Numeričko rješenje Schrödingerove jednadžbe

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Kvantna fizika, vježbe

Diskretizacija Schrödingerove jednadžbe

- vremenski neovisna Schrödingerova jednadžba

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)$$

- pretpostavimo da valna funkcija iščezava izvan intervala $[x_{min}, x_{max}]$ duljine L
- interval podijelimo na N podintervala duljine $h = (x_{max} - x_{min})/N$

$$x_j = x_{min} + jh, \quad j = 0, \ldots, N$$

- aproksimiramo drugu derivaciju

$$\frac{d^2}{dx^2}\psi(x_j) = \frac{1}{h^2}\left[\psi(x_{j-1}) - 2\psi(x_j) + \psi(x_{j+1})\right]$$

- definiramo veličine

$$d = \frac{\hbar^2}{mh^2}, \quad u = \frac{\hbar^2}{2mh^2}$$

- Schrödingerova jednadžba svodi se na sustav linearnih jednadžbi

$$-u\psi_{j-1} + (d + V_j)\psi_j - u\psi_{j+1} = E\psi_j$$

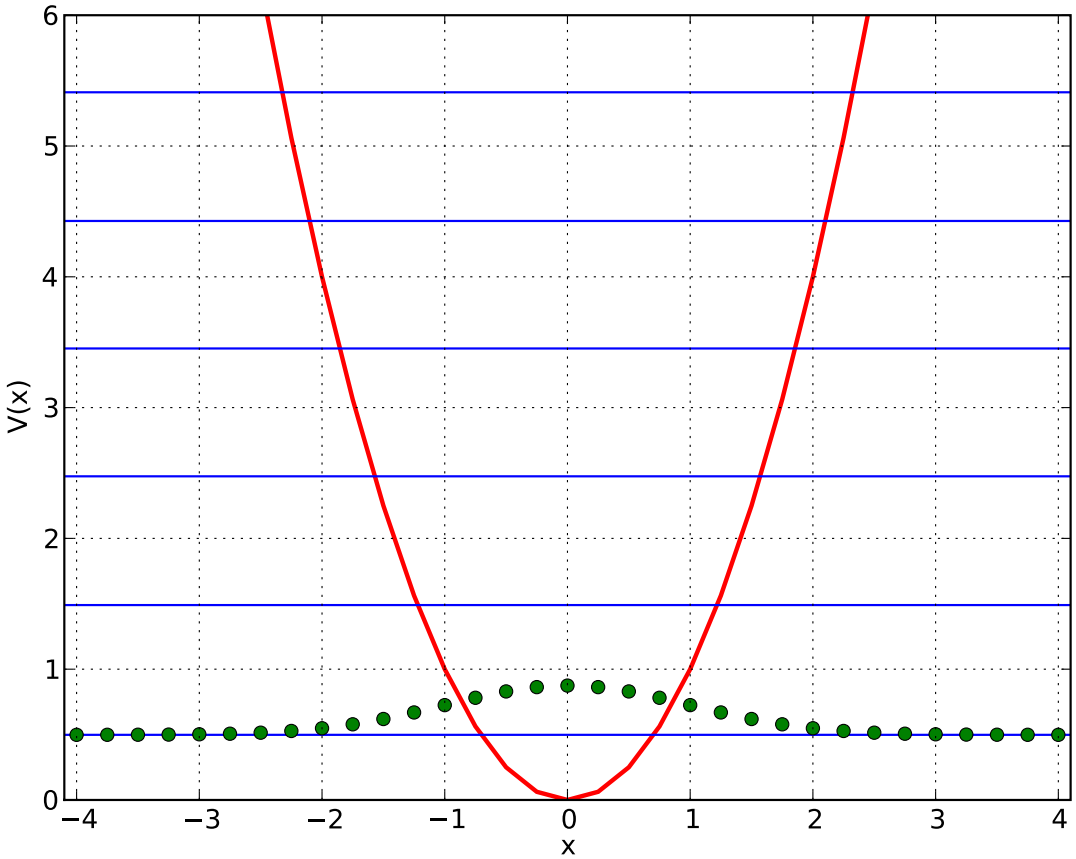
- svodi se na dijagonalizaciju tridijagonalne matrice

$$\begin{pmatrix} d+V_1 & -u & 0 & 0 & \cdots \\ -u & d+V_2 & -u & 0 & \cdots \\ 0 & -u & d+V_3 & -u & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & -u & d+V_{n-1} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_{N-1} \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_{N-1} \end{pmatrix}$$

- pritom smo iskoristili rubne uvjete

$$\psi_0 = 0 \quad \text{i} \quad \psi_N = 0$$

- rezultat su
  - energije pojedinih stanja E_0, E_1,...
  - valne funkcije u točkama mreže $\psi^{(0)}(x_j), \ldots, \psi^{(N)}(x_j)$



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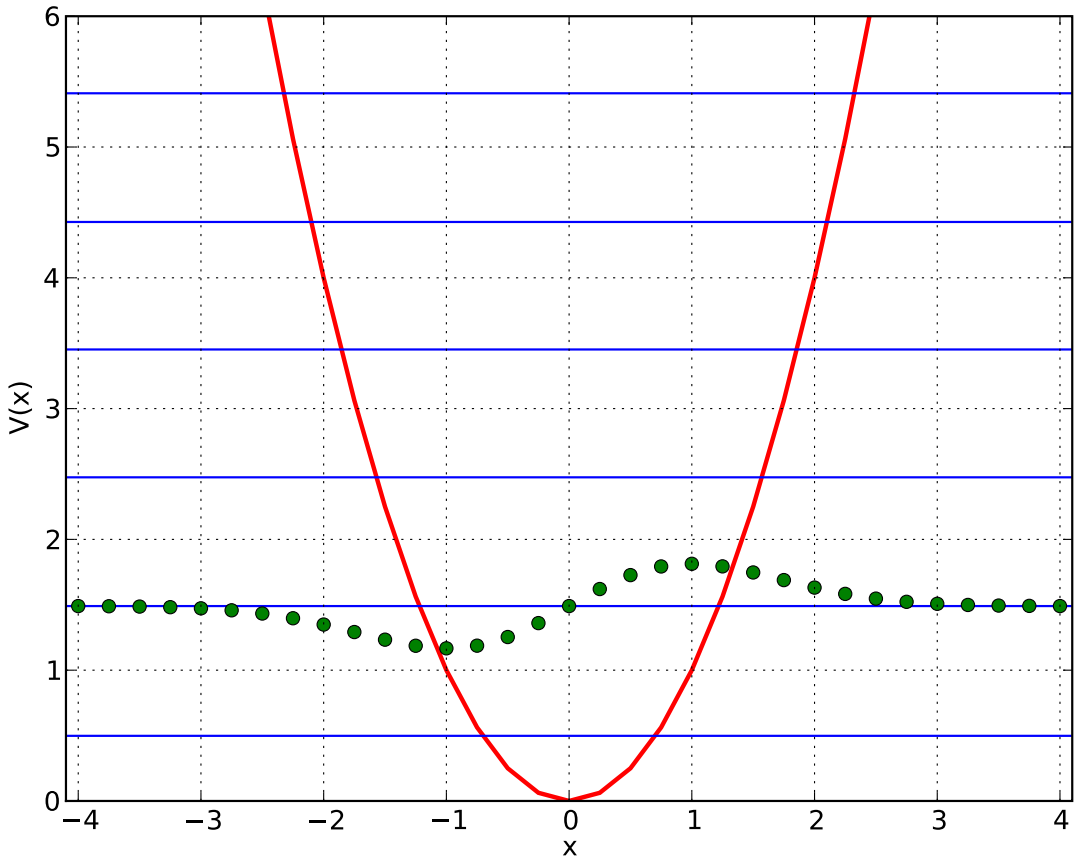

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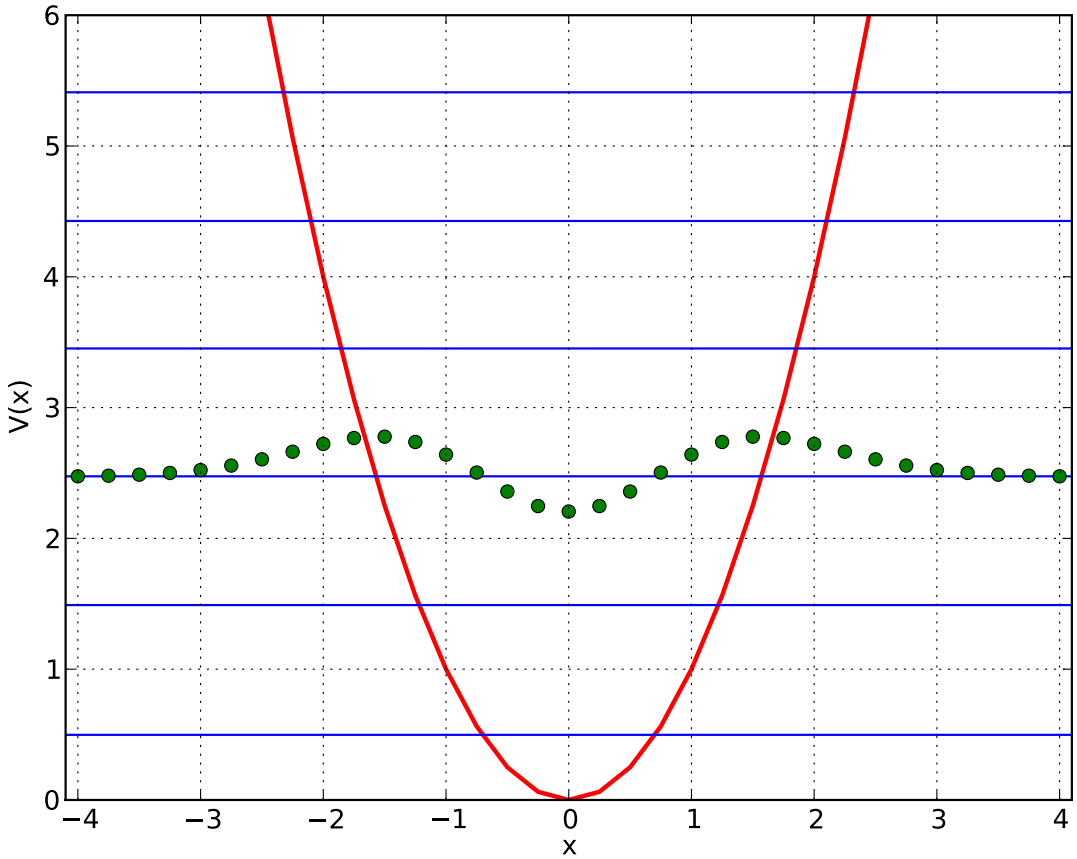

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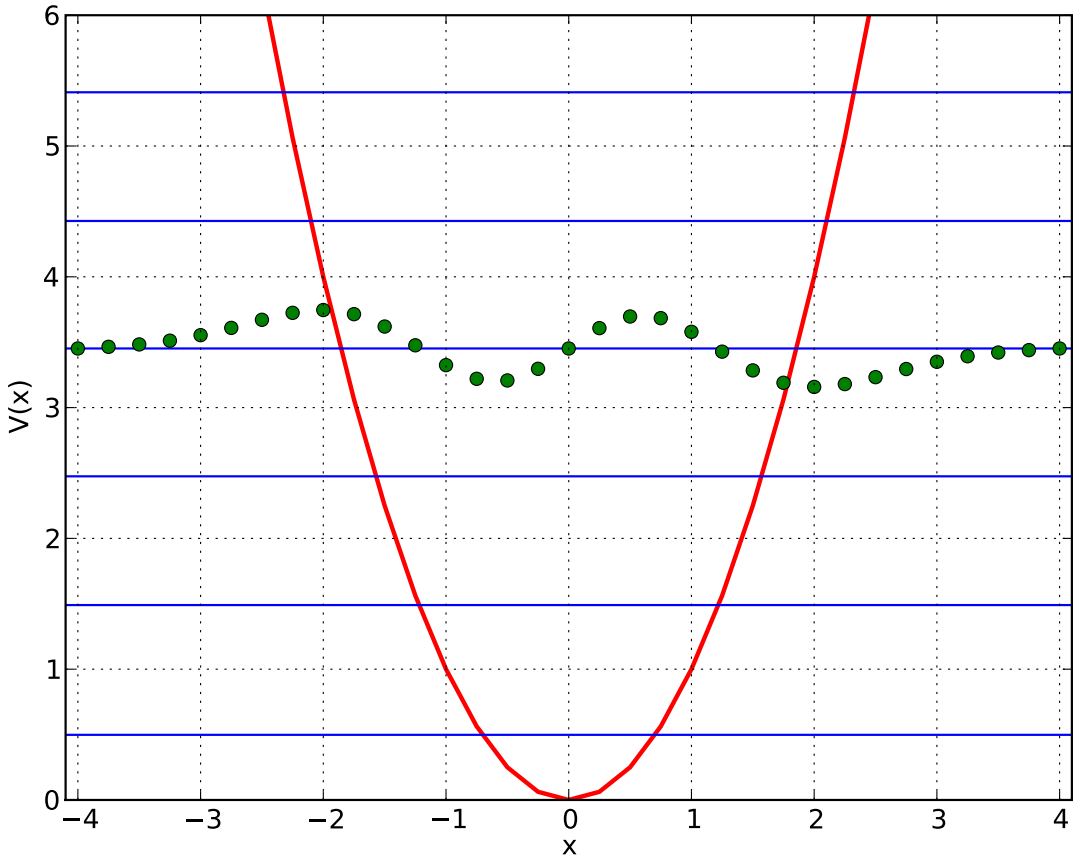

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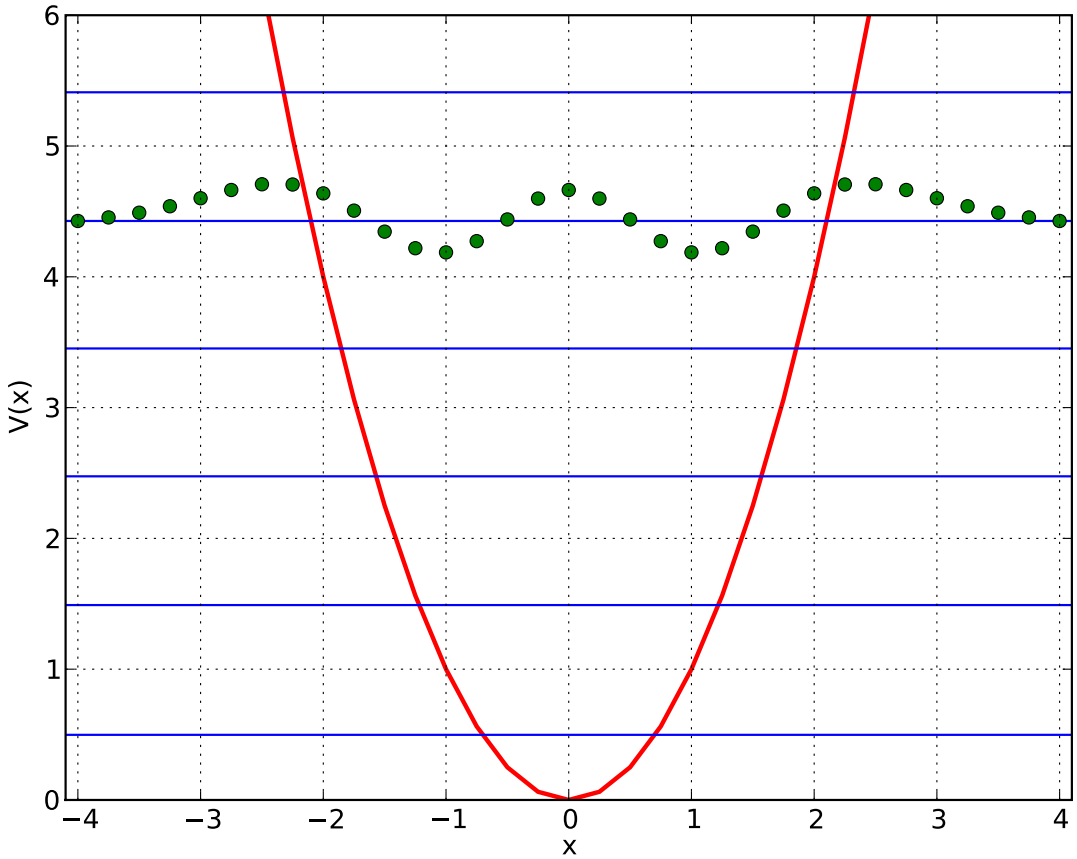
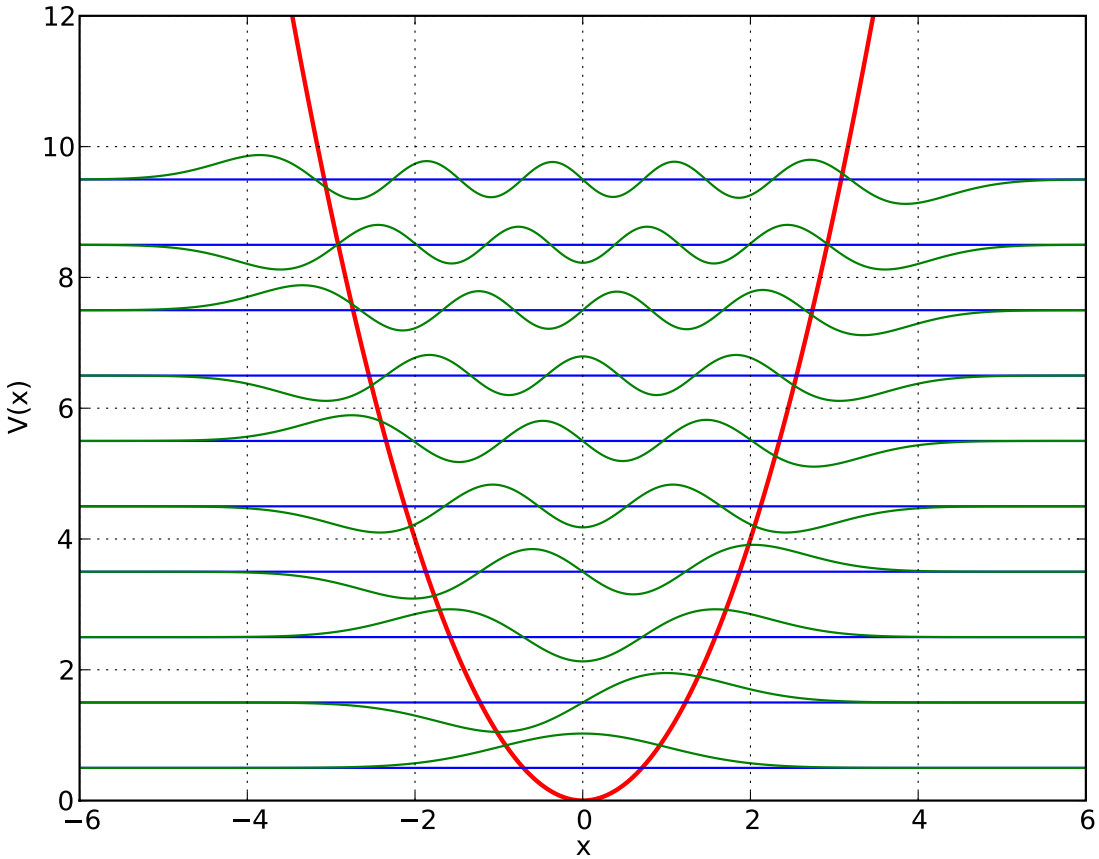


Primjer: harmonički oscilator

- potencijal harmoničkog oscilatora (analitički rješiv)

$$V(x) = \frac{1}{2} m\omega^2 x^2$$



Primjer: anaharmonički oscilator

- potencijal anaharmoničkog oscilatora (nije rješiv analitički)

$$V(x) = \frac{1}{2} m\omega^2 x^2 + \epsilon_1 (\alpha x)^3 + \epsilon_2 (\alpha x)^4$$

- promatramo slučaj $\epsilon_2 \ll \epsilon_1$

stanje	numerički	račun smetnje
n=0	-0.0076	-0.0075
n=1	-0.0560	-0.0537
n=2	-0.1582	-0.1466
n=3	-0.3208	-0.2868
n=4	-0.5527	-0.4750
n=5	-0.8626	-0.7119
n=6	-1.2513	-0.9980
n=7	-1.6948	-1.3340

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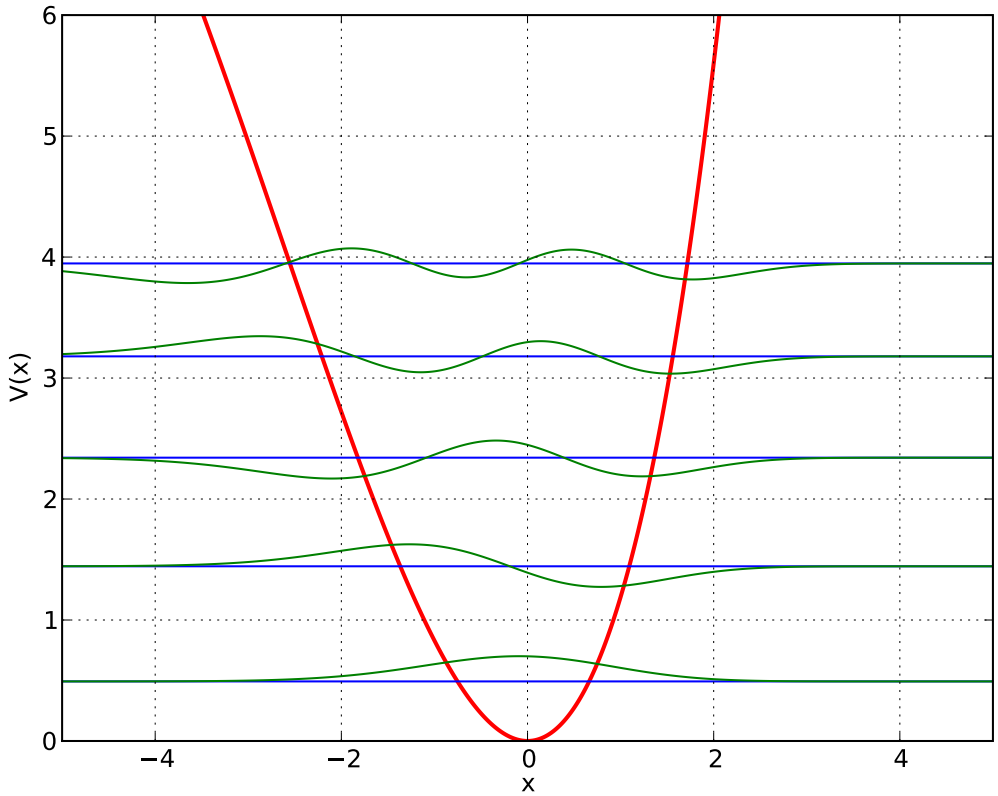

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- promatramo slučaj $\epsilon_1 = 0$

stanje	numerički	račun smetnje
n=0	0.0326	0.0309
n=1	0.1534	0.1359
n=2	0.3737	0.2953
n=3	0.6758	0.4453
n=4	1.0484	0.5222
n=5	1.4835	0.4622

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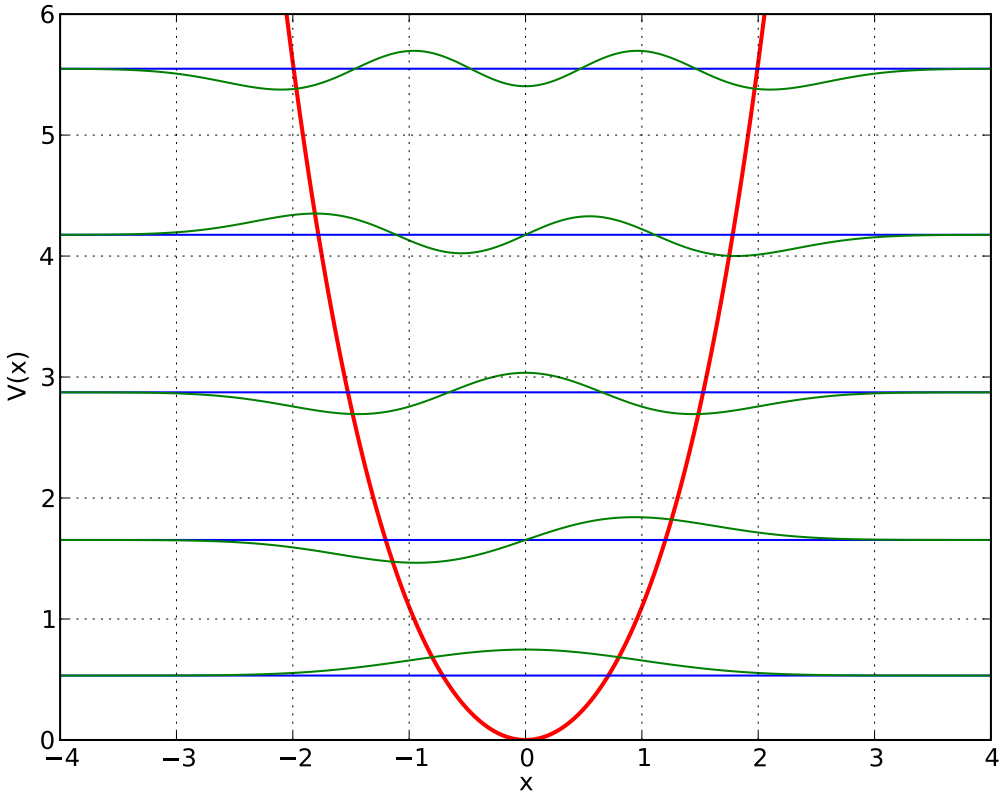
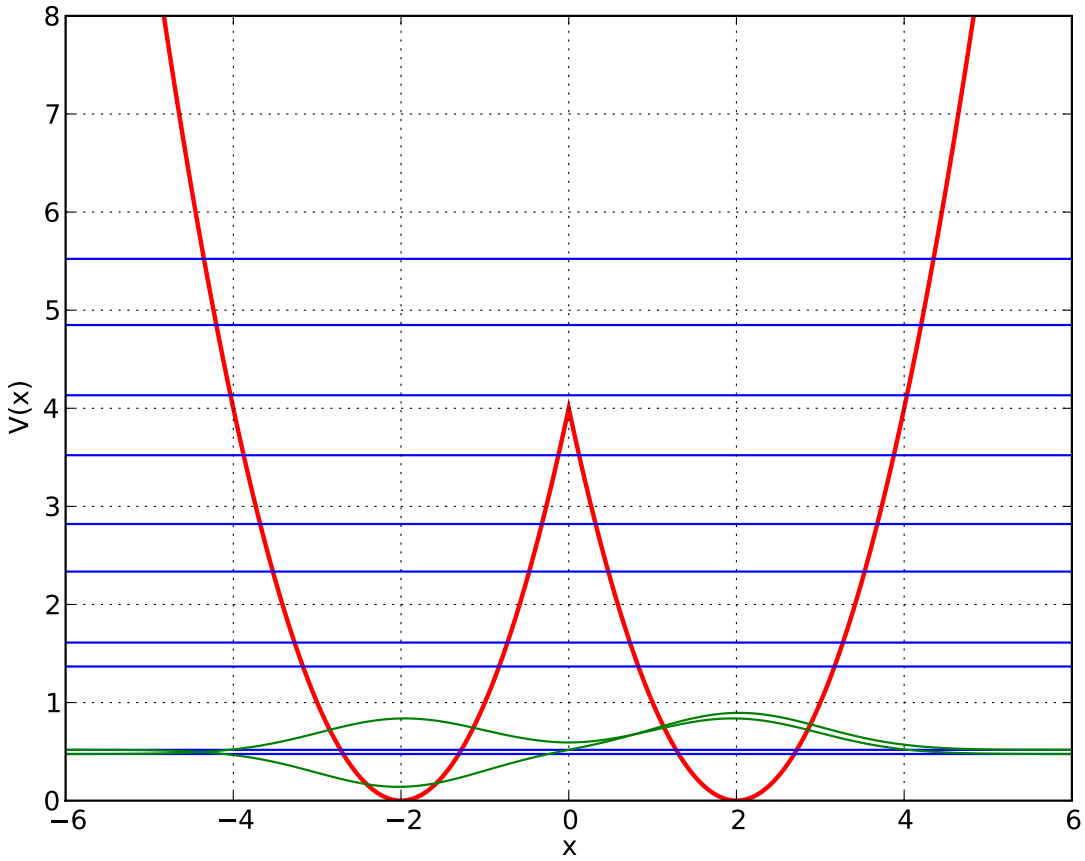


Dvije harmoničke jame

- najniže energije

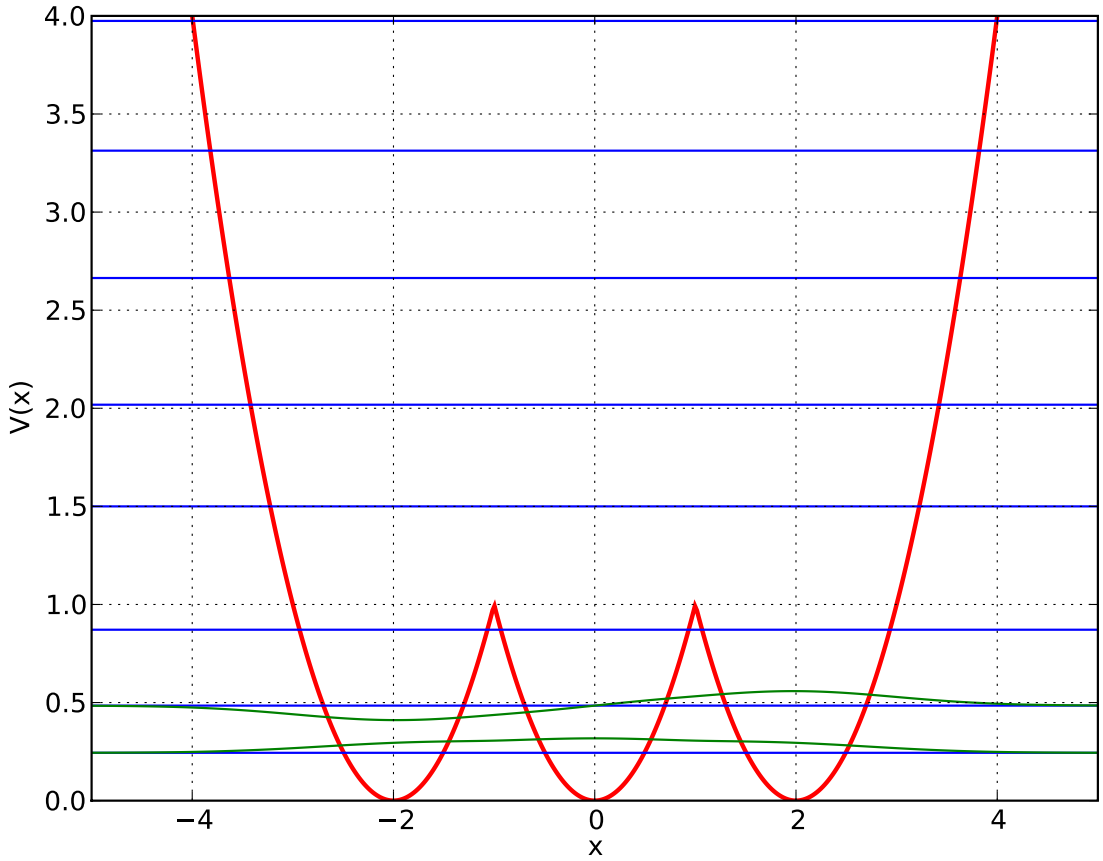
$$E_0 = 0.4757, \quad E_1 = 0.5179, \quad E_2 = 1.3675, \quad E_3 = 1.6114$$



Tri harmoničke jame

- najniže energije

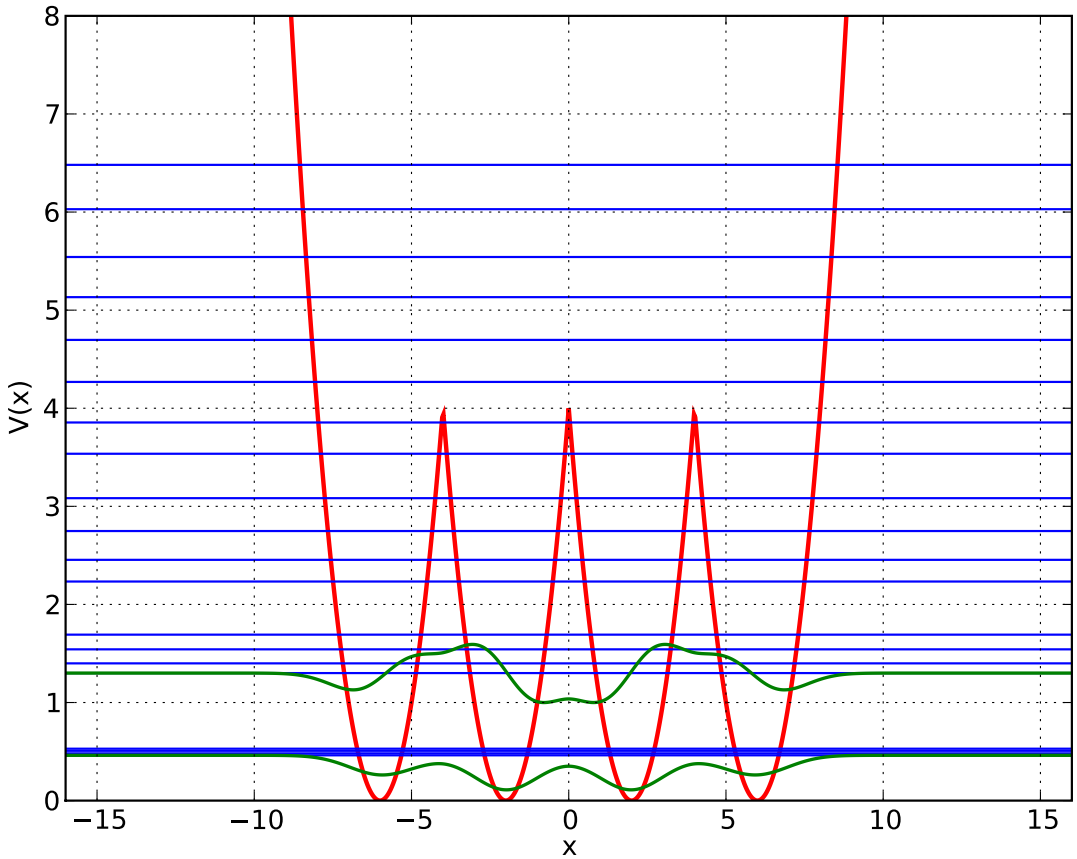
$$E_0 = 0.2439, \quad E_1 = 0.4844, \quad E_2 = 0.8713, \quad E_3 = 1.4999$$



Četiri harmoničke jame

- najniže energije

$$E_0 = 0.4617, \quad E_1 = 0.4819, \quad E_2 = 0.5078, \quad E_3 = 0.5293$$
$$E_4 = 1.3001, \quad E_5 = 1.3992, \quad E_6 = 1.5421, \quad E_7 = 1.6919$$



Šest harmoničkih jama

- najniže energije

$$E_0 = 0.458,\ E_1 = 0.469,\ E_2 = 0.485,\ E_3 = 0.503,\ E_4 = 0.521,\ E_5 = 0.533$$

$$E_6 = 1.282,\ E_7 = 1.334,\ E_8 = 1.413,\ E_9 = 1.513,\ E_{10} = 1.624,\ E_{11} = 1.72$$