1. zadaća iz kvantne fizike

26. listopad 2009.

Zadatak 1

Odrediti koji su od sljedećih oblika valne funkcije fizikalno dopustivi:

(a) $\psi(x) = A_0 x^2$

(b) $\psi(x) = A_0 x^n e^{-x^2}$

(c) $\psi(x) = A_0 x^n e^{-x}$

(d) $\psi(x) = A_n \dfrac{P_n(x)}{Q_n(x)}$

n je prirodni broj, $P_n(x)$ i $Q_n(x)$ polinomi n-tog stupnja. Komentirati zašto i u kojim situacijama to vrijedi.

(a) $\psi(x) = A_0 x^n$

Na $\langle -\infty, \infty \rangle$ nije normalizabilna

Na bilo kojem konačnom intervalu ne iščezava na granicama.

$\Longrightarrow$ nije dopustiva

(b) $\psi(x) = A_0 x^n e^{-x^2}$

Normalizabilna na $\langle -\infty, \infty \rangle$, neprekidna i konačna. $\Longrightarrow$ dopustiva

(c) $\underline{\Psi(x) = A_0 x^n e^{-x}}$

U $x \to -\infty$ Ψ divergira

$\Rightarrow$ nije normalizabilna pa nije dopustiva na $\langle -\infty, \infty \rangle$

Na $[0, \infty\rangle$ je dopustiva jer je $\Psi(0) = 0$, normalizabilna je, neprekidna i konačna.

(d) $\underline{\Psi(x) = A_0 \frac{P_n(x)}{Q_n(x)}}$

Za $x \to \pm\infty$ vodeći članovi u polinomima su reda $\sim x^n$, ali istog reda su u brojniku i nazivniku $\Rightarrow \Psi(x \to \pm\infty) \sim$ konst.

$\Rightarrow$ nije normalizabilna na $\langle -\infty, \infty \rangle$

Također, ako Q_n ima korijen m-tog reda u x_0, a P_n nema korijen istog ili većeg reda, Ψ divergira u x_0.

Jedini dopustivi slučaj je da je Ψ ograničena na interval ograničen nultočkama P_n i da nemamo unutar njega divergencije zbog Q_n.

Zadatak 2

Izvršiti separaciju varijabli za Schrödingerovu jednadžbu u potencijalu koji ovisi samo o udaljenosti od z-osi.

U cilindričnom koordinatnom sistemu:

$\rho = \sqrt{x^2+y^2} \rightsquigarrow \underline{V(\vec{r}) = V(\rho)}$

Schrödingerova:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r}) + V(\rho)\Psi(\vec{r}) = E\Psi(\vec{r})$$

$$\nabla^2 = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2} + \frac{\partial^2}{\partial z^2}$$

Pretpostavimo $\Psi(\vec{r}) = R(\rho)\varphi(\theta)Z(z)$

$$\rightsquigarrow \frac{\varphi Z}{\rho}\frac{d}{d\rho}\left(\rho\frac{dR}{d\rho}\right) + \frac{RZ}{\rho^2}\frac{d^2\varphi}{d\theta^2} + R\varphi\frac{d^2 Z}{dz^2} =$$

$$= \frac{2m}{\hbar^2}V(\rho)R\varphi Z - \frac{2m}{\hbar^2}ER\varphi Z \quad / : R\varphi Z$$

$$\frac{1}{R\rho}\frac{d}{d\rho}\left(\rho\frac{dR}{d\rho}\right) + \frac{1}{\rho^2\varphi}\frac{d^2\varphi}{d\theta^2} + \frac{1}{Z}\frac{d^2Z}{dz^2} = \frac{2m}{\hbar^2}\left(V(\rho)-E\right)$$

$$\frac{1}{Z}\frac{d^2Z}{dz^2} = -\frac{1}{\rho R}\frac{d}{d\rho}\left(\rho\frac{dR}{d\rho}\right) - \frac{1}{\rho^2\varphi}\frac{d^2\varphi}{d\theta^2} + \frac{2m}{\hbar^2}\left(V(\rho)-E\right)$$

Lijeva strana zadnje jednadžbe ovisi samo o z varijabli, dok desna ovisi samo o ρ i θ varijablama. Jednakost vrijedi $\forall z, \rho, \theta$ $\Rightarrow$ lijeva i desna strana jednake su nekoj konstanti λ.

$$\frac{d^2 Z}{dz^2} = \lambda Z$$

Imamo 3 različita rješenja u ovisnosti o λ:

1) $\underline{\lambda > 0}$

$$\rightarrow \quad Z(z) = A e^{\sqrt{\lambda} z} + B e^{-\sqrt{\lambda} z}$$

To je neprihvatljivo rješenje jer se konačna Ψ ne bi dala normalizirati

2) $\underline{\lambda = 0}$

$$\rightarrow \quad Z(z) = Az + B$$

Također vodi na nenormalizabilnu Ψ

3) $\underline{\lambda < 0}$, $|\lambda| = k^2$

$$\rightarrow \quad Z(z) = A e^{ikz} + B e^{-ikz}$$

Ravni valovi u z-smjeru prihvatljivo rješenje.

Od Schrödingerove je ostalo:

$$-k^2 = -\frac{1}{\rho R}\frac{d}{d\rho}\left(\rho\frac{dR}{d\rho}\right) - \frac{1}{\rho^2 \varphi}\frac{d^2\varphi}{d\vartheta^2} + \frac{2m}{\hbar^2}\left(V(\rho)-E\right)$$

$$\rightarrow \frac{1}{\varphi}\frac{d^2\varphi}{d\vartheta^2} = -\frac{\rho}{R}\frac{d}{d\rho}\left(\rho\frac{dR}{d\rho}\right) + \frac{2m\rho^2}{\hbar^2}\left(V(\rho)-E\right) + k^2\rho^2$$

$$\Rightarrow \underline{\frac{1}{\varphi}\frac{d^2\varphi}{d\vartheta^2} = \mu}$$

Ovdje imamo rubni uvjet koji je zahtjev koordinatnog sustava: $\underline{\varphi(0) = \varphi(2\pi)}$

1) $\underline{\mu > 0}$

$$\rightarrow \varphi(\vartheta) = A e^{\sqrt{\mu}\vartheta} + B e^{-\sqrt{\mu}\vartheta}$$

Ne može zadovoljiti rubni uvjet.

2) $\underline{\mu = 0}$

$$\rightarrow \varphi(\vartheta) = A\vartheta + B$$

$$\varphi(0) = \varphi(2\pi) \Rightarrow \underline{\varphi(\vartheta) = B}, \quad A = 0$$

3) $\underline{\mu < 0}$, $|\mu| = m^2$

$$\rightarrow \varphi(\vartheta) = \underline{A e^{im\vartheta} + B e^{-im\vartheta}}$$

$$\varphi(0) = \varphi(2\pi) \Rightarrow m \in \mathbb{N}$$

$e^{im\vartheta}$ i $e^{-im\vartheta}$ su linearno nezavisne.

Ako pustimo da m može biti negativan imamo:

$$\underline{\varphi(\vartheta) = A e^{im\vartheta}} \quad , \quad m \in \mathbb{Z}$$

(uključili smo i slučaj 2.1)

Preostaje jednadžba po ρ, koja ovisi o obliku potencijala:

$$\underline{\frac{1}{\rho}\frac{d}{d\rho}\left(\rho\frac{dR}{d\rho}\right) = \frac{2m}{\hbar^2}\left(V(\rho)-E\right)R + \left(k^2+\frac{m^2}{\rho}\right)R}$$

Zadatak 3

Valna funkcija čestice dana je sa

$$\psi(x) = \left(\frac{\pi}{a}\right)^{-\frac{1}{4}} e^{-\frac{1}{2}ax^2}$$

Izračunati Δx i Δp, te provjeriti relacije neodređenosti. (Napomena: $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$)

$$\langle x\rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x)\, x\, \psi(x) =$$

$$= \sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} dx\, e^{-ax^2} x = 0$$ podintegralna funkcija je neparna

$$\langle x^2\rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x)\, x^2 \psi(x) =$$

$$= \sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} dx\, x^2 e^{-ax^2} =$$

$$= \sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} dx\, \frac{\partial}{\partial a}\left(-e^{-ax^2}\right) =$$

$$= -\sqrt{\frac{a}{\pi}} \frac{d}{da} \int_{-\infty}^{\infty} dx\, e^{-ax^2} = \sqrt{\frac{a}{\pi}} \frac{d}{da}\left(\sqrt{\frac{\pi}{a}}\right) =$$

$$= -\sqrt{\frac{a}{\pi}} \left(-\frac{\sqrt{\pi}}{2} \frac{1}{a^{3/2}}\right) = \frac{1}{2a}$$

$$\rightarrow \Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \frac{1}{\sqrt{2a}}$$

$$\langle p \rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x)\, \hat{p}\, \psi(x) =$$

$$= -i\hbar \int_{-\infty}^{\infty} dx\, \psi^*(x) \frac{d\psi}{dx} =$$

$$= -i\hbar \sqrt{\frac{a}{\pi}}\, (-a) \int_{-\infty}^{\infty} dx\, e^{-ax^2} x \;\; = 0 \quad \Big\{ \text{neparna podintegralna funkcija}$$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x)\, \hat{p}^2 \psi(x) =$$

$$= -\hbar^2 \sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}ax^2} \frac{d^2}{dx^2}\left(e^{-\frac{1}{2}ax^2}\right) =$$

$$= -\hbar^2 \sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}ax^2} \frac{d}{dx}\left(-ax\, e^{-\frac{1}{2}ax^2}\right) =$$

$$= -\hbar^2 \sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}ax^2} \left(-a e^{-\frac{1}{2}ax^2} + a^2x^2 e^{-\frac{1}{2}ax^2}\right) =$$

$$= \hbar^2 a \sqrt{\frac{a}{\pi}} \left(\int_{-\infty}^{\infty} dx\, e^{-ax^2} - a \int_{-\infty}^{\infty} dx\, x^2 e^{-ax^2}\right) =$$

$$= \hbar^2 a \sqrt{\frac{a}{\pi}} \left(\sqrt{\frac{\pi}{a}} - a \frac{1}{2a} \sqrt{\frac{\pi}{a}}\right) = \frac{\hbar^2 a}{2}$$

$$\longrightarrow \quad \Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \hbar \sqrt{\frac{a}{2}}$$

$$\Longrightarrow \quad \Delta x \Delta p = \frac{1}{\sqrt{2a}} \times \hbar \sqrt{\frac{a}{2}} = \underline{\frac{\hbar}{2} \geq \frac{\hbar}{2}}$$

Zadatak 4

Čestica se nalazi u potencijalu harmoničkog oscilatora. Izračunajte vjerojatnost da se nalazi u klasično zabranjenom području za prva tri svojstvena stanja Hamiltonijana. Komentirati.

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \quad , \quad E_0 = \frac{1}{2}\hbar\omega$$

$$\psi_1(x) = \left(\frac{m\omega}{\hbar}\right)^{3/4} \frac{\sqrt{2}}{\pi^{1/4}}\, x \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \quad , \quad E_1 = \frac{3}{2}\hbar\omega$$

$$\psi_2(x) = \frac{1}{\sqrt{2}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(2\frac{m\omega}{\hbar}x^2 - 1\right) \exp\left(-\frac{m\omega}{2\hbar}x^2\right),$$

$$E_3 = \frac{5}{2}\hbar\omega$$

Klasične točke obrata:

$$E = V(x)$$

$$E = \frac{1}{2}m\omega^2 x^2 \longrightarrow x = \pm\sqrt{\frac{2E}{m\omega^2}}$$

$$\rightarrow \quad x_0 = \sqrt{\frac{\hbar}{m\omega}} \quad , \quad x_1 = \sqrt{\frac{3\hbar}{m\omega}} \quad , \quad x_2 = \sqrt{\frac{5\hbar}{m\omega}}$$

$$P_0 = \int_{-\infty}^{-x_0} dx\, \psi_0^* \psi_0 + \int_{x_0}^{\infty} dx\, \psi_0^* \psi_0 =$$

$$= 1 - \int_{-x_0}^{x_0} dx\, \psi_0^* \psi_0$$

$$P_0 = 1 - \sqrt{\frac{m\omega}{\pi\hbar}} \int_{-x_0}^{x_0} dx \; \exp\left(-\frac{m\omega}{\hbar} x^2\right)$$

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

$$= 1 - \frac{1}{\sqrt{\pi}} \int_{-1}^{1} dz\, e^{-z^2} = 1 - \frac{2}{\sqrt{\pi}} \int_{0}^{1} dz\, e^{-z^2} =$$

$$= \underline{1 - \operatorname{erf}(1)} = \underline{0.1573}$$

$$P_1 = \int_{-\infty}^{-x_1} dx\, \psi_1^*(x)\psi_1(x) + \int_{x_1}^{\infty} dx\, \psi_1^*(x)\, \psi_1(x) =$$

$$= 1 - \int_{-x_1}^{x_1} dx\, \psi_1^*(x)\, \psi_1(x) =$$

$$= 1 - \left(\frac{m\omega}{\hbar}\right)^{3/2} \frac{2}{\sqrt{\pi}} \int_{-x_1}^{x_1} x^2 \exp\left(-\frac{m\omega}{\hbar} x^2\right) dx =$$

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

$$= 1 - \frac{2}{\sqrt{\pi}} \int_{-\sqrt{3}}^{\sqrt{3}} dz\;\; z^2 e^{-z^2} =$$

$$= 1 - \frac{4}{\sqrt{\pi}} \int_{0}^{\sqrt{3}} dz\; z^2 e^{-z^2} =$$

$$= 1 + \frac{4}{\sqrt{\pi}} \int_{0}^{\sqrt{3}} dz \left(\frac{\partial}{\partial \alpha} e^{-\alpha z^2}\right)\Bigg|_{\alpha=1} =$$

$$= 1 + \frac{4}{\sqrt{\pi}} \left(\frac{d}{d\alpha} \int_0^{\sqrt{3}} dz \, e^{-\alpha z^2} \right) \Bigg|_{\alpha=1} = \left\{ \begin{aligned} y &= \sqrt{\alpha}\, z \\ dz &= \frac{1}{\sqrt{\alpha}} dy \end{aligned} \right.$$

$$= 1 + \frac{4}{\sqrt{\pi}} \frac{d}{d\alpha} \left(\frac{1}{\sqrt{\alpha}} \int_0^{\sqrt{3\alpha}} dy \, e^{-y^2} \right) \Bigg|_{\alpha=1} =$$

$$= 1 + 2 \frac{d}{d\alpha} \left(\frac{1}{\sqrt{\alpha}} \operatorname{erf}\left(\sqrt{3\alpha}\right) \right) \Bigg|_{\alpha=1} =$$

$$= 1 + 2 \left(-\frac{1}{2\alpha^{3/2}} \operatorname{erf}\left(\sqrt{3\alpha}\right) \right) \Bigg|_{\alpha=1} + 2 \left(\frac{1}{\sqrt{\alpha}} \frac{2}{\sqrt{\pi}} e^{-3\alpha} \frac{\sqrt{3}}{2\sqrt{\alpha}} \right) \Bigg|_{\alpha=1}$$

$$= \underline{1 - \operatorname{erf}(\sqrt{3}) + 2\sqrt{\frac{3}{\pi}}\, e^{-3}} = \underline{0.1116}$$

$$P_2 = \int_{-\infty}^{-x_2} dx \, \psi_2^* \psi_2 + \int_{x_2}^{\infty} dx \, \psi_2^* \psi_2 =$$

$$= 1 - \int_{-x_2}^{x_2} dx \, \psi_2^* \psi_2 =$$

$$= 1 - \frac{1}{2} \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} \int_{-x_2}^{x_2} dx \left(2 \frac{m\omega}{\hbar} x^2 - 1 \right)^2 \exp\left(-\frac{m\omega}{\hbar} x^2 \right)$$

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

$$= 1 - \frac{1}{2\sqrt{\pi}} \int_{-\sqrt{5}}^{\sqrt{5}} dz \left(2z^2 - 1 \right)^2 \exp\left(-z^2 \right) =$$

$$= 1 - \frac{1}{\sqrt{\pi}} \int_0^{\sqrt{5}} dz \left(4z^4 - 4z^2 + 1 \right) e^{-z^2} =$$

$$= 1 - \frac{4}{\sqrt{\pi}} \int_0^{\sqrt{5}} dz\, z^4 e^{-z^2} + \frac{4}{\sqrt{\pi}} \int_0^{\sqrt{5}} dz\, z^2 e^{-z^2} - \frac{1}{\sqrt{\pi}} \int_0^{\sqrt{5}} dz\, e^{-z^2}$$

$$= 1 - \frac{1}{2} erf(\sqrt{5}) - \frac{4}{\sqrt{\pi}} \int_0^{\sqrt{5}} dz \left(\frac{\partial^2}{\partial \alpha^2} e^{-\alpha z^2} \right) \Bigg|_{\alpha=1} -$$

$$- \frac{4}{\sqrt{\pi}} \int_0^{\sqrt{5}} dz \left(\frac{\partial}{\partial \alpha} e^{-\alpha z^2} \right) =$$

$$= 1 - \frac{1}{2} erf(\sqrt{5}) - \frac{4}{\sqrt{\pi}} \left(\frac{d^2}{d\alpha^2} \int_0^{\sqrt{5}} dz\, e^{-\alpha z^2} \right) \Bigg|_{\alpha=1} -$$

$$- \frac{4}{\sqrt{\pi}} \frac{d}{d\alpha} \left(\int_0^{\sqrt{5}} dz\, e^{-\alpha z^2} \right) \Bigg|_{\alpha=1} =$$

$$\left\{ y = \sqrt{\alpha}\, z \;, \quad dz = \frac{1}{\sqrt{\alpha}} dy \right\}$$

$$= 1 - \frac{1}{2} erf(\sqrt{5}) - \frac{4}{\sqrt{\pi}} \left(\frac{d^2}{d\alpha^2} \left(\frac{1}{\sqrt{\alpha}} \int_0^{\sqrt{5\alpha}} dy\, e^{-y^2} \right) \right) \Bigg|_{\alpha=1} -$$

$$- \frac{4}{\sqrt{\pi}} \left(\frac{d}{d\alpha} \left(\frac{1}{\sqrt{\alpha}} \int_0^{\sqrt{5\alpha}} dy\, e^{-y^2} \right) \right) \Bigg|_{\alpha=1} =$$

$$= 1 - \frac{1}{2} erf(\sqrt{5}) - 2 \left(\frac{d^2}{d\alpha^2} \left(\frac{1}{\sqrt{\alpha}} efr\left(\sqrt{5\alpha}\right) \right) \right) \Bigg|_{\alpha=1} -$$

$$- 2 \left(\frac{d}{d\alpha} \left(\frac{1}{\sqrt{\alpha}} erf\left(\sqrt{5\alpha}\right) \right) \right) \Bigg|_{\alpha=1} =$$

$$= 1 - \frac{1}{2}\,\mathrm{erf}(\sqrt{5}) -$$

$$-2\frac{d}{d\alpha}\left(-\frac{1}{2\alpha^{3/2}}\,\mathrm{erf}(\sqrt{5\alpha}) + \frac{1}{\alpha}\sqrt{\frac{5}{\pi}}\,e^{-5\alpha}\right)\Bigg|_{\alpha=1} -$$

$$-2\left(-\frac{1}{2\alpha^{3/2}}\,\mathrm{erf}(\sqrt{5\alpha}) + \frac{1}{\alpha}\sqrt{\frac{5}{\pi}}\,e^{-5\alpha}\right)\Bigg|_{\alpha=1} =$$

$$= 1 + \frac{1}{2}\,\mathrm{erf}(\sqrt{5}) - 2\sqrt{\frac{5}{\pi}}\,e^{-5\alpha} -$$

$$-2\left(\frac{3}{4\alpha^{5/2}}\,\mathrm{erf}(\sqrt{5\alpha}) - \frac{1}{2\alpha^{2}}\sqrt{\frac{5}{\pi}}\,e^{-5\alpha} - \frac{1}{\alpha^{2}}\sqrt{\frac{5}{\pi}}\,e^{-5\alpha} -\right.$$

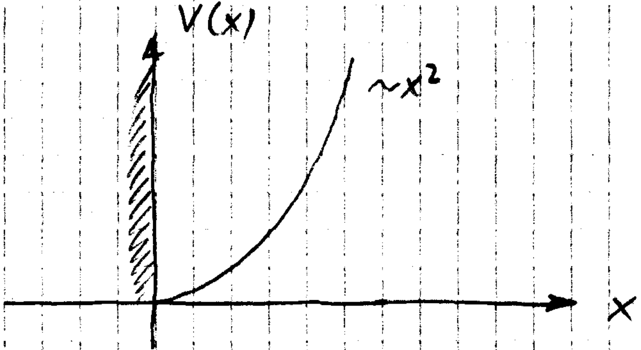
$$\left. - \frac{5}{\alpha}\sqrt{\frac{5}{\pi}}\,e^{-5\alpha}\right)\Bigg|_{\alpha=1} =$$

$$= \underline{1 - \mathrm{erf}(\sqrt{5}) + 11\sqrt{\frac{5}{\pi}}\,e^{-5}} = \underline{0.0951}$$

Zadatak 5

Riješiti Schrödingerovu jednadžbu za potencijal

$$V(x)=\begin{cases}\frac{1}{2}m\omega^2x^2 , & x>0\\ \infty , & x\leq 0\end{cases}$$



$\underline{\psi(0)=0}$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi \qquad (x>0)$$

$$\frac{d^2\psi}{dx^2}-\frac{m^2\omega^2}{\hbar^2}x^2\psi=-\frac{2mE}{\hbar^2}\psi$$

Ispitajmo ponašanje ψ za $x\to\infty$.
Dominantni član linearan u ψ je onaj uz x^2

$$\rightsquigarrow \quad \frac{d^2\psi}{dx^2}\approx\frac{m^2\omega^2}{\hbar^2}x^2\psi$$

Probajmo sa $\psi(x\to\infty)\approx Ae^{Bx^2}$

$$\frac{d\psi}{dx}=2ABxe^{Bx^2}$$

$$\frac{d^2\psi}{dx^2}=2ABe^{Bx^2}+4AB^2x^2e^{Bx^2}\approx 4AB^2x^2e^{Bx^2}$$

$$\Rightarrow \quad 4\cancel{A}B^2\cancel{x^2}\cancel{e^{Bx^2}}=\frac{m^2\omega^2}{\hbar^2}\cancel{A}\cancel{e^{Bx^2}}$$

$$\Rightarrow \quad B = \pm \frac{m\omega}{2\hbar}$$

Moramo odabrati predznak minus, jer u suprotnom imamo problema sa normalizacijom ψ.

Ponašanje u $x \to \infty$ nam sugerira ansatz:

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

Uvrstimo to u Schrödingerovu:

$$\frac{d\psi}{dx} = \frac{d\varphi}{dx} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) - \frac{m\omega}{\hbar} \varphi x \exp\left(-\frac{m\omega}{2\hbar}x^2\right)$$

$$\frac{d^2\psi}{dx^2} = \frac{d^2\varphi}{dx^2} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) - 2\frac{m\omega}{\hbar} x \frac{d\varphi}{dx} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) -$$

$$- \frac{m\omega}{\hbar} \varphi \exp\left(-\frac{m\omega}{2\hbar}x^2\right) + \frac{m^2\omega^2}{\hbar^2} x^2 \varphi \exp\left(-\frac{m\omega}{2\hbar}x^2\right)$$

$$\Rightarrow \quad \frac{d^2\varphi}{dx^2} - \frac{2m\omega}{\hbar} x \frac{d\varphi}{dx} + \left(\frac{2mE}{\hbar^2} - \frac{m\omega}{\hbar}\right)\varphi = 0$$

Uz definicije: $x = \sqrt{\frac{\hbar}{m\omega}}\, z \quad , \quad \varepsilon = \frac{2E}{\hbar\omega}$

$$\Rightarrow \quad \underline{\frac{d^2\varphi}{dz^2} - 2z\frac{d\varphi}{dz} + (\varepsilon - 1)\varphi = 0} \qquad (*)$$

Rješavamo Frobeniusovom metodom.

Pretpostavka: $\varphi(z) = \sum_{n=0}^{\infty} A_n z^{n+\lambda}$, $\underline{A_0 \neq 0}$

$$\frac{d\varphi}{dz} = \sum_{n=0}^{\infty} A_n (n+\lambda) z^{n+\lambda-1}$$

$$\frac{d^2\varphi}{dz^2} = \sum_{n=0}^{\infty} A_n (n+\lambda)(n+\lambda-1) z^{n+\lambda-2} =$$

$$= A_0 \lambda(\lambda-1) z^{\lambda} + A_1 \lambda(\lambda+1) z^{\lambda+1} +$$

$$+ \sum_{n=2}^{\infty} A_n (n+\lambda)(n+\lambda-1) z^{n+\lambda-2} =$$

$$= A_0 \lambda(\lambda-1) z^{\lambda} + A_1 \lambda(\lambda+1) z^{\lambda+1} +$$

$$+ \sum_{n=0}^{\infty} A_{n+2} (n+\lambda+2)(n+\lambda+1) z^{n+\lambda}$$

Uvrstimo to u ⊛:

$$A_0 \lambda(\lambda-1) z^{\lambda} + A_1 \lambda(\lambda+1) z^{\lambda+1} +$$

$$+ \sum_{n=0}^{\infty} \Big[A_{n+2} (n+\lambda+2)(n+\lambda+1) + A_n \big(\varepsilon - 1 - 2(n+\lambda)\big) \Big] z^{n+\lambda} \underline{= 0}$$

$A_0 \neq 0 \implies \lambda(\lambda-1) = 0$ (indicijalna jednadžba)

$\rightarrow \underline{\lambda_1 = 0}$, $\underline{\lambda_2 = 1}$

Dobili smo dva rješenja. No, ako uzmemo $\lambda_1 = 0$ imamo rješenje oblika:

$$\varphi(z) = \sum_{n=0}^{\infty} A_n z^n = A_0 + \sum_{n=1}^{\infty} A_n z^n$$

Tada ćemo zbog $A_0 \neq 0$ imati da je
$\psi(0) \neq 0$ što nam nije dobro rješenje.
Sa $\lambda_2 = 1$ nemamo takvih problema

$$\Rightarrow \underline{\lambda = 1} \qquad \underline{\varphi(z) = z \sum_{n=0}^{\infty} A_n z^n}$$

$$\lambda = 1 \Rightarrow \underline{A_1 = 0}$$

Preostaje nam riješiti rekurzivnu relaciju:

$$A_{n+2} = \frac{2n + 2\lambda + 1 - \varepsilon}{(n+\lambda+1)(n+\lambda+2)} A_n$$

$$A_{n+2} = \frac{2n + 3 - \varepsilon}{(n+2)(n+3)} A_n$$

$$A_1 = 0 \Rightarrow A_{2k+1} = 0, \quad k \in \mathbb{N}$$

Provjerimo kako se ponašaju koeficijenti A za velike n :

$$A_{n+2} \approx \frac{2}{n} A_n \Rightarrow A_n \approx \frac{1}{(n/2)!}$$

$$\varphi(z) \approx \sum_{n=0}^{\infty} \frac{1}{n!} z^{2n} \sim e^{z^2}$$

Pošto imamo $\psi(z) = \varphi(z) e^{-\frac{z^2}{2}} \sim$

$\sim e^{z^2} e^{-\frac{1}{2}z^2} \sim e^{\frac{1}{2}z^2}$ ψ bi divergiralo u ∞!

$\Rightarrow$ moramo negdje odrezati red da φ ostane konačno u $x \to \infty$.

$$A_{k+2} = \frac{2k+3-\varepsilon}{(k+2)(k+3)} A_k$$

$$\Rightarrow \quad \underline{\varepsilon = 2N+3} \quad \Rightarrow \boxed{E_N = \left(N + \frac{3}{2}\right)\hbar\omega}$$

kvantizacija energije

k je paran broj, pa je $N = 2n$, $n \in \mathbb{N}_0$

$$\Rightarrow \quad \underline{\underline{E_n = \left(2n + \frac{3}{2}\right)\hbar\omega}}$$

$$\Rightarrow \quad \varphi(z) = z \sum_{k=0}^{n} A_{2k} z^{2k} =$$

$$= \sum_{k=0}^{n} A_{2k} z^{2k+1} \equiv \sum_{k=0}^{n} B_{2k+1} z^{2k+1}$$

$$\rightsquigarrow \quad B_{2k+3} = A_{2k+2} = \frac{2(2k-2n)}{(2k+2)(2k+3)} A_{2k} =$$

$$= \frac{2(2k-2n)}{(2k+2)(2k+3)} B_{2k+1} =$$

$$= \frac{2\left((2k+1)-(2n+1)\right)}{\left((2k+1)+1\right)\left((2k+1)+2\right)} B_{2k+1}$$

$$\Rightarrow \quad B_{k+2} = \frac{2\,(k - (2n+1))}{(k+1)(k+2)}\, B_k$$

Gornja rekurzijska relacija definira Hermiteov polinom $(2n+1)$-og stupnja (do na konstantu $B_1 = A_0$).

$$\Rightarrow \quad \varphi(z) = A_0\, H_{2n+1}(z)$$

$$\Rightarrow \quad \psi(z) = A_0\, H_{2n+1}(z)\, e^{-z^2/2}$$

Pa, konačno, za valnu funkciju imamo:

$$\psi_n(x) = N_n\, H_{2n+1}\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) \exp\left(-\frac{m\omega}{2\hbar} x^2\right), \quad x > 0$$

$$E_n = \left(2n + \frac{3}{2}\right) \hbar\omega$$

(gdje je N_n norma)