psi_n^{(0)}(x) =$$

$$= \frac{\alpha}{\sqrt{2^{n+k} n! k!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \int_{-\infty}^{\infty} dx\, H_k\left(\sqrt{\frac{m\omega}{\hbar}} x\right) x^4 H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right) \exp\left(-\frac{m\omega}{\hbar} x^2\right)$$

$$\left\{ \quad z = \sqrt{\frac{m\omega}{\hbar}} x \qquad dx = \sqrt{\frac{\hbar}{m\omega}} \quad \right\}$$

$$= \frac{\alpha}{\sqrt{\pi 2^{n+k} n! k!}} \left(\frac{\hbar}{m\omega}\right)^2 \int_{-\infty}^{\infty} dz\, H_k(z)\, z^4 H_n(z) \exp\left(-z^2\right)$$

Raspisat ćemo $z^4 H_n(z)$ koristeći rekurzijsku relaciju:

$$\underline{H_{n+1}(z) = 2z H_n(z) - 2n H_{n-1}(z)}$$

$$z H_n(z) = \frac{1}{2} H_{n+1}(z) + n H_{n-1}(z)$$

$$z^2 H_n = z\left(\frac{1}{2} H_{n+1} + n H_{n-1}\right) =$$

$$= \frac{1}{2} z H_{n+1} + n z H_{n-1} =$$

$$= \frac{1}{2}\left(\frac{1}{2} H_{n+2} + (n+1) H_n\right) + n\left(\frac{1}{2} H_n + (n-1) H_{n-2}\right) =$$

$$= \frac{1}{4} H_{n+2} + \frac{2n+1}{2} H_n + n(n-1) H_{n-2}$$

$$z^3 H_n = \frac{1}{4} z H_{n+2} + \frac{2n+1}{2} z H_n + n(n-1) z H_{n-2} =$$

$$= \frac{1}{4}\left(\frac{1}{2} H_{n+3} + (n+2) H_{n+1}\right) + \frac{2n+1}{2}\left(\frac{1}{2} H_{n+1} + n H_{n-1}\right) +$$

$$+ n(n-1)\left(\frac{1}{2} H_{n-1} + (n-2) H_{n-3}\right) =$$

$$= \frac{1}{8} H_{n+3} + \frac{3(n+1)}{4} H_{n+1} + \frac{3n^2}{2} H_{n-1} + n(n-1)(n-2) H_{n-3}$$

$$\underline{\underline{z^4 H_n}} = \frac{1}{8} z H_{n+3} + \frac{3(n+1)}{4} z H_{n+1} + \frac{3n^2}{2} z H_{n-1} +$$

$$+ n(n-1)(n-2) z H_{n-3} =$$

$$= \frac{1}{8}\left(\frac{1}{2} H_{n+4} + (n+3) H_{n+2}\right) + \frac{3(n+1)}{4}\left(\frac{1}{2} H_{n+2} + (n+1) H_n\right) +$$

$$+ \frac{3n^2}{2}\left(\frac{1}{2} H_n + (n-1) H_{n-2}\right) + n(n-1)(n-2)\left(\frac{1}{2} H_{n-2} + (n-3) H_{n-4}\right) =$$

$$= \frac{1}{16} H_{n+4} + \frac{2n+3}{4} H_{n+2} + \frac{3(2n^2+2n+1)}{4} H_n +$$

$$+ n(n-1)(2n-1) H_{n-2} + n(n-1)(n-2)(n-3) H_{n-4}$$

U gornjem raspisu se za $n = 0, 1, 2, 3$ pojavljuju nedefinirani Hermiteovi polinomi negativnog reda. Međutim, faktor koji stoji ispred njih je nula u tim slučajevima pa nam je gornja relacija operativna.

Sljedeće, koristimo ortogonalnost Hermiteovih polinoma:

$$\int_{-\infty}^{\infty} dz\, H_n(z) H_m(z) e^{-z^2} = \delta_{nm}\, 2^n n! \sqrt{\pi}$$

$$\underline{\underline{\langle \psi_k^{(0)} | \delta V | \psi_m^{(0)} \rangle}} = \frac{\alpha}{\sqrt{\pi\, 2^{m+k}\, m!\, k!}} \left(\frac{\hbar}{m\omega}\right)^2 \times$$

$$\times \left[\frac{1}{16} \int_{-\infty}^{\infty} dz\, H_{m+4}(z)\, H_k(z)\, e^{-z^2} + \frac{2m+3}{4} \int_{-\infty}^{\infty} dz\, H_{m-2}(z)\, H_k(z)\, e^{-z^2} + \right.$$

$$+ \frac{3(2m^2+2m+1)}{4} \int_{-\infty}^{\infty} dz\, H_m(z)\, H_k(z)\, e^{-z^2} +$$

$$+ m(m-1)(2m-1) \int_{-\infty}^{\infty} dz\, H_{m-2}(z)\, H_k(z)\, e^{-z^2} +$$

$$\left. + m(m-1)(m-2)(m-3) \int_{-\infty}^{\infty} dz\, H_{m-4}(z)\, H_k(z)\, e^{-z^2} \right] =$$

$$= \alpha \left(\frac{\hbar}{m\omega}\right)^2 \left[\frac{1}{16} \sqrt{\frac{2^k k!}{2^m m!}}\, \delta_{m+4,k} + \frac{2m+3}{4} \sqrt{\frac{2^k k!}{2^m m!}}\, \delta_{m+2,k} + \right.$$

$$+ \frac{3(2m^2+2m+1)}{4} \sqrt{\frac{2^k k!}{2^m m!}}\, \delta_{m,k} + m(m-1)(2m-1) \sqrt{\frac{2^k k!}{2^m m!}}\, \delta_{m-2,k} +$$

$$\left. + m(m-1)(m-2)(m-3) \sqrt{\frac{2^k k!}{2^m m!}}\, \delta_{m-4,k} \right] =$$

$$= \alpha \left(\frac{\hbar}{m\omega}\right)^2 \left[\frac{1}{16} \sqrt{\frac{2^{m+4}(m+4)!}{2^m m!}}\, \delta_{m+4,k} + \frac{2m+3}{4} \sqrt{\frac{2^{m+2}(m+2)!}{2^m m!}}\, \delta_{m+2,k} + \right.$$

$$+ \frac{3(2m^2+2m+1)}{4} \sqrt{\frac{2^m m!}{2^m m!}}\, \delta_{m,k} + m(m-1)(2m-1) \sqrt{\frac{2^{m-2}(m-2)!}{2^m m!}}\, \delta_{m-2,k} +$$

$$\left. + m(m-1)(m-2)(m-3) \sqrt{\frac{2^{m-4}(m-4)!}{2^m m!}}\, \delta_{m-4,k} \right] =$$

$$= \alpha \left(\frac{\hbar}{m\omega}\right)^2 \left[\frac{1}{4}\sqrt{(n+1)(n+2)(n+3)(n+4)}\ \delta_{n+4,k} + \right.$$

$$+ \frac{2n+3}{2}\sqrt{(n+1)(n+2)}\ \delta_{n+2,k} + \frac{3(2n^2+2n+1)}{4}\ \delta_{n,k} +$$

$$\left. + \frac{2n-1}{2}\sqrt{n(n-1)}\ \delta_{n-2,k} + \frac{1}{4}\sqrt{n(n-1)(n-2)(n-3)}\ \delta_{n-4,k} \right] \tag{1}$$

Za prvu popravku imamo:

$$\Delta E_n^{(1)} = \langle \psi_n^{(0)} | \delta V | \psi_n^{(0)} \rangle = \underline{\underline{3\,(2n^2+2n+1)\,\alpha \left(\frac{\hbar}{2m\omega}\right)^2}} \tag{2}$$

Za drugu popravku imamo:

$$\Delta E_n^{(2)} = \sum_{\substack{n=0\\ n\neq k}}^{\infty} \frac{|\langle \psi_k^{(0)} | \delta V | \psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}} =$$

$$= \frac{1}{\hbar\omega} \sum_{\substack{n=0\\ n\neq k}}^{\infty} \frac{|\langle \psi_n^{(0)} | \delta V | \psi_k^{(0)} \rangle|^2}{(n-k)}$$

$$= \frac{\alpha^2}{\hbar\omega}\left(\frac{\hbar}{m\omega}\right)^4 \left[\frac{(n+1)(n+2)(n+3)(n+4)}{(-4)\cdot 16} + \right.$$

$$+ \frac{(2n+3)^2}{(-2)\cdot 4}(n+1)(n+2) + \frac{(2n-1)^2}{2\cdot 4} n(n-1) +$$

$$\left. + \frac{n(n-1)(n-2)(n-3)}{4\cdot 16} \right] =$$

$$\underline{\underline{= -\frac{\alpha^2}{\hbar\omega}\left(\frac{\hbar}{2m\omega}\right)^4 \left[42 + 118n + 102n^2 + 68n^3 \right]}} \tag{3}$$

Harmonička aproksimacija više ne vrijedi kada je prva popravka energije reda veličine $\hbar\omega$ (razmaka između energijskih nivoa harmoničkog oscilatora). To je ispunjeno za stanje:

$$3(2n^2+2n+1)\,\alpha\left(\frac{\hbar}{2m\omega}\right)^2 \sim \hbar\omega$$

Uzmimo da je $\dfrac{\hbar\omega}{\alpha\left(\frac{\hbar}{2m\omega}\right)^2} = \dfrac{1}{\eta}$, gdje je η neki jako mali broj.

$$\Rightarrow \quad n^2+n+\frac{1}{2}-\frac{1}{3\eta} \sim 0$$

Pa je gruba granica gdje prestaje važiti harmonička aproksimacija:

$$n_{granično} \sim \frac{1}{2}\left(-1+\sqrt{\frac{4}{3\eta}-1}\right)$$

Dakle, ne vrijedi za $n > n_{granično}$.

Za ilustraciju:

$\eta = 0.1 \longrightarrow n_{granično} \sim 1$

$\eta = 0.01 \longrightarrow n_{granično} \sim 5$

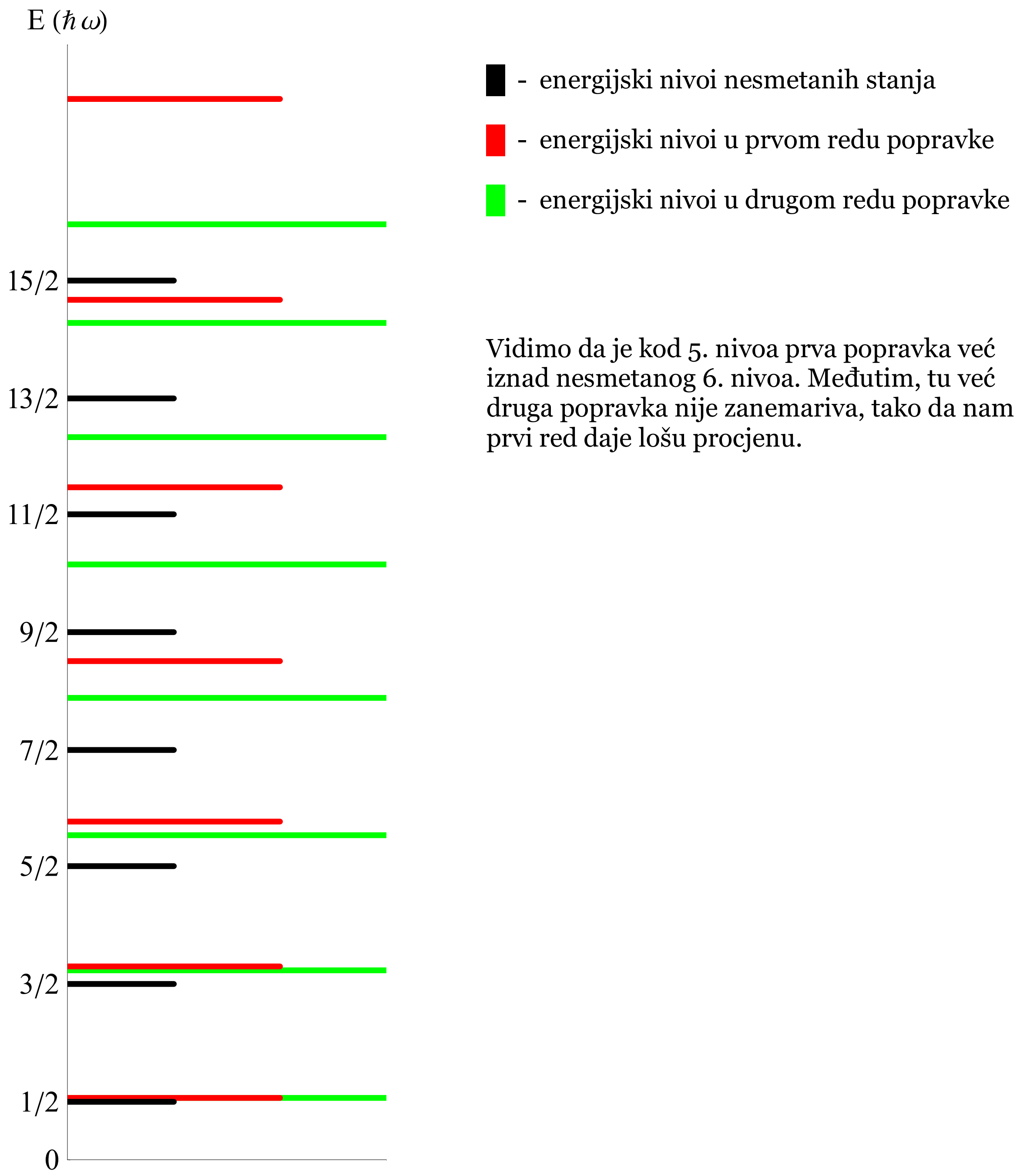
$\eta = 10^{-3} \longrightarrow n_{granično} \sim 17$

$\eta = 10^{-4} \longrightarrow n_{granično} \sim 57$

$\eta = 10^{-5} \longrightarrow n_{granično} \sim 182$

Naravno, ovo su grube procjene jer za velike n druga popravka postaje usporediva sa prvom popravkom i račun smetnje ne daje dobre rezultate u tako niskom redu.

Enerijski dijagram za prvih osam nivoa za $\frac{a}{\hbar\omega}\left(\frac{\hbar}{2m\omega}\right)^2 = 0.01$



Vidimo da je kod 5. nivoa prva popravka već iznad nesmetanog 6. nivoa. Međutim, tu već druga popravka nije zanemariva, tako da nam prvi red daje lošu procjenu.

Rezultat (1) možemo dobiti i pomoću operatora podizanja i spuštanja za harmonički oscilator :

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{i}{m\omega}p\right)$$

$$a^{+} = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{i}{m\omega}p\right) \quad , \quad [a, a^{+}] = 1$$

Oni imaju svojstva da je : $a|\psi_n^{(0)}\rangle = \sqrt{n}\,|\psi_{n-1}^{(0)}\rangle$

$a^{+}|\psi_n^{(0)}\rangle = \sqrt{n+1}\,|\psi_{n+1}^{(0)}\rangle$

Pa smetnju možemo raspisati pomoću njih :

$$x = \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^{+})$$

$$\delta V = \alpha x^4 = \alpha\left(\frac{\hbar}{2m\omega}\right)^2 (a+a^{+})^4 \equiv A\,(a+a^{+})^4$$

$$\langle \psi_n^{(0)} | \alpha x^4 | \psi_n^{(0)} \rangle = ?$$

$$x^4 |\psi_n^{(0)}\rangle = A\,(a+a^{+})^3 (a+a^{+}) |\psi_n^{(0)}\rangle =$$

$$= A\,(a+a^{+})^3 \left[\sqrt{n}\,|\psi_{n-1}^{(0)}\rangle + \sqrt{n+1}\,|\psi_{n+1}^{(0)}\rangle \right] =$$

$$= A\,(a+a^{+})^2 \left[\sqrt{n(n-1)}\,|\psi_{n-2}^{(0)}\rangle + (2n+1)\,|\psi_n^{(0)}\rangle + \right.$$

$$\left. + \sqrt{(n+1)(n+2)}\,|\psi_{n+2}^{(0)}\rangle \right] =$$

$$= A\,(a+a^{+}) \left[\sqrt{n(n-1)(n-2)}\,|\psi_{n-3}^{(0)}\rangle + 3n\sqrt{n}\,|\psi_{n-1}^{(0)}\rangle + \right.$$

$$\left. + 3(n+1)\sqrt{n+1}\,|\psi_{n+1}^{(0)}\rangle + \sqrt{(n+1)(n+2)(n+3)}\,|\psi_{n+3}^{(0)}\rangle \right] =$$

$$= A \Big[\sqrt{n(n-1)(n-2)(n-3)}\,|\psi_{n-4}^{(0)}\rangle + 2(n-2)\sqrt{n(n-1)}\,|\psi_{n-2}^{(0)}\rangle +$$

$$+ 3(2n^2+2n+1)\,|\psi_n^{(0)}\rangle + 2(2n+3)\sqrt{(n+1)(n+2)}\,|\psi_{n+2}^{(0)}\rangle +$$

$$+ \sqrt{(n+1)(n+2)(n+3)(n+4)}\,|\psi_{n+4}^{(0)}\rangle \Big]$$

$$\Rightarrow \quad \underline{\langle \psi_k^{(0)} | \delta V | \psi_n^{(0)} \rangle} =$$

$$= \alpha \left(\frac{\hbar}{2m\omega}\right)^2 \Big[\sqrt{n(n-1)(n-2)(n-3)}\;\delta_{k,n-4} +$$

$$+ 2(2n-1)\sqrt{n(n-1)}\;\delta_{k,n-2} + 3(2n^2+2n+1)\;\delta_{k,n} +$$

$$+ 2(2n+3)\sqrt{(n+1)(n+2)}\;\delta_{k,n+2} +$$

$$+ \sqrt{(n+1)(n+2)(n+3)(n+4)}\;\delta_{k,n+4} \Big]$$

Gornji rezultat je isto što i (1) i iz njega slijede (2) i (3).

Zadatak 5

Izračunati u prvom redu računa smetnje energetski pomak osnovnog stanja elektrona u atomu sličnom vodiku (atomski broj Z, samo jedan elektron) do kojeg dolazi jer naboj jezgre nije točkast. Promatrati jezgru kao homogeno nabijenu kuglu polumjera R i naboja Ze. Odrediti ovisnost korekcije o atomskom broju atoma.

Potencijalna energija elektrona u potencijalu jezgre (homogeno nabijene kuglice) je:

$$V(r) = \begin{cases} -\dfrac{Ze^2}{r} & , \quad r > R \\ \dfrac{Ze^2}{R}\left(\dfrac{1}{2}\left(\dfrac{r}{R}\right)^2 - \dfrac{3}{2}\right) & , \quad r < R \end{cases}$$

Potencijal na području $r < R$ smatramo da je potencijal točkastog naboja + smetnja. Točnije:

$$V(r) = -\frac{Ze^2}{r} + \delta V(r) \quad , \quad \text{gdje je smetnja:}$$

$$\delta V(r) = \begin{cases} \dfrac{Ze^2}{R}\left(\dfrac{1}{2}\left(\dfrac{r}{R}\right)^2 - \dfrac{3}{2}\right) + \dfrac{Ze^2}{R} & , \quad r < R \\ 0 & , \quad r > R \end{cases}$$

Osnovno stanje elektrona u atomu s točkastom jezgrom naboja Ze opisano je valnom funkcijom:

$$\psi_{100}(\vec{r}) = \frac{1}{\sqrt{\pi a^3}} \exp\left(-\frac{r}{a}\right) \quad ; \quad a = \frac{\hbar^2}{m_e Z e^2} = \frac{a_0}{Z}$$

Pa je popravka energije elektrona u prvom redu (zbog konačnih dimenzija jezgre):

$$\Delta E = \langle \psi_{100} | \delta V | \psi_{100} \rangle = \int d^3r \, \psi_{100}^*(\vec{r}) \delta V(\vec{r}) \psi_{100}(\vec{r}) =$$

$$= \frac{1}{\pi a^3} \int_0^R dr \int_0^\pi d\vartheta \int_0^{2\pi} d\varphi \; r^2 \sin\vartheta \, e^{-\frac{2r}{a}} \left[\frac{Ze^2}{2R^3} r^2 - \frac{3Ze^2}{2R} + \frac{Ze^2}{r} \right] =$$

$$= \frac{4}{a^3} \frac{Ze^2}{R} \int_0^R dr \, r^2 e^{-\frac{2r}{a}} \left[\frac{r^2}{2R^2} - \frac{3}{2} + \frac{R}{r} \right] =$$

$$= \frac{4}{a^3} \frac{Ze^2}{R} \left[\frac{1}{2R^2} \int_0^R dr \, r^4 e^{-\frac{2r}{a}} - \frac{3}{2} \int_0^R dr \, r^2 e^{-\frac{2r}{a}} + R \int_0^R dr \frac{e^{-\frac{2r}{a}}}{r} \right] =$$

$$= \frac{4Ze^2}{Ra^3} \left[\frac{1}{2R^2} \left(\frac{3a^5}{4} - \frac{a}{4} e^{-\frac{2R}{a}} \left(3a^4 + 6a^3R + 6a^2R^2 + 4aR^3 + 2R^4 \right) \right) \right.$$

$$\left. - \frac{3}{2} \cdot \frac{a}{4} \left(a^2 - e^{-\frac{2R}{a}} \left(a^2 + 2aR + 2R^2 \right) \right) + R \frac{a}{4} \left(a - e^{-\frac{2R}{a}} (a + 2R) \right) \right]$$

$$= \frac{Ze^2}{2R} \left[3 \left(\frac{a}{R} \right)^2 - 3 + 2 \left(\frac{R}{a} \right) - 3 \left(\left(\frac{a}{R} \right)^2 + 2 \left(\frac{a}{R} \right) + 1 \right) e^{-\frac{2R}{a}} \right]$$

Uvrstimo za Bohrov radijus $a(Z)$:

$$\Delta E(Z) = \frac{Ze^2}{2R} \left[\frac{3}{Z^2} \left(\frac{a_0}{R} \right)^2 + 2Z \left(\frac{R}{a_0} \right) - 3 - \right.$$

$$\left. - 3 \left(\frac{1}{Z} \left(\frac{a_0}{R} \right) + 1 \right)^2 \exp\left(-2Z \left(\frac{R}{a_0} \right) \right) \right]$$

$\longrightarrow$ ovisnost popravke energije o atomskom broju Z.

Promotrimo kolika je popravka u odnosu na energiju neperturbiranog stanja $E_0 = -\frac{Ze^2}{2a_0}$:

$$\frac{\Delta E}{|E_0|} = \frac{a_0}{R}\left[\frac{3}{Z^2}\left(\frac{a_0}{R}\right)^2 + 2Z\left(\frac{R}{a_0}\right) - 3 - \right.$$

$$\left. - 3\left(\frac{1}{Z^2}\left(\frac{a_0}{R}\right)^2 + \frac{2}{Z}\left(\frac{a_0}{R}\right) + 1\right)\exp\left(-2Z\left(\frac{R}{a_0}\right)\right)\right]$$

Tipično je $\frac{R}{a_0} \sim 10^{-3} << 1$ pa razvijemo eksponencijalni član po $\frac{R}{a_0}$: (do trećeg reda)

$$\exp\left(-2Z\left(\frac{R}{a_0}\right)\right) \approx 1 - 2Z\left(\frac{R}{a_0}\right) + 2Z^2\left(\frac{R}{a_0}\right)^2 - \frac{4Z^2}{3}\left(\frac{R}{a_0}\right)^3$$

Uvrštavanjem toga u $\frac{\Delta E}{|E_0|}$ dobijemo:

$$\left|\frac{\Delta E}{E_0}\right| \approx \frac{4}{5}\left(\frac{R}{a_0}\right)^2 Z^3$$

$\longrightarrow$ popravka energije raste sa 4. potencijom Z

Vidimo da postoje atomski brojevi Z za koje prvi red računa daje besmisleni rezultat. Kada je $|\Delta E| > E_0$ imamo da je energija veća od nule, što znači da imamo slobodnu česticu!

$$\frac{|\Delta E|}{E_0} > 1 \longrightarrow Z > \left[\frac{5}{4}\left(\frac{a_0}{R}\right)^2\right]^{1/3} \sim 100$$

$\longrightarrow$ Prvi red računa smetnje ima smisla samo za lake jezgre.