Periodični potencijali

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Kvantna fizika, vježbe

Floquetov teorem

- neka je $V(x)$ periodički potencijal s periodom a

$$V(x+a) = V(x)$$

- Schrödingerova jednadžba je invarijantna s obzirom na traslacije za cjelobrojni višekratnik od a
- označimo s $u_1(x)$ i $u_2(x)$ dva linearno nezavisna rješenja Schrödingerove jednadžbe
- $u_1(x+a)$ i $u_2(x+a)$ su također rješenja pa ih možemo napisati kao linearnu kombinaciju rješenja $u_1(x)$ i $u_2(x)$

$$u_1(x+a) = C_{11} u_1(x) + C_{12} u_2(x),$$
$$u_2(x+a) = C_{21} u_1(x) + C_{22} u_2(x)$$

- *Floquetov teorem*: među rješenjima postoje dva, ψ_1 i ψ_2 sa svojstvom

$$\psi(x+a) = \lambda\psi(x),$$

pri čemu je λ konstantni faktor

- Floquetov teorem dokazujemo tako da rješenje $\psi(x)$ napišemo kao linearnu kombinaciju rješenja $u_1(x)$ i $u_2(x)$

$$\psi(x) = Au_1(x) + Bu_2(x)$$

- slijedi

$$\psi(x+a) = \lambda\psi(x) = (AC_{11} + BC_{21})u_1(x) + (AC_{12} + BC_{22})u_2(x)$$

- došli smo do sustava jednadžbi

$$AC_{11} + BC_{21} = \lambda A$$
$$AC_{12} + BC_{22} = \lambda B$$

- da bi sustav imao rješenje, determinanta mu mora iščezavati

$$\begin{vmatrix} C_{11}-\lambda & C_{21} \\ C_{12} & C_{22}-\lambda \end{vmatrix} = 0 \Longrightarrow \lambda^2 - (C_{11}+C_{22})\lambda + C_{11}C_{22} - C_{12}C_{21} = 0$$

- iz prethodne kvadratne jednadžbe možemo izračunati konstantu λ

- Wronskijan sustava $W = \psi_1\psi_2' - \psi_2\psi_1'$ zadovoljava sljedeću relaciju

$$D = \psi_1\psi_2' - \psi_2\psi_1' \Longrightarrow D(x+a) = \lambda_1\lambda_2 D(x)$$

- Wronskijan mora biti konstanta pa vrijedi

$$\lambda_1\lambda_2 = 1$$

- da bi rješenje bilo omeđeno mora vrijediti $|\lambda| < 1$

$$\lambda_1 = e^{iKa} \quad \text{i} \quad \lambda_2 = e^{-iKa}, \quad K \in \mathcal{R}$$

- budući da vrijedi relacija

$$e^{2\pi in} = 1,$$

  K možemo ograničiti na interval

$$-\frac{\pi}{a} \leq K \leq \frac{\pi}{a}$$

- za sva omeđena rješenja vrijedi

$$\psi(x+na) = e^{inKa}\psi(x) \Longrightarrow \psi(x) = e^{iKx}u_K(x),$$

pri čemu je $u_K(x)$ periodička funkcija od x

$$u_K(x) = u_K(x+a)$$

- Blochov teorem
- poznavajući rješenje na intervalu $0 \leq x \leq a$, možemo konstruirati rješenje na svakom sljedećem intervalu

$$\psi(x) = e^{iKa}\left[Au_1(x-a) + Bu_2(x-a)\right]$$

Primjer: Diracov "češalj"

- zadan je potencijal u obliku niza δ-funkcija razmaknutih za udaljenost a

$$V(x) = \frac{\hbar^2}{m}\Omega \sum_{n=-\infty}^{+\infty} \delta(x + na)$$

- ograničimo se na područje $0 < x < a$
- čestica je slobodna pa dva linearno nezavisna rješenja glase

$$u_1(x) = e^{ikx} \quad \text{i} \quad u_2(x) = e^{-ikx}$$

- opće rješenje je njihova linearna kombinacija

$$u(x) = Ae^{ikx} + Be^{-ikx}$$

- koristeći Floquetov teorem

$$u(x + a) = e^{iKa}u(x),$$

  možemo se ograničiti na područje $0 \leq x \leq a$

- u području $a \leq x \leq 2a$ vrijedi

$$u(x) = e^{iKa}\left[Au_1(x-a) + Bu_2(x-a)\right]$$

- spojimo rješenja na granici

$$u(a+0) = u(a-0) \quad \text{i} \quad u'(a+0) = u'(a-0) + 2\Omega u(a)$$

- član $2\Omega u(a)$ dolazi od δ-funkcije u potencijalu
- došli smo do sustava od dvije jednadžbe s dvije nepoznanice (koeficijenti A i B)

$$\begin{aligned} e^{iKa}(A+B) &= Ae^{ika} + Be^{-ika} \\ ike^{iKa}(A-B) &= ik\left(Ae^{ika} - Be^{-ika}\right) + 2\Omega\left(Ae^{ika} + Be^{-ika}\right) \end{aligned}$$

- uredimo sustav jednadžbi

$$\begin{aligned} A\left(e^{iKa} - e^{ika}\right) + B\left(e^{iKa} - e^{-ika}\right) &= 0 \\ A\left(e^{iKa} - e^{ika} - \frac{2\Omega}{ik}e^{ika}\right) - B\left(e^{iKa} - e^{-ika} + \frac{2\Omega}{ik}e^{-ika}\right) &= 0 \end{aligned}$$

- da bi homogeni sustav imao rješenje determinanta mu mora iščezavati

$$\cos Ka = \cos ka + \frac{\Omega}{k} \sin ka$$

- da bi rješenje postojalo, mora vrijediti

$$\left| \cos ka + \frac{\Omega}{k} \sin ka \right| \leq 1$$

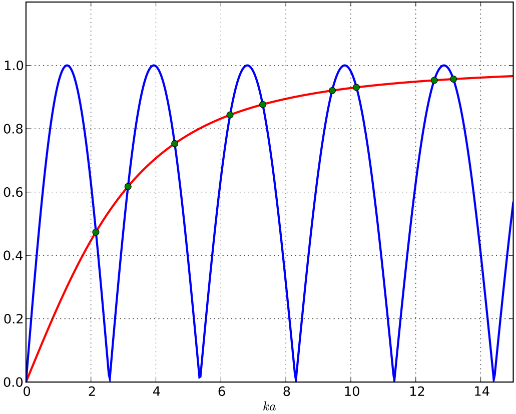
- prethodni uvjet nam daje dozvoljene energijske vrpce, a možemo ga napisati i u malo drugačijem obliku

$$\left| \cos \left(ka - \arctan \frac{\Omega a}{ka} \right) \right| \leq \frac{1}{\sqrt{1 + (\Omega a/ka)^2}}$$

- bez obzira na vrijednost *ka*, uvijek postoji raspon zabranjenih energija

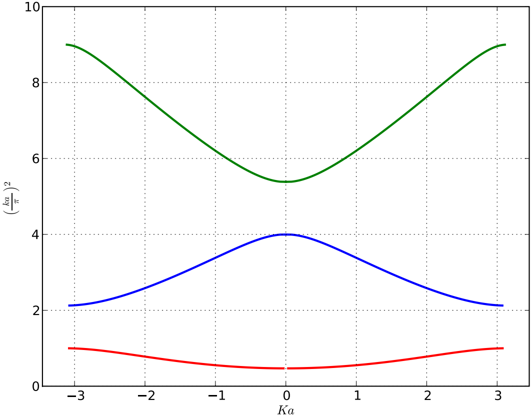
Određivanje raspona dozvoljenih energija ($\Omega a = 4$)

$$\left|\cos\left(ka - \arctan\frac{\Omega a}{ka}\right)\right| \leq \frac{1}{\sqrt{1 + (\Omega a / ka)^2}}$$



Ovisnost energije o *Ka*

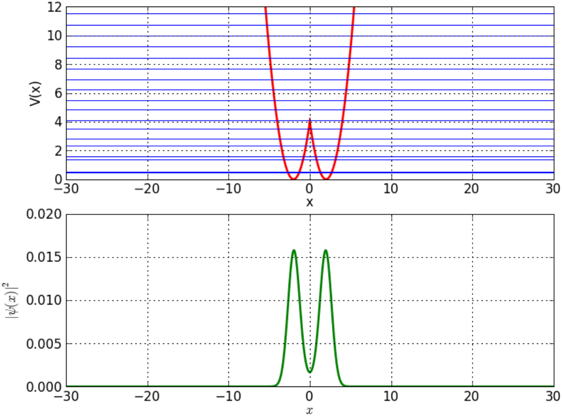
$$\cos Ka = \cos ka + \frac{\Omega}{k} \sin ka$$



Dvije harmoničke jame

- najniže energije

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



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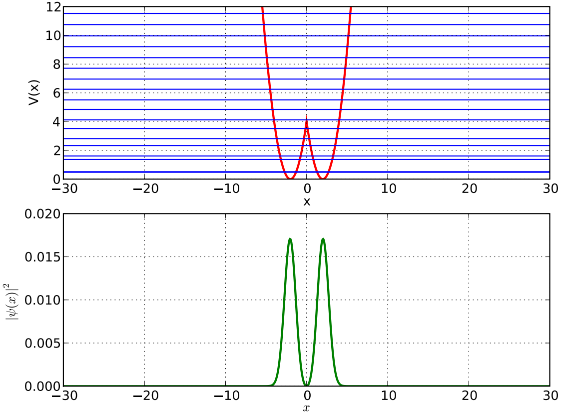

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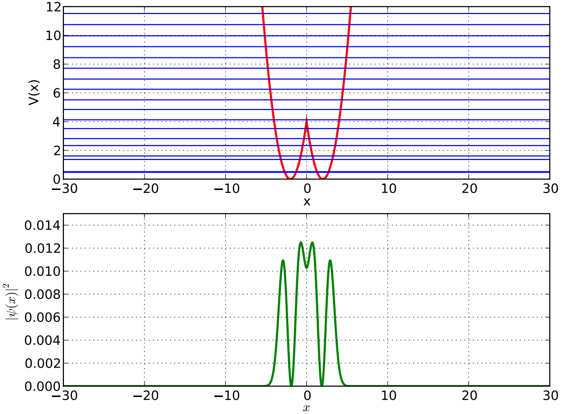

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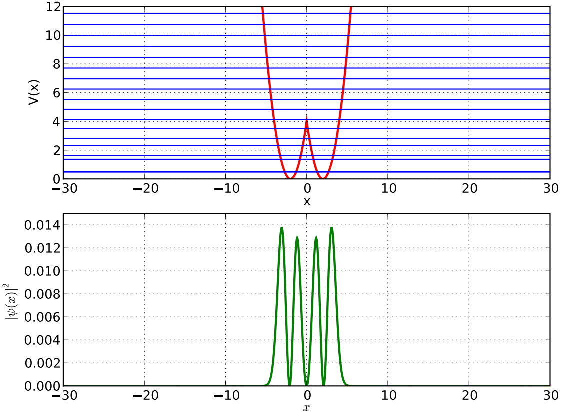

Četiri harmoničke jame

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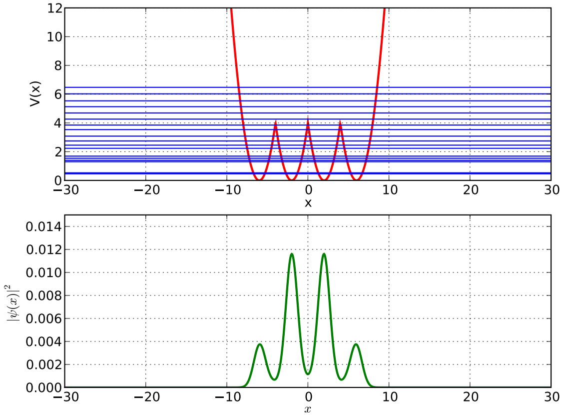
$$E_0 = 0.4617, \quad E_1 = 0.4819, \quad E_2 = 0.5078, \quad E_3 = 0.5293$$
$$E_4 = 1.3001, \quad E_5 = 1.3992, \quad E_6 = 1.5421, \quad E_7 = 1.6919$$



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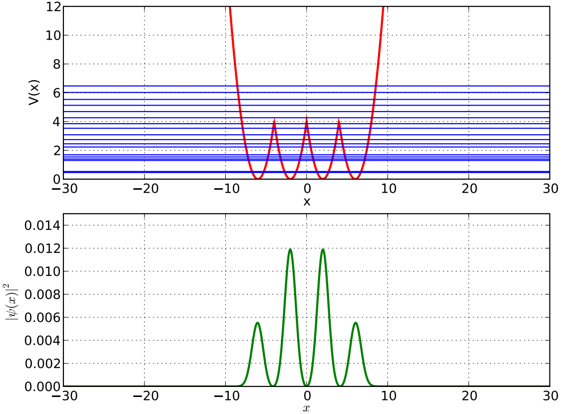

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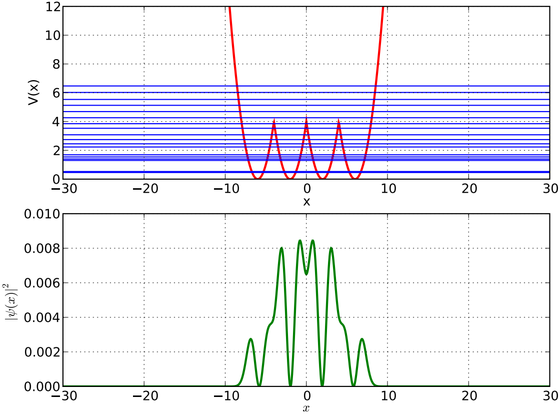

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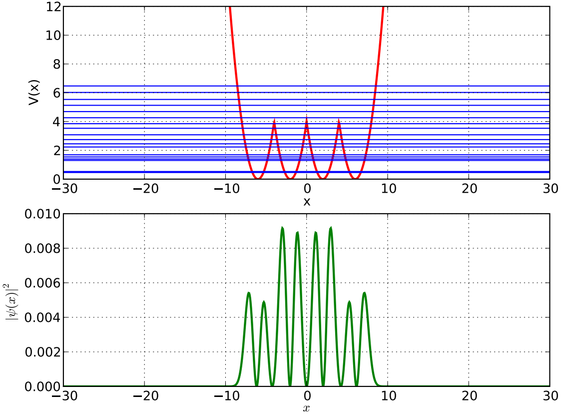
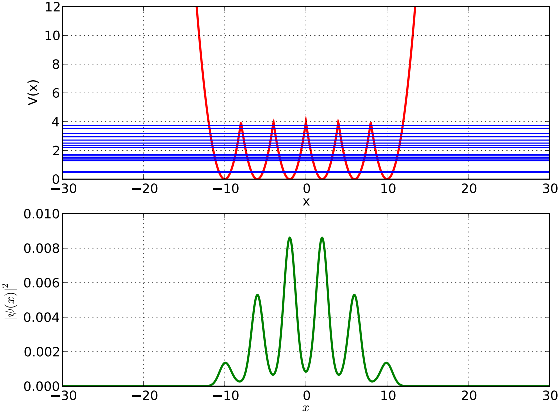


Šest harmoničkih jama

- najniže energije

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

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



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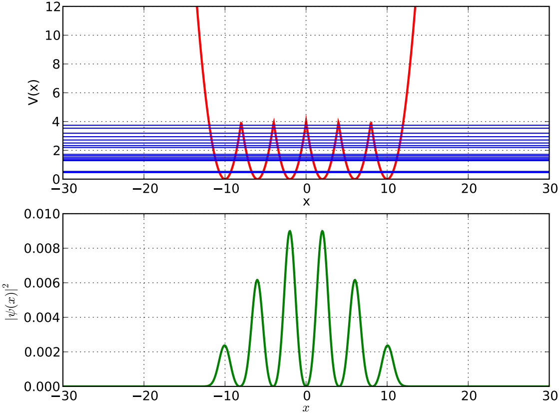

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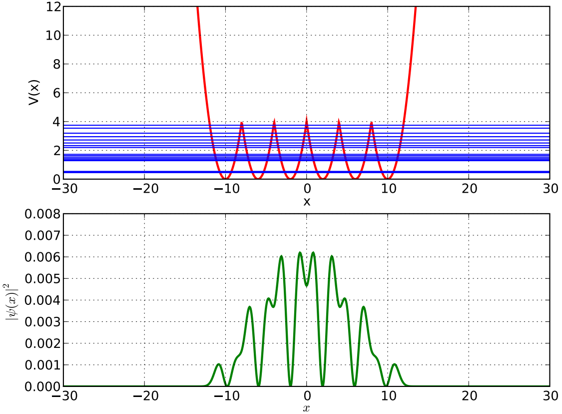

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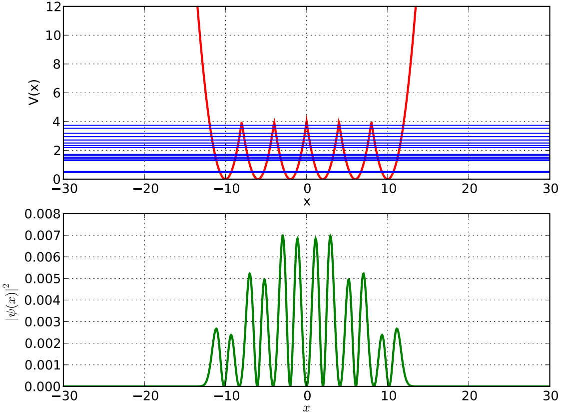

Osam harmoničkih jama

- najniže energije

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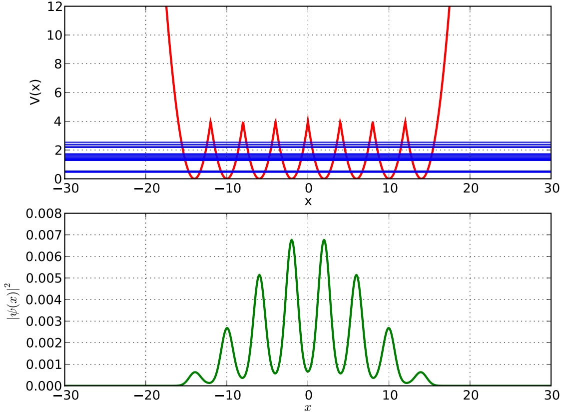
$$E_8 = 1.275, \ldots \; E_{15} = 1.736$$



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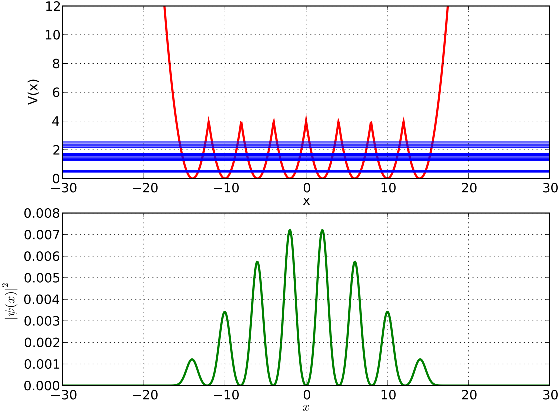

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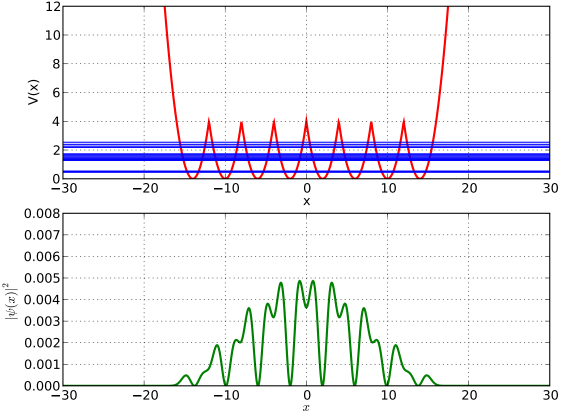

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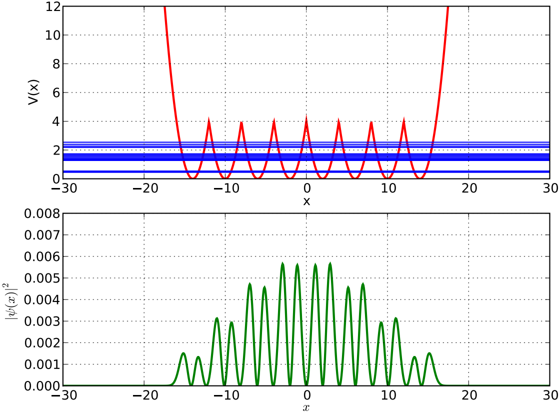

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$$E_0 = 0.455, \ldots, \; E_{13} = 0.536$$
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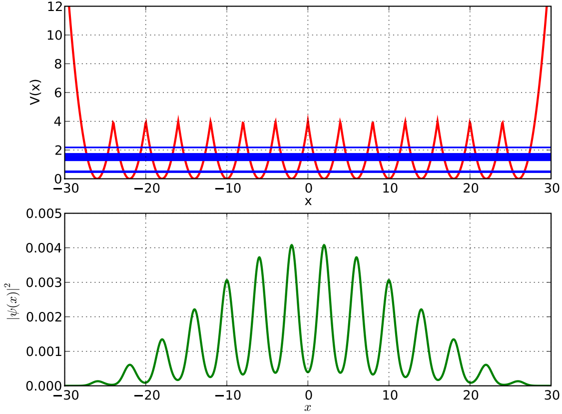

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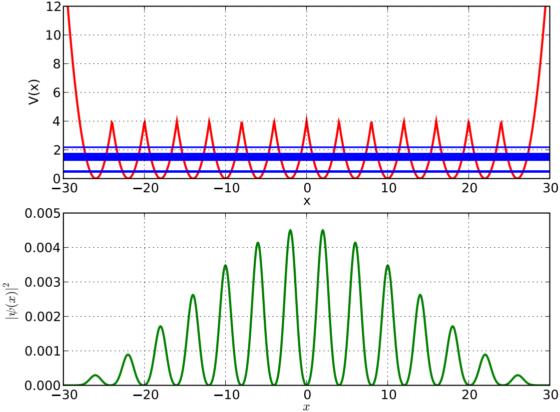

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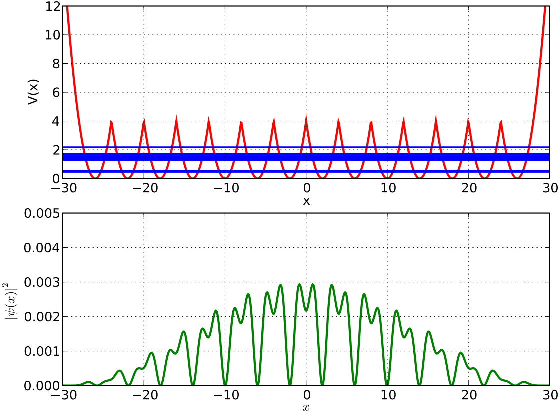

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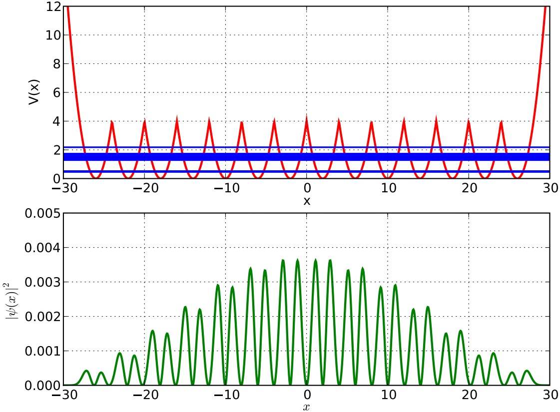
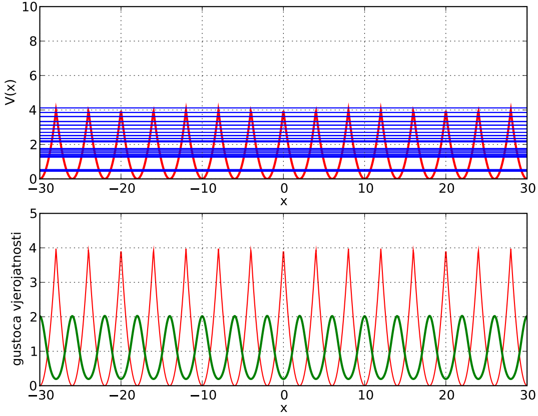


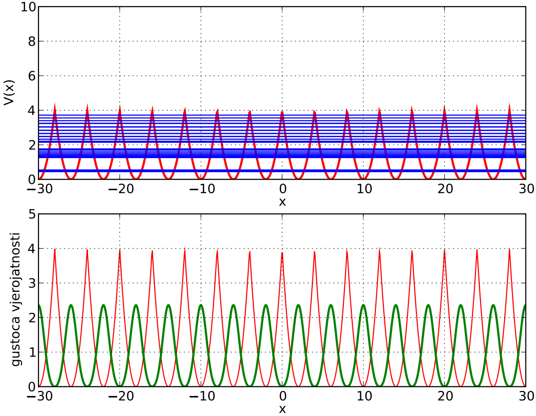
Periodički rubni uvjeti

- "zatvaramo" krajeve u krug: $\psi(x_0) = \psi(x_N)$
- prvo stanje u prvoj vrpci ($E = 0.454$)



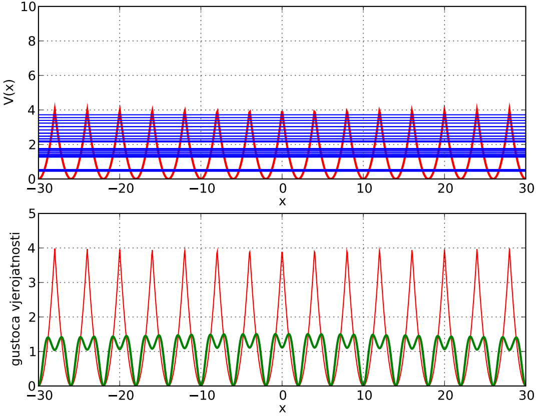
Periodički rubni uvjeti

- "zatvaramo" krajeve u krug: $\psi(x_0) = \psi(x_N)$
- zadnje stanje u prvoj vrpci ($E = 0.537$)



Periodički rubni uvjeti

- "zatvaramo" krajeve u krug: $\psi(x_0) = \psi(x_N)$
- prvo stanje u drugoj vrpci ($E = 1.264$)



Periodički rubni uvjeti

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- zadnje stanje u prvoj vrpci ($E = 1.764$)