Delec v jami kvadratne oblike z električnim poljem

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April 6, 2006

1 Navodilo

Na kvantni piki oblike kvadrata na površini polprevodnika se nahaja elektron. Kvantno piko predstavimo z neskončno potencialno jamo oblike kvadrata. Kako se spremenita energiji stanj, ki ustrezata prvi vzbujeni energiji, ko vklopimo potencial oblike $V(x,y) = A\,\left(x-\frac{a}{2}\right)\,\left(y-\frac{a}{2}\right)$. Pri matričnem računanju se omejimo na bazo $B = \{|1,2\rangle, |2,1\rangle\}$.

2 2-D neskončna potencialna jama - $\hat{H}_0$

Stacionarna Sch. enačba za tak potencial se glasi:

$$\hat{H}_0\,|\psi\rangle = E\,|\psi\rangle$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y) + V(x,y) = E\,\psi(x,y)$$

$$V(x,y) = \begin{cases} 0 & (x,y) \in [0,a]\times[0,a] \\ \infty & \text{sicer} \end{cases}$$

Rešitve te enačbe so lastne funkcije operatoraja $\hat{H}_0$.

$$\psi_{nm}(x,y) = \frac{2}{a}\,\sin(\frac{n\pi}{a}\,x)\,\sin(\frac{m\pi}{a}\,y)\,.$$

Pripadajoče lastne vrednosti so:

$$E_{nm} = \frac{\hbar^2\pi^2}{2\,m\,a^2}\left(n^2+m^2\right)$$

V izbrani bazi $B = \{|1,2\rangle, |2,1\rangle\}$ lahko zapišemo matriko operatorja $\hat{H}_0$ kot:

$$H_0 = \frac{\hbar^2\pi^2}{2\,m\,a^2}\begin{pmatrix} 5 & 0 \\ 0 & 5 \end{pmatrix},$$

3 Operator potenciala $\hat{V}$ v izbrani bazi B

Kot je zapisano v navodilu naloge ima potencial obliko:

$$V(x,y) = A\left(x - \frac{a}{2}\right)\left(y - \frac{a}{2}\right).$$

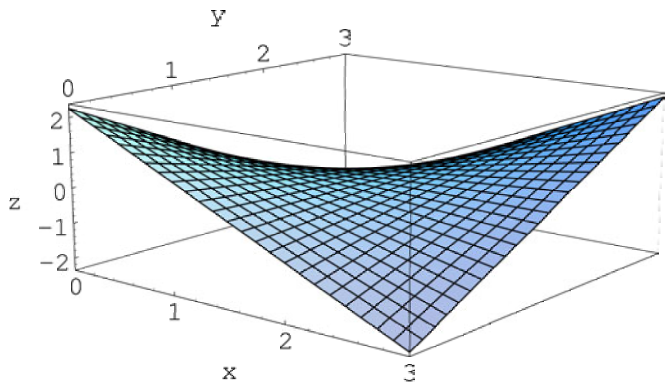

Figure 1: graf potenciala za $A = 1$, $a = 3$ na območju kvantne pike $[0, a] \times [0, a]$

Do matričnih elementov potenciala $\hat{V}$ pridemo po znani poti:

$$\begin{aligned}
V_{11} =& \quad \langle 1,2|\hat{V}|1,2\rangle \\
V_{22} =& \quad \langle 2,1|\hat{V}|2,1\rangle \\
V_{12} =& \quad \langle 1,2|\hat{V}|2,1\rangle \\
V_{21} =& \quad \langle 2,1|\hat{V}|1,2\rangle
\end{aligned}$$

To zapišemo z integrali.

$$\begin{aligned}
V_{11} =& \quad A\left(\tfrac{2}{a}\right)^2 \textstyle\int_0^a \int_0^a \sin(\tfrac{\pi}{a}x)\,\sin(\tfrac{2\pi}{a}y)\left[\left(x-\tfrac{a}{2}\right)\left(y-\tfrac{a}{2}\right)\right]\sin(\tfrac{\pi}{a}x)\,\sin(\tfrac{2\pi}{a}y)\,dx\,dy \\
V_{22} =& \quad A\left(\tfrac{2}{a}\right)^2 \textstyle\int_0^a \int_0^a \sin(\tfrac{2\pi}{a}x)\,\sin(\tfrac{\pi}{a}y)\left[\left(x-\tfrac{a}{2}\right)\left(y-\tfrac{a}{2}\right)\right]\sin(\tfrac{2\pi}{a}x)\,\sin(\tfrac{\pi}{a}y)\,dx\,dy \\
V_{12} =& \quad A\left(\tfrac{2}{a}\right)^2 \textstyle\int_0^a \int_0^a \sin(\tfrac{\pi}{a}x)\,\sin(\tfrac{2\pi}{a}y)\left[\left(x-\tfrac{a}{2}\right)\left(y-\tfrac{a}{2}\right)\right]\sin(\tfrac{2\pi}{a}x)\,\sin(\tfrac{\pi}{a}y)\,dx\,dy \\
V_{21} =& \quad A\left(\tfrac{2}{a}\right)^2 \textstyle\int_0^a \int_0^a \sin(\tfrac{2\pi}{a}x)\,\sin(\tfrac{\pi}{a}y)\left[\left(x-\tfrac{a}{2}\right)\left(y-\tfrac{a}{2}\right)\right]\sin(\tfrac{\pi}{a}x)\,\sin(\tfrac{2\pi}{a}y)\,dx\,dy
\end{aligned}$$

Za izračun zgornih integralov uporabimo Mathematico. Lahko pa upoštevamo naslednje enačbe:

$$\int_0^a \sin^2\left(\frac{k\pi t}{a}\right)\,dt = \frac{a}{2}$$

$$\int_0^a \sin^2\left(\frac{k\pi t}{a}\right) t\,dt = \frac{a^2}{4}$$

$$\int_0^a \sin\left(\frac{k\pi t}{a}\right)\sin\left(\frac{l\pi t}{a}\right) t\,dt = \frac{a^2}{2\pi^2}\left[\frac{1-\cos((k+l)\pi)}{(k+l)^2} - \frac{\cos((k-l)\pi)-1}{(k-l)^2}\right]$$

Tako dobimo matrične elemente za dodani potencial v bazi $B = \{|1,2\rangle, |2,1\rangle\}$.

$$\begin{aligned} V_{11} &= 0 \\ V_{22} &= 0 \\ V_{12} &= \tfrac{256}{81}\tfrac{A}{\pi^4}a^2 \\ V_{21} &= \tfrac{256}{81}\tfrac{A}{\pi^4}a^2 \end{aligned}$$

Sedaj lahko zapišemo matriko, ki pripada operatorju $\hat{V}$.

$$V = \begin{pmatrix} 0 & \frac{256}{81}\frac{A}{\pi^4}a^2 \\ \frac{256}{81}\frac{A}{\pi^4}a^2 & 0 \end{pmatrix},$$

4 Nov Hamiltonjan

Zapišimo nov Hamiltonov operator $\hat{H} = \hat{H}_0 + \hat{V}$, v matrični obliki:

$$H = H_0 + V = \frac{\hbar^2\pi^2}{2\,m\,a^2}\begin{pmatrix} 5 & 0 \\ 0 & 5 \end{pmatrix} + \begin{pmatrix} 0 & \frac{256}{81}\frac{A}{\pi^4}a^2 \\ \frac{256}{81}\frac{A}{\pi^4}a^2 & 0 \end{pmatrix},$$

kar za preglednejše računanje prevedemo na:

$$H = \begin{pmatrix} p & q \\ q & p \end{pmatrix},$$

z vpeljavo konstant p in q.

$$p := 5\,\frac{\hbar^2\pi^2}{2\,m\,a^2}$$

$$q := \frac{256}{81}\frac{A}{\pi^4}a^2$$

Ker nas zanimajo energije tega Hamiltonjana, pogledamo kakšne so njegove lastne vrednosti.

$$\begin{vmatrix} p-\lambda & q \\ q & p-\lambda \end{vmatrix} = 0,$$

$$(p-\lambda)^2 - q^2 = 0$$

$$\lambda^2 - 2\,p\lambda + p^2 - q^2 = 0$$

$$\lambda_{1,2} = \frac{2\,p \pm \sqrt{4\,p^2 - 4\,p^2 + 4\,q^2}}{2}$$

$$\lambda_{1,2} = p \pm q$$

Poglejmi si še pripadajoče lastne vektorje zapisane v originalni bazi $B = \{|1,2\rangle, |2,1\rangle\}$.

$$\lambda = p + q$$

$$\left|\begin{array}{cc|c} p-p-q & q & 0 \\ q & p-p-q & 0 \end{array}\right|$$

$$\left|\begin{array}{cc|c} -q & q & 0 \\ q & -q & 0 \end{array}\right|$$

$$|\psi_1\rangle = \tfrac{1}{\sqrt{2}}\left(|1,2\rangle + |2,1\rangle\right)$$

$$\lambda = p - q$$

$$\left|\begin{array}{cc|c} p-p+q & q & 0 \\ q & p-p+q & 0 \end{array}\right|$$

$$\left|\begin{array}{cc|c} q & q & 0 \\ q & q & 0 \end{array}\right|$$

$$|\psi_2\rangle = \tfrac{1}{\sqrt{2}}\left(|1,2\rangle - |2,1\rangle\right)$$

5 Grafi novih lastnih funkcij

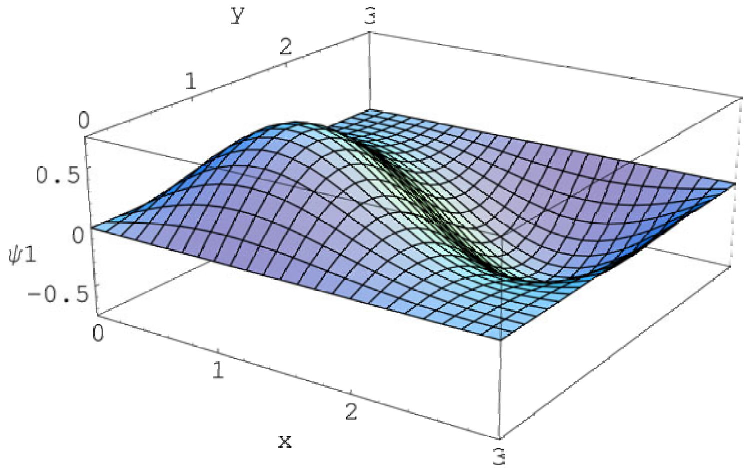

Figure 2: graf za $\psi_1(x, y)$

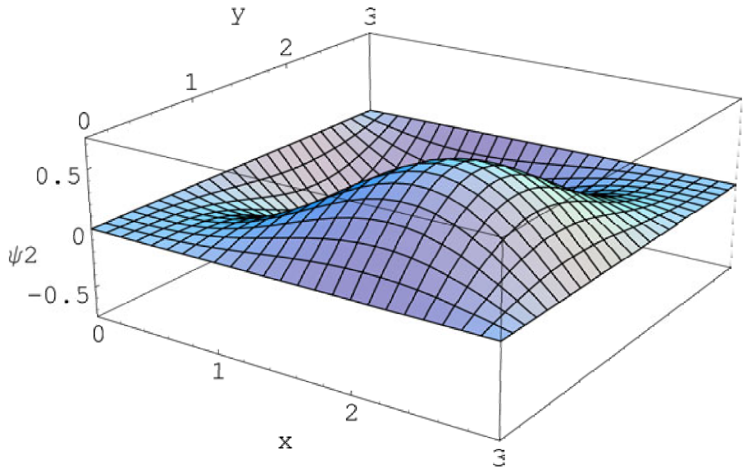

Figure 3: graf za $\psi_2(x, y)$

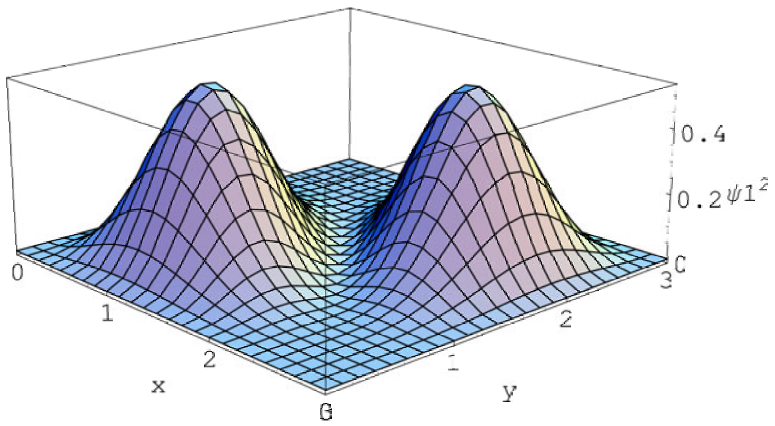

Figure 4: vrjetnostna gostota $|\psi_1(x,y)|^2$

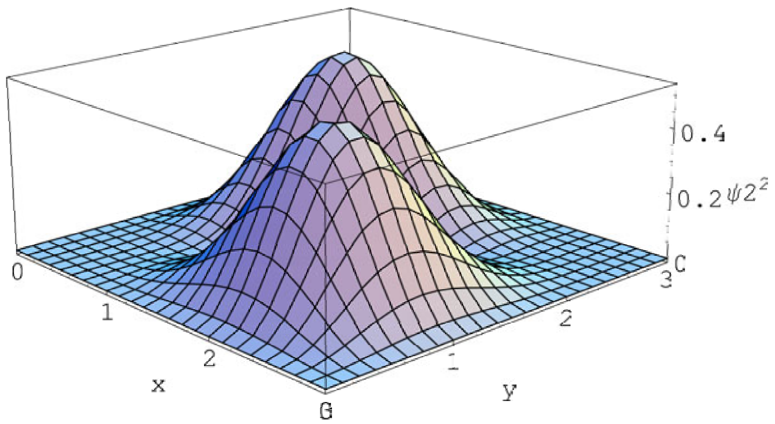

Figure 5: vrjetnostna gostota $|\psi_2(x,y)|^2$