

Zadatak 1.

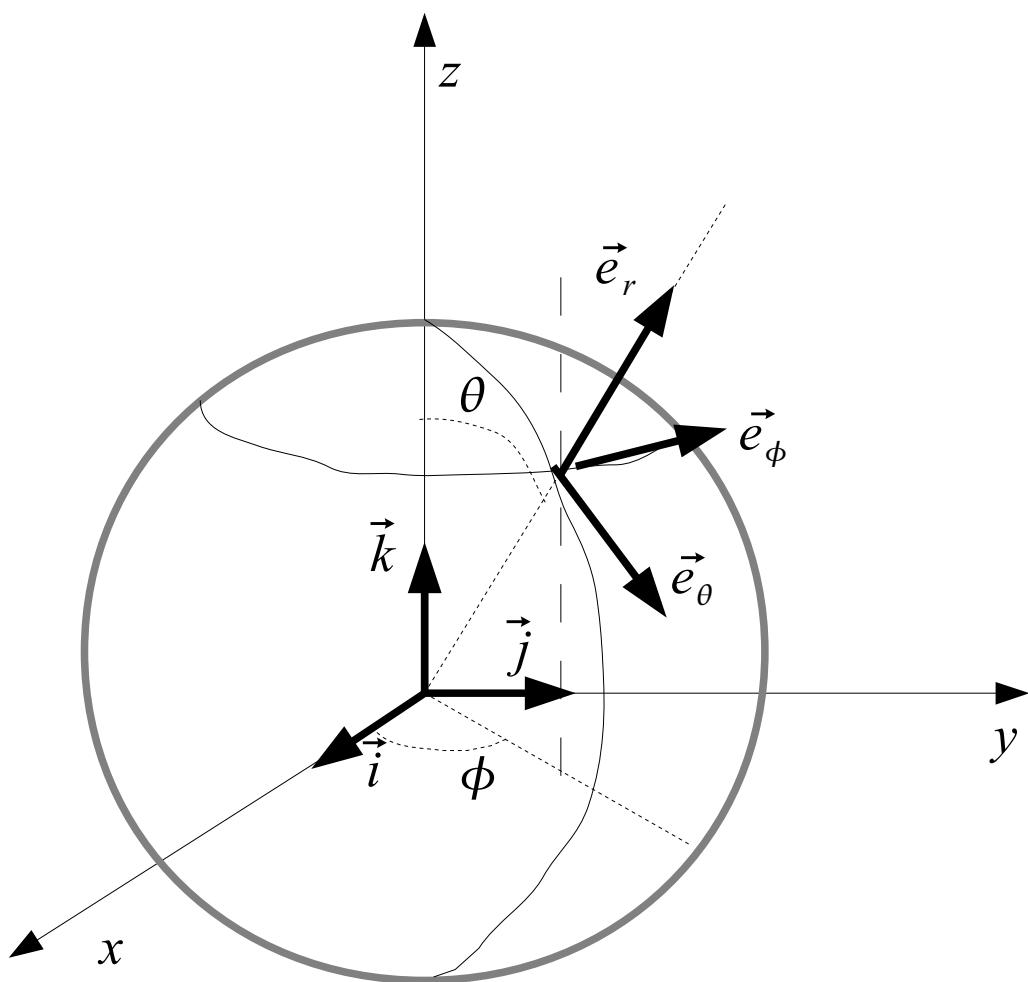
Napišite operator gradijenta u sfernim koordinatama.

Rješenje:

U kartezijevim pravokutnim koordinatama operator gradijenta je jednak

$$\vec{\nabla} = \vec{i} \frac{\partial}{\partial x} + \vec{j} \frac{\partial}{\partial y} + \vec{k} \frac{\partial}{\partial z}$$

Sferni se koordinatni sustav satoji od tri koordinate r, θ, ϕ kojima moramo pridružiti tri jedinična vektora $\vec{e}_r, \vec{e}_\theta, \vec{e}_\phi$



Odnos između koordinata i jediničnih vektora kartezijevog i sfernog sustava je

$$\begin{aligned}x &= r \sin(\theta) \cos(\phi) \\y &= r \sin(\theta) \sin(\phi) \\z &= r \cos(\theta)\end{aligned}$$

$$\begin{aligned}\vec{e}_r &= \vec{i} \sin(\theta) \cos(\phi) + \vec{j} \sin(\theta) \sin(\phi) + \vec{k} \cos(\theta) \\ \vec{e}_\theta &= \vec{i} \cos(\theta) \cos(\phi) + \vec{j} \cos(\theta) \sin(\phi) - \vec{k} \sin(\theta) \\ \vec{e}_\phi &= -\vec{i} \sin(\phi) + \vec{j} \cos(\phi)\end{aligned}$$

$$\begin{aligned}\vec{i} &= \vec{e}_r \sin(\theta) \cos(\phi) + \vec{e}_\theta \cos(\theta) \cos(\phi) - \vec{e}_\phi \sin(\phi) \\ \vec{j} &= \vec{e}_r \sin(\theta) \sin(\phi) + \vec{e}_\theta \cos(\theta) \sin(\phi) + \vec{e}_\phi \cos(\phi) \\ \vec{k} &= \vec{e}_r \cos(\theta) - \vec{e}_\theta \sin(\theta)\end{aligned}$$

Sada još treba izraziti derivacije po x, y, z s pomoću derivacija po r, θ, ϕ . Imamo

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x} \frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial x} \frac{\partial}{\partial \phi}$$

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial y} \frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial y} \frac{\partial}{\partial \phi}$$

$$\frac{\partial}{\partial z} = \frac{\partial r}{\partial z} \frac{\partial}{\partial r} + \frac{\partial \theta}{\partial z} \frac{\partial}{\partial \theta} + \frac{\partial \phi}{\partial z} \frac{\partial}{\partial \phi}$$

$$\frac{\partial r}{\partial x} = \frac{x}{r} = \sin(\theta)\cos(\phi), \quad \frac{\partial r}{\partial y} = \frac{y}{r} = \sin(\theta)\sin(\phi), \quad \frac{\partial r}{\partial z} = \frac{z}{r} = \cos(\theta)$$

$$\frac{\partial \theta}{\partial x} = \frac{\cos(\theta)\cos(\phi)}{r}, \quad \frac{\partial \theta}{\partial y} = \frac{\cos(\theta)\sin(\phi)}{r}, \quad \frac{\partial \theta}{\partial z} = -\frac{\sin(\theta)}{r}$$

$$\frac{\partial \phi}{\partial x} = -\frac{1}{r} \frac{\sin(\phi)}{\sin(\theta)}, \quad \frac{\partial \phi}{\partial y} = \frac{1}{r} \frac{\cos(\phi)}{\sin(\theta)}, \quad \frac{\partial \phi}{\partial z} = 0$$

Sada imamo

$$\frac{\partial}{\partial x} = \sin(\theta)\cos(\phi) \frac{\partial}{\partial r} + \frac{\cos(\theta)\cos(\phi)}{r} \frac{\partial}{\partial \theta} - \frac{1}{r} \frac{\sin(\phi)}{\sin(\theta)} \frac{\partial}{\partial \phi}$$

$$\frac{\partial}{\partial y} = \sin(\theta)\sin(\phi) \frac{\partial}{\partial r} + \frac{\cos(\theta)\sin(\phi)}{r} \frac{\partial}{\partial \theta} + \frac{1}{r} \frac{\cos(\phi)}{\sin(\theta)} \frac{\partial}{\partial \phi}$$

$$\frac{\partial}{\partial z} = \cos(\theta) \frac{\partial}{\partial r} - \frac{\sin(\theta)}{r} \frac{\partial}{\partial \theta}$$

Konačni rezultat (detalje prikazati na ploči):

$$\vec{\nabla} = \vec{e}_r \frac{\partial}{\partial r} + \vec{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \vec{e}_\phi \frac{1}{r \sin(\theta)} \frac{\partial}{\partial \phi}$$

Zadatak 2.

Napišite operator zamaha $\vec{L} = \vec{r} \times \vec{p}$ u kartezijevim i sfernim koordinatama.

Rješenje:

Po zakonu vektorskog množenja imamo:

$$\begin{aligned}
 L_x &= -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) = \\
 &= -i\hbar \left[r \sin(\theta) \sin(\phi) \left(\cos(\theta) \frac{\partial}{\partial r} - \frac{\sin(\theta)}{r} \frac{\partial}{\partial \theta} \right) - \right. \\
 &\quad \left. - r \cos(\theta) \left(\sin(\theta) \sin(\phi) \frac{\partial}{\partial r} + \frac{\cos(\theta) \sin(\phi)}{r} \frac{\partial}{\partial \theta} + \frac{1}{r \sin(\theta)} \cos(\phi) \frac{\partial}{\partial \phi} \right) \right] = \\
 &= -i\hbar \left[-\sin(\phi) \frac{\partial}{\partial \theta} - \cot(\theta) \cos(\phi) \frac{\partial}{\partial \phi} \right] = \\
 &= i\hbar \left[\sin(\phi) \frac{\partial}{\partial \theta} + \cot(\theta) \cos(\phi) \frac{\partial}{\partial \phi} \right]
 \end{aligned}$$

$$\begin{aligned}
 L_y &= -i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) = \\
 &= i\hbar \left(-\cos(\phi) \frac{\partial}{\partial \theta} + \cot(\theta) \sin(\phi) \frac{\partial}{\partial \phi} \right)
 \end{aligned}$$

$$L_z = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) = -i\hbar \frac{\partial}{\partial \phi}$$

Zadatak 3.

Napišite operatore $L_{\pm} = L_x \pm i L_y, L_z$ u sfernim koordinatama i izvedite njihova komutacijska pravila.

Rješenje:

$$L_{\pm} = i \hbar e^{\pm i \phi} \left(\frac{\partial}{\partial \theta} \pm i \cot(\theta) \frac{\partial}{\partial \phi} \right), \quad L_z = -i \hbar \frac{\partial}{\partial \phi}$$

$$[L_z, L_{\pm}] = \hbar^2 \left[\frac{\partial}{\partial \phi}, e^{\pm i \phi} \right] \frac{\partial}{\partial \theta} \pm i \hbar^2 \left[\frac{\partial}{\partial \phi}, e^{\pm i \phi} \right] \cot(\theta) \frac{\partial}{\partial \phi} = \pm \hbar L_{\pm}$$

$$[L_+, L_-] = 2 \hbar L_z$$

Zadatak 4.

Dokažite da operator

$$\vec{L}^2 = L_x^2 + L_y^2 + L_z^2$$

komutira s L_x, L_y i L_z

Zadatak 5.

Izrazite operator \vec{p}^2 u sfernim koordinatama i povežite ga s operatorom \vec{L}^2 .

Zadatak 6.

Napišite Schrödingerovu jednadžbu za česticu koja se giba po kružnici.

Rješenje:

Gibanje po kružnici je ravninsko gibanje, koje opisujemo dvjema prostornim koordinatama x i y . Zbog toga je pogodno uzeti cilindrične koordinate

$$x = r \cos(\phi) , \quad y = r \sin(\phi)$$

i izraziti operator \vec{p}^2 s pomoću koordinata ρ, ϕ . Imamo

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x} \frac{\partial}{\partial r} + \frac{\partial \phi}{\partial x} \frac{\partial}{\partial \phi} = \cos(\phi) \frac{\partial}{\partial r} - \frac{\sin(\phi)}{r} \frac{\partial}{\partial \phi}$$

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y} \frac{\partial}{\partial r} + \frac{\partial \phi}{\partial y} \frac{\partial}{\partial \phi} = \sin(\phi) \frac{\partial}{\partial r} + \frac{\cos(\phi)}{r} \frac{\partial}{\partial \phi}$$

Kvadrirajmo ove operatore:

$$\begin{aligned} \frac{\partial^2}{\partial x^2} &= \cos^2(\phi) \frac{\partial^2}{\partial r^2} - \cos(\phi) \sin(\phi) \left(-\frac{1}{r^2} \frac{\partial}{\partial \phi} + \frac{\partial^2}{\partial \phi \partial r} \right) + \\ &+ \frac{\sin^2(\phi)}{r} \frac{\partial}{\partial r} - \frac{\sin(\phi) \cos(\phi)}{r} \frac{\partial^2}{\partial \phi \partial r} + \frac{\sin(\phi) \cos(\phi)}{r^2} \frac{\partial}{\partial \phi} + \\ &+ \frac{\sin^2(\phi)}{r^2} \frac{\partial^2}{\partial \phi^2} \end{aligned}$$

$$\begin{aligned} \frac{\partial^2}{\partial y^2} = & \sin^2(\phi) \frac{\partial^2}{\partial r^2} + \cos(\phi) \sin(\phi) \left(-\frac{1}{r^2} \frac{\partial}{\partial \phi} + \frac{\partial^2}{\partial \phi \partial r} \right) + \\ & + \frac{\cos^2(\phi)}{r} \frac{\partial}{\partial r} + \frac{\sin(\phi) \cos(\phi)}{r} \frac{\partial^2}{\partial \phi \partial r} - \frac{\sin(\phi) \cos(\phi)}{r^2} \frac{\partial}{\partial \phi} + \\ & + \frac{\cos^2(\phi)}{r^2} \frac{\partial^2}{\partial \phi^2} \end{aligned}$$

Zbrajanjem dviju prethodnih jednadžbi dobivamo

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2}$$

Gibanje po kružnici znači da valna funkcija ne ovisi o r . Prema tome Schrödingerova jednadžba je

$$-\frac{\hbar^2}{2mr^2} \frac{\partial^2}{\partial \phi^2} \psi(\phi) = E \psi(\phi)$$

No, derivacija po kutu je zapravo operator zamaha, pa imamo

$$\frac{L_z^2}{2I} \psi = E \psi$$

gdje je I moment tromosti čestice.

KVANTNA KEMIJA 6. vježbe