1 Teorija motnje

Anharmonski oscilator. V Hamiltonian harmonskega oscilatorja dodamo motnjo, na primer

$$H = \frac{p^2}{2m} = \frac{1}{2}kx^2 + \lambda x^4$$

Hamiltonian nemotenega oscilatorja označimo s H_0:

$$H_0 \left|n\right\rangle^0 = E_n^0 \left|n\right\rangle^0, \qquad E_n^0 = \hbar\omega\left(n + \frac{1}{2}\right)$$

V prvem redu popravka je

$$E_n = E_n^0 + {}^0\left\langle n\right| H' \left|n\right\rangle^0$$

Po dogovoru lastne funkcije nemotenega oscilatorja označimo kar z $\left|n\right\rangle^0 = \left|n\right\rangle$. Zdaj si oglejmo motnjo:

$$\left\langle n\right| \lambda x^4 \left|n\right\rangle = \lambda \left\langle x^2 n \,\middle|\, x^2 n\right\rangle$$

Operator x^2 zapišemo z operatorjema a in $a^\dagger$.

$$x = \frac{x_0}{\sqrt{2}}\left(a^\dagger + a\right)$$

$$x^2 = \frac{x_0^2}{2}\left(a^\dagger + a\right)^2$$

$$= \frac{x_0^2}{2}\left({a^\dagger}^2 + a^\dagger a + a a^\dagger + a^2\right)$$

Vemo, da je komutator teh operatorjev

$$[a^\dagger, a] = 1$$

. Sledi:

$$x^2 = \frac{x_0^2}{2}\left({a^\dagger}^2 + 1 + 2a^\dagger a + a^2\right)$$

$$\left|x^2 n\right\rangle = \frac{x_0^2}{2}\left({a^\dagger}^2 \left|n\right\rangle + 1\left|n\right\rangle + 2a^\dagger a\left|n\right\rangle + a^2\left|1\right\rangle\right)$$

$$= \frac{x_0^2}{2}\left(\sqrt{(n+1)(n+2)}\left|n+2\right\rangle + \left|n\right\rangle + 2n\left|n\right\rangle + \sqrt{(n(n-1))}\left|n-2\right\rangle\right)$$

$$\lambda\left\langle x^2 n \,\middle|\, x^2 n\right\rangle = \lambda\frac{x_0^4}{4}\left((n+1)(n+2) + (2n+1)^2 + n(n-1)\right)$$

$$= \cdots = \frac{3}{8}\lambda x_0^4\left(n^2 + n + \frac{1}{2}\right)$$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) + \frac{3}{8}\lambda x_0^4\left(n^2 + n + \frac{1}{2}\right)$$

Vodikov atom v električnem polju. Električno polje kaže v smeri z. Tako imamo Hamiltonian

$$H = \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 r} - e\varepsilon z$$

Izračunati bomo morali matriko skalarnih produktov stanj $\left|lm\right\rangle$:

$$\begin{array}{cc} & \begin{array}{cccc} \left|0,\,0\right\rangle & \left|1,\,1\right\rangle & \left|1,\,0\right\rangle & \left|1,\,-1\right\rangle \end{array} \\ \begin{array}{c} \left\langle 0,\,0\right| \\ \left\langle 1,\,1\right| \\ \left\langle 1,\,0\right| \\ \left|1,\,-1\right\rangle \end{array} & \begin{bmatrix} 0 & 0 & u & 0 \\ 0 & 0 & 0 & 0 \\ u^* & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

V pomoč zapišemo nekaj fundamentalnih dejstev:

1.)

$$[H',\, L_z] = 0, \quad [H,\, L_z] = 0 \;\rightarrow\; \langle lm|\, H'\, |l'm'\rangle = 0 \text{ za } m' \neq m$$

2.) Če označimo operator $P : \overrightarrow{r} \mapsto -\overrightarrow{r}$:

$$[H_0,\, P] = \{H',\, P\} = 0$$

3.) V sferičnih koordinatah bo imela ψ obliko $\psi_{nlm}(\overrightarrow{r}) = R_{nl}(r) Y_{lm}(\vartheta, \varphi)$.

$$P Y_{lm}(\vartheta, \varphi) = (-1)^l Y_{lm}(\vartheta, \varphi)$$

Da so po diagonali ničle, sledi iz teh dejstev:

$$\langle lm|\, \{H',\, P\}\, |l'm'\rangle = \langle lm|\, H'P + PH'\, |l'm'\rangle =$$

$$\langle lm|\, PH'\, |l'm'\rangle + \langle lm|\, H'P\, |l'm'\rangle = \left((-1)^{l'} + (-1)^l\right) \langle lm|\, H'\, |l'm'\rangle$$

Če je $l = l'$, je $\langle lm|\, H'\, |l'm'\rangle = 0$, torej imamo na diagonali ničle. Izračunati moramo še u in u^*:

$$u = \langle 0,\, 0|\, H'\, |1,\, 0\rangle = \int R_{20}^*(r) Y_{00}^*(\vartheta, \varphi)\, (-e\varepsilon z)\, R_{21}(r) Y_{10}(\vartheta, \varphi)\, \mathrm{d}^3\overrightarrow{r}$$

Uporabimo:

$$\begin{aligned}
R_{20}^* &= \frac{2}{(2r_B)^{3/2}} \left(1 - \frac{r}{2r_B}\right) e^{-r/2r_B} \\
Y_{00}^* &= \frac{1}{\sqrt{4\pi}} \\
R_{21} &= \frac{1}{\sqrt{3}} \frac{1}{(2r_B)^{3/2}} \frac{r}{r_B} e^{-r/2r_B} \\
Y_{10} &= \sqrt{\frac{3}{4\pi}} \cos\vartheta \\
z &= r\cos\vartheta
\end{aligned}$$

$$\begin{aligned}
u &= -\frac{e\varepsilon}{(2r_B)^3} \frac{2}{4\pi} \int_0^\infty r^2 \left(1 - \frac{r}{2r_B}\right) \frac{r^2}{r_B} e^{-r/r_B}\, \mathrm{d}r \int_0^{2\pi} \mathrm{d}\varphi \int_{-1}^{1} \cos^2\vartheta\, \mathrm{d}(\cos\vartheta) \\
&= -\frac{e\varepsilon}{(2r_B)^3} \frac{2}{4\pi} \int_0^\infty \frac{r^2}{r_B^2} \left(1 - \frac{1}{2}\frac{r}{r_B}\right) \frac{r^2}{r_B^2} e^{-r/r_B} r_B^2\, \mathrm{d}\left(\frac{r}{r_B}\right) 2\pi\, \frac{2}{3} \\
&= -\frac{e\varepsilon}{12 r_B} \int_0^\infty u^4 \left(1 - \frac{u}{2}\right) e^{-u}\, \mathrm{d}u = -\frac{e\varepsilon}{12 r_B} \left(\Gamma(3) - \frac{1}{2}\Gamma(4)\right) \\
&= -\frac{e\varepsilon}{12 r_B}(24 - 60) = 3e\varepsilon/r_B
\end{aligned}$$

Zdaj imamo matrične elemente matrike skalarnih produktov. Vidimo, da imamo takoj lastni vrednosti $\lambda_{12} = 0$ in pripadajoča lastna vektorja $|1,\, 1\rangle$ in $|1,\, -1\rangle$. Iščemo še lastne vrednosti matrike

$$\begin{bmatrix} 0 & u \\ u & 0 \end{bmatrix}$$

Dobimo $\lambda_{34} = \pm u$. Posebej iščemo lastne vektorje za vsako možnost.

1. $\lambda = -u$:

$$\begin{bmatrix} u & u \\ u & u \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \Rightarrow \quad \begin{matrix} \alpha = -\beta \\ \begin{pmatrix} \alpha \\ -\alpha \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \end{matrix}$$

   Torej je lastno stanje $\frac{1}{\sqrt{2}} (|0,\, 0\rangle - |1,\, 0\rangle) \equiv |-\rangle$

2. $\lambda = u$: Po popolnoma enakem postopku dobimo lastno stanje $\frac{1}{\sqrt{2}} (|0,\, 0\rangle + |1,\, 0\rangle) \equiv |+\rangle$

Označili smo lastna vektorja $|-\rangle$ in $|+\rangle$, izračunamo lahko npr.

$$\langle -|\, z\, |-\rangle = \ldots = 3r_B$$

$$\langle +|\, z\, |+\rangle = \ldots = -3r_B$$