Playing with Quantum Mechanics on the lattice

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Humboldt University (Berlin), Oct. 30, 2012

CM, QM, repeat some basics

classical mechanics, Hamilton's (!!!) formulation:

$$H = H(p,x)\left[= \frac{p^2}{2m} + V(x)\right], \quad \frac{dx}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial x}$$

prepare/choose $x(0), p(0)$, solve DEs, pre/postdict $x(t), p(t)$ for all t

C→Q: state = point in $x - p$ plane → direction in an infinite dimensional Hilbert space $|\psi\rangle$

time evolution, Schrödinger:

$$i\hbar \frac{d}{dt}|\psi\rangle = \hat{H}|\psi\rangle \Rightarrow |\psi(t)\rangle \quad [\,|\psi(0)\rangle \text{ must be known first}]$$

$\hat{H}$ operator, formed as $\hat{H} = H(\hat{p}, \hat{x})$
what are ops $\hat{p}$, $\hat{x}$?

Heisenberg commutation relation: ops obey

$$\hat{p}\hat{x} - \hat{x}\hat{p} = [\hat{p}\,,\hat{x}] = \frac{\hbar}{i}$$

standard solution:

choose $\hat{x}$ diagonal, ON basis (continuously infinite set of vectors):

$$\{|y\rangle\}, \quad \hat{x}\,|y\rangle = y|y\rangle \quad [y = \text{eigenvalue}] \quad \langle y|z\rangle = \delta(y-z)$$

define $\hat{p}$ as shift:

$$\mathrm{e}^{\frac{i}{\hbar}u\,\hat{p}}\,|x\rangle = |x-u\rangle$$

then:

$$\left[\mathrm{e}^{\frac{i}{\hbar}\varepsilon\,\hat{p}}, \hat{x}\right]|x\rangle = \varepsilon\,|x-\varepsilon\rangle \underbrace{\Rightarrow}_{\mathrm{O}(\varepsilon)} \frac{i}{\hbar}[\hat{p}\,,\hat{x}]|x\rangle = |x\rangle \Rightarrow \text{Heisenberg}$$

now (for a while):

$$\hat{H} = \frac{1}{2m}\,\hat{p}^2 + \frac{m\omega^2}{2}\,\hat{x}^2 \qquad (V = \text{harmonic oscillator})$$

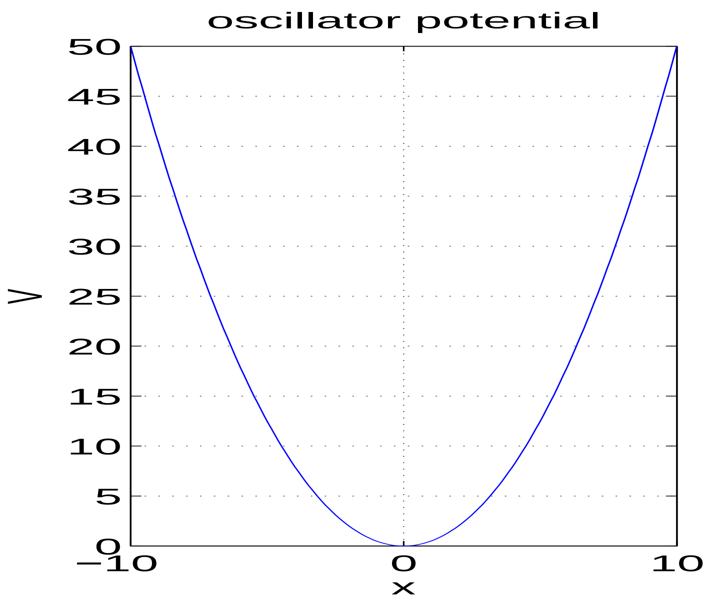
take units of length, time, mass such that $1 = m = \omega = \hbar$ holds

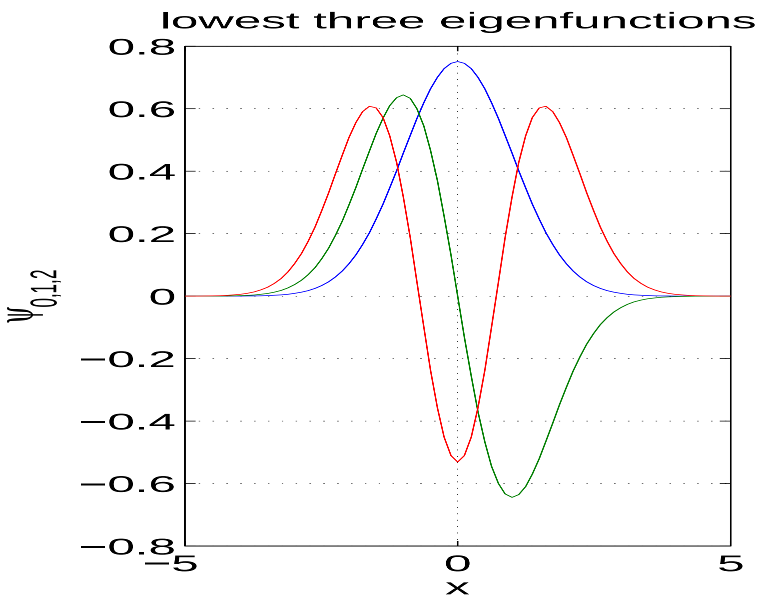
$$\hat{H} = \frac{1}{2}(\hat{p}^2 + \hat{x}^2)$$

complete set of energy eigenstates:

$$\hat{H}\,|n\rangle = E_n|n\rangle, \quad E_n = n + 1/2, \quad n = 0, 1, 2, \ldots, \infty$$

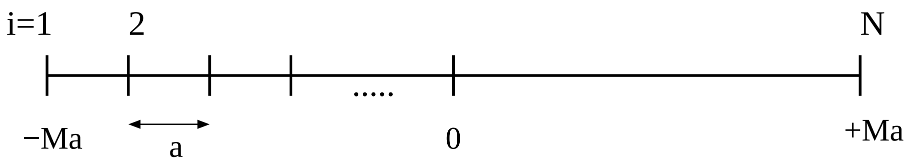
$$\psi_n(x) = \langle x|n\rangle, \quad \psi_n(x) = \mathrm{e}^{-x^2/2} \times (\text{polynomial of deg.}\, n)$$





Make it all finite

- neither computers like nor labs measure values in $\mathbb{R}$
- replace the infinite real line by a finite set $\{x_i, i=1,2,\ldots N\}$ of equally spaced points:



- $x_1 = -Ma,\ x_N = +Ma,\ N = 2M+1$
- $\langle x_i | x_j \rangle = \delta_{ij}, \quad |\psi\rangle = \sum_{i=1}^{N} \psi_i |x_i\rangle,$ state space $= \mathbb{C}^N$

now operator $\hat{x}$ → diagonal $N \times N$ matrix, $|\psi\rangle \to$ column:

$$\hat{x} \triangleq \begin{pmatrix} x_1 & 0 & \cdots & 0 \\ 0 & x_2 & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & & x_N \end{pmatrix}, \qquad |\psi\rangle \triangleq \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix}$$

lattice momentum operator:

$$e^{i\,(n\,a)\,\hat{p}}\,|x_i\rangle = |x_i - n\,a\rangle = |x_{i-n}\rangle$$

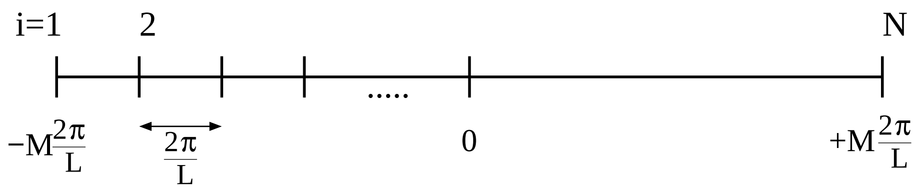
we use periodic boundary conditions $\leftrightarrow$ subscripts modulo N

$$|x_0\rangle \equiv |x_N\rangle, \quad |x_{N+1}\rangle \equiv |x_1\rangle, \quad |x_{i\pm N}\rangle \equiv |x_i\rangle \equiv |x+L\rangle \quad [L = Na]$$

second (momentum) basis (alternative to $\{|x_i\rangle\}$)

$$\hat{p}\,|q_i\rangle = q_i|q_i\rangle \Rightarrow \langle q_k|x_j\rangle = \langle q_k|e^{-i\,x_j\,\hat{p}}\,|x_0\rangle = e^{-i\,q_k x_j}\langle q_k|x_0\rangle = e^{-i\,q_k x_j}/\sqrt{N}$$

- choice $\langle q_k|x_0\rangle = 1/\sqrt{N} \Rightarrow$ normalization $\langle p_i|p_j\rangle = \delta_{ij}$
- periodicity $\Rightarrow e^{-i\,q_k L} = 1 \Rightarrow q_k = \frac{2\pi}{L}\,k$



- same dimension N (of course...)

Now there is an obvious realization of $\hat{p}$ as a $N \times N$ matrix as well:

$$(\hat{p})_{ij} = \sum_{k=1}^{N} \langle x_i | p_k \rangle p_k \langle p_k | x_j \rangle = \frac{1}{N} \sum_{k=1}^{N} p_k \mathrm{e}^{i p_k (x_i - x_j)}$$

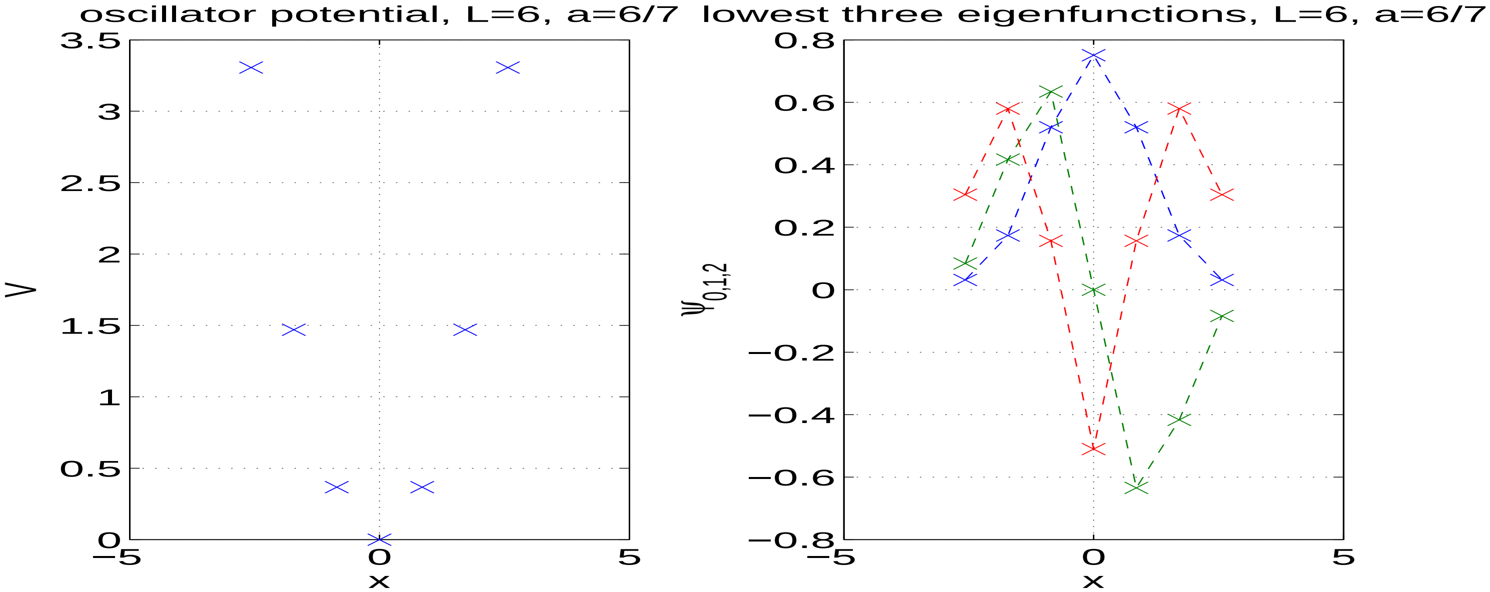
If we now take (very crude!) $N = 7$, $L = 6 \Rightarrow a = 6/7$:

$$\hat{H} = \frac{1}{2}(\hat{p}^2 + \hat{x}^2) = \hat{H}^\top =$$

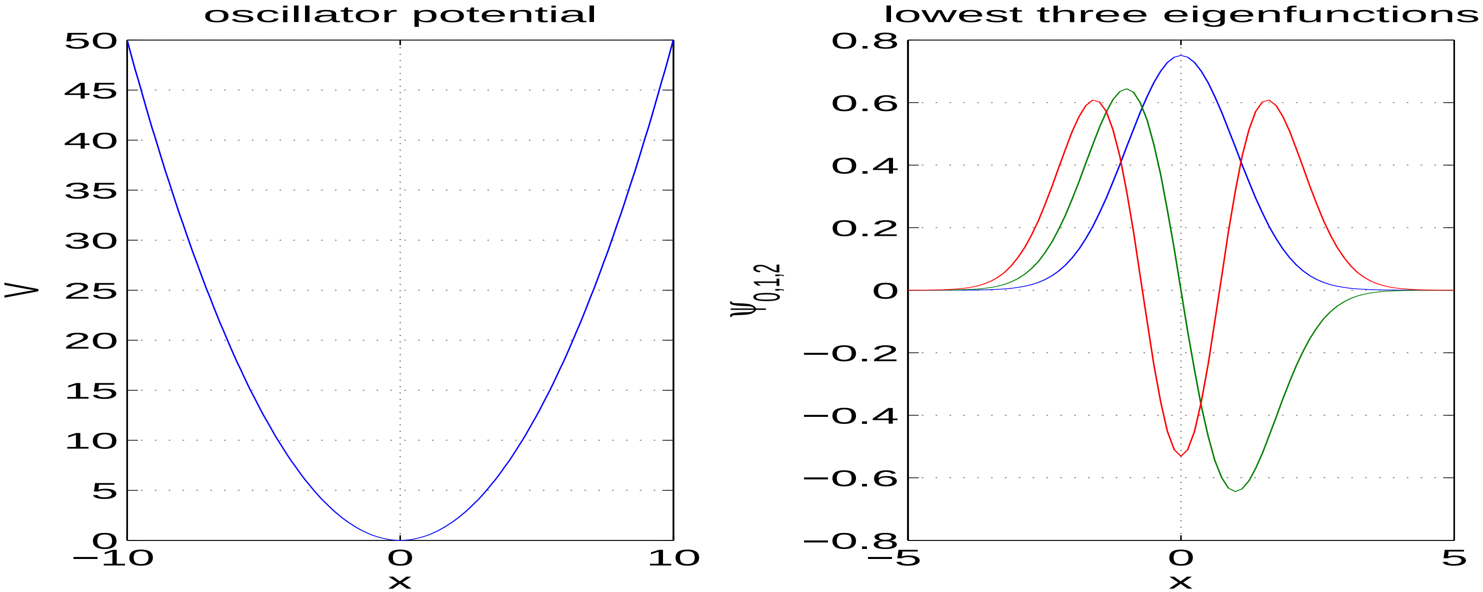
$$= \begin{pmatrix} 5.499 & -1.312 & 0.280 & -0.064 & -0.064 & 0.280 & -1.312 \\ \bullet & 3.663 & -1.312 & 0.280 & -0.064 & -0.064 & 0.280 \\ \bullet & \bullet & 2.561 & -1.312 & 0.280 & -0.064 & -0.064 \\ \bullet & \bullet & \bullet & 2.193 & -1.312 & 0.280 & -0.064 \\ \bullet & \bullet & \bullet & \bullet & 2.561 & -1.312 & 0.280 \\ \bullet & \bullet & \bullet & \bullet & \bullet & 3.663 & -1.312 \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & 5.499 \end{pmatrix}$$

`matlab`: $\mathrm{eig}(\hat{H}) = 0.4995 \quad 1.5067 \quad 2.4389 \quad 3.7007 \quad 4.0529 \quad 5.8278 \quad 7.6119$

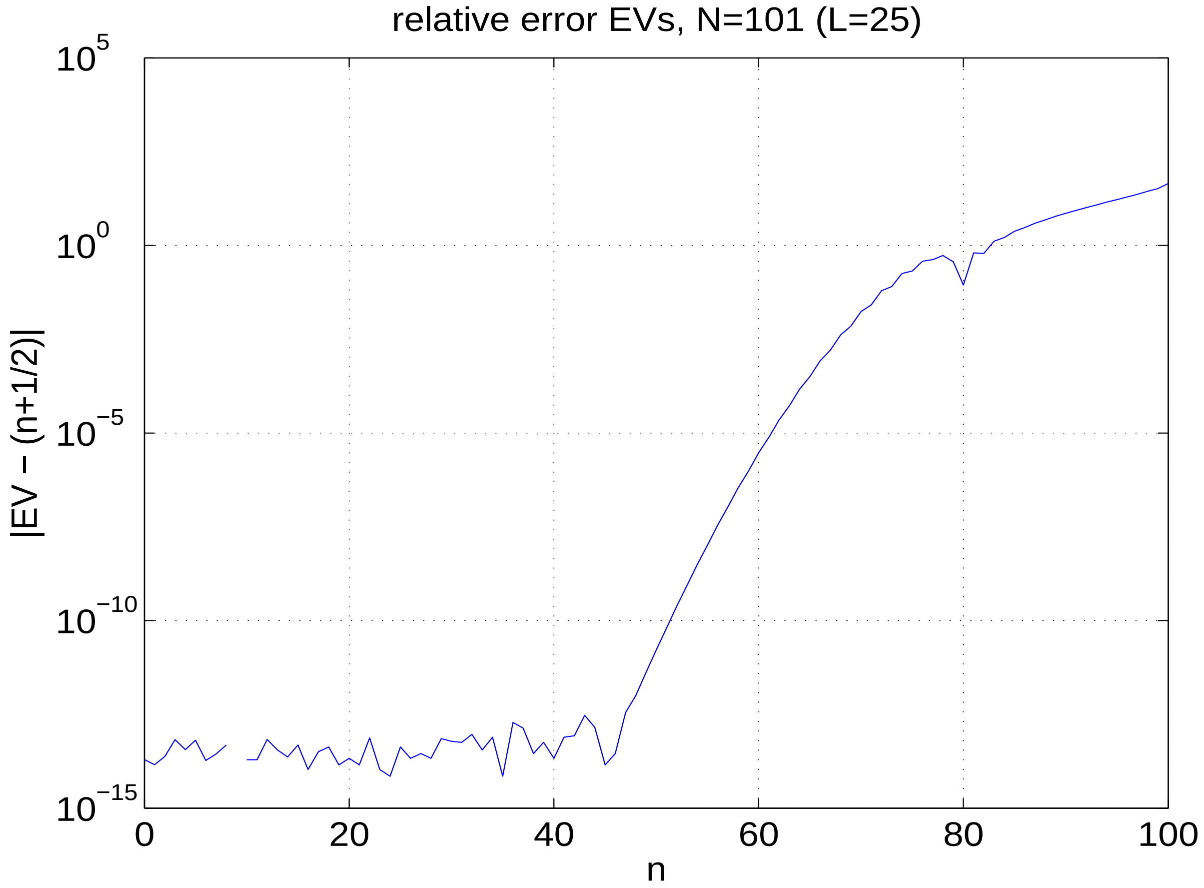
vs. $\quad 1/2 \quad 3/2 \quad 5/2 \quad 7/2 \quad 9/2 \quad 11/2 \quad 13/2$


oscillator potential, L=6, a=6/7
lowest three eigenfunctions, L=6, a=6/7
V
x
$\psi_{0,1,2}$
x

instead of:


oscillator potential
lowest three eigenfunctions
V
x
$\psi_{0,1,2}$
x

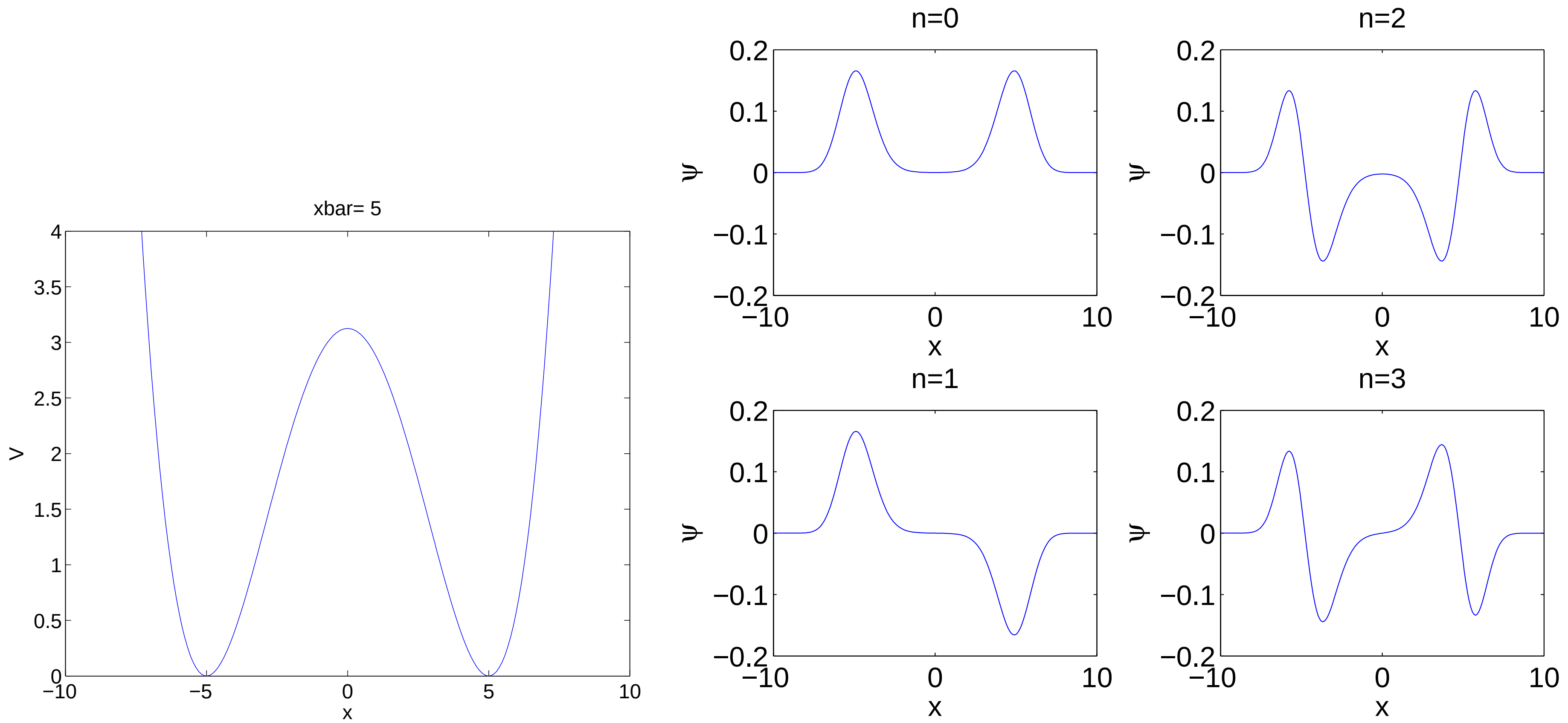
.... but with $N = 101$:



anharmonic case, for example `matlab:` $\mathrm{eig}\Big(\frac{1}{2}(\hat{p}^2 + \hat{x}^4)\Big) =$
0.5302 1.8998 3.7278 5.8224 8.1309 10.6192 13.2642 16.0493 18.9615

Application: tunneling and symmetry breaking (not really)

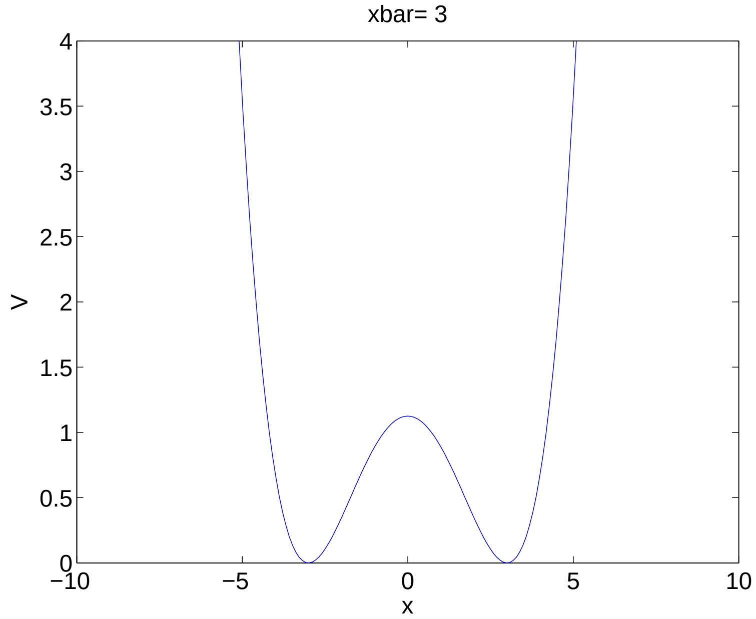
$$V(x) = \frac{1}{8\bar{x}^2}(x-\bar{x})^2(x+\bar{x})^2\,[\Rightarrow V''(\pm\bar{x}) = 1], \qquad N = 201, L = 20$$

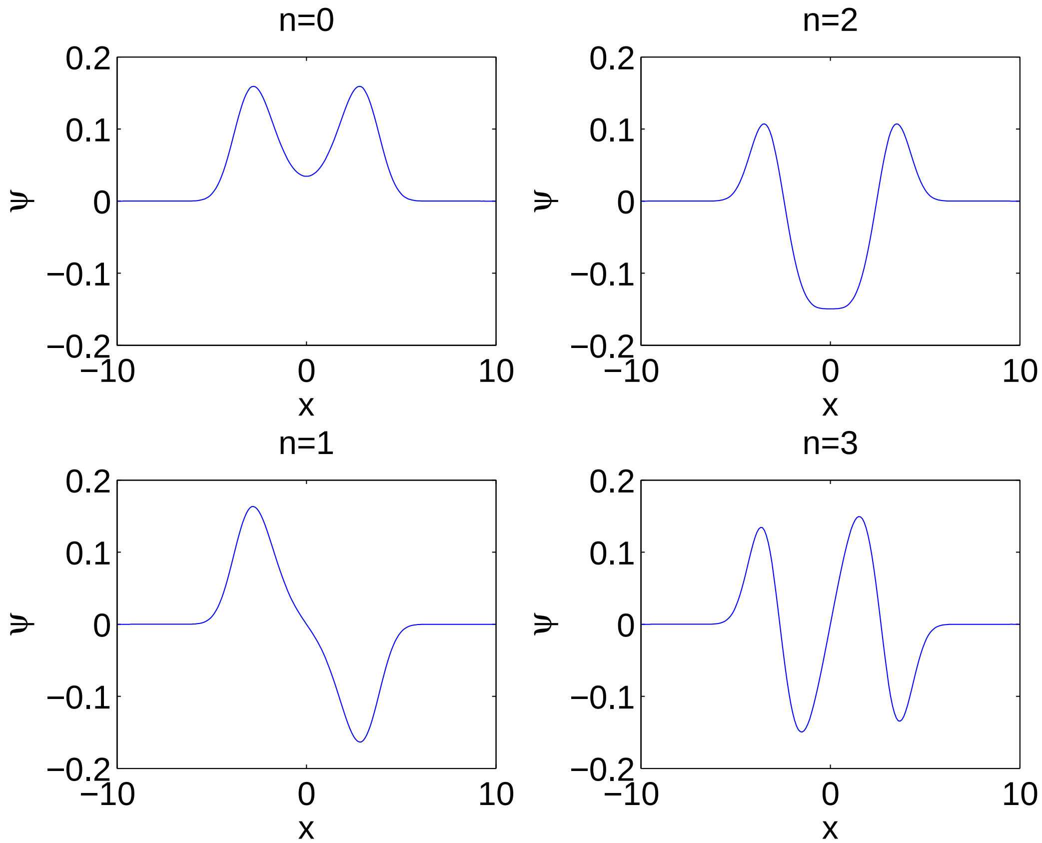


$$E_{0\ldots3} = 0.4895\ 0.4895\ 1.4218\ 1.4219 \quad [E_1 - E_0 = 6.12\times10^{-7}]$$

Application: [some] tunneling

$$V(x) = \frac{1}{8\bar{x}^2}(x-\bar{x})^2(x+\bar{x})^2\,[\Rightarrow V''(\pm\bar{x})=1], \qquad N=201, L=20$$

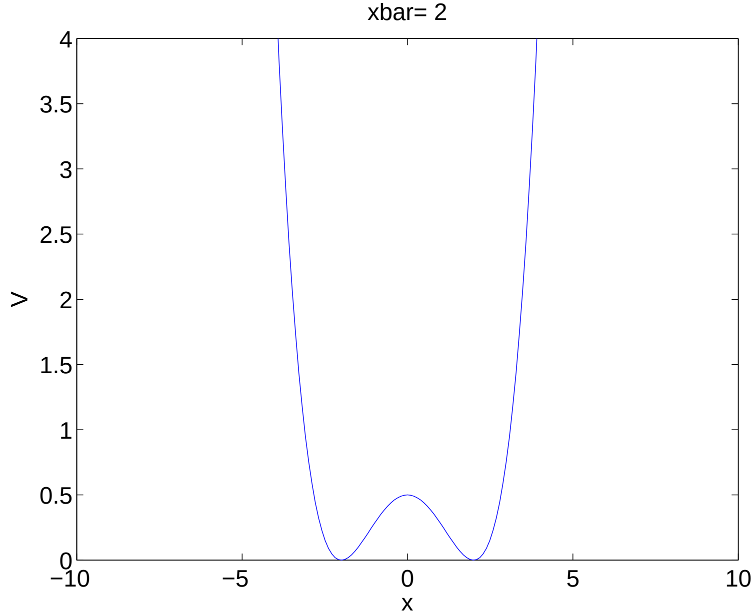


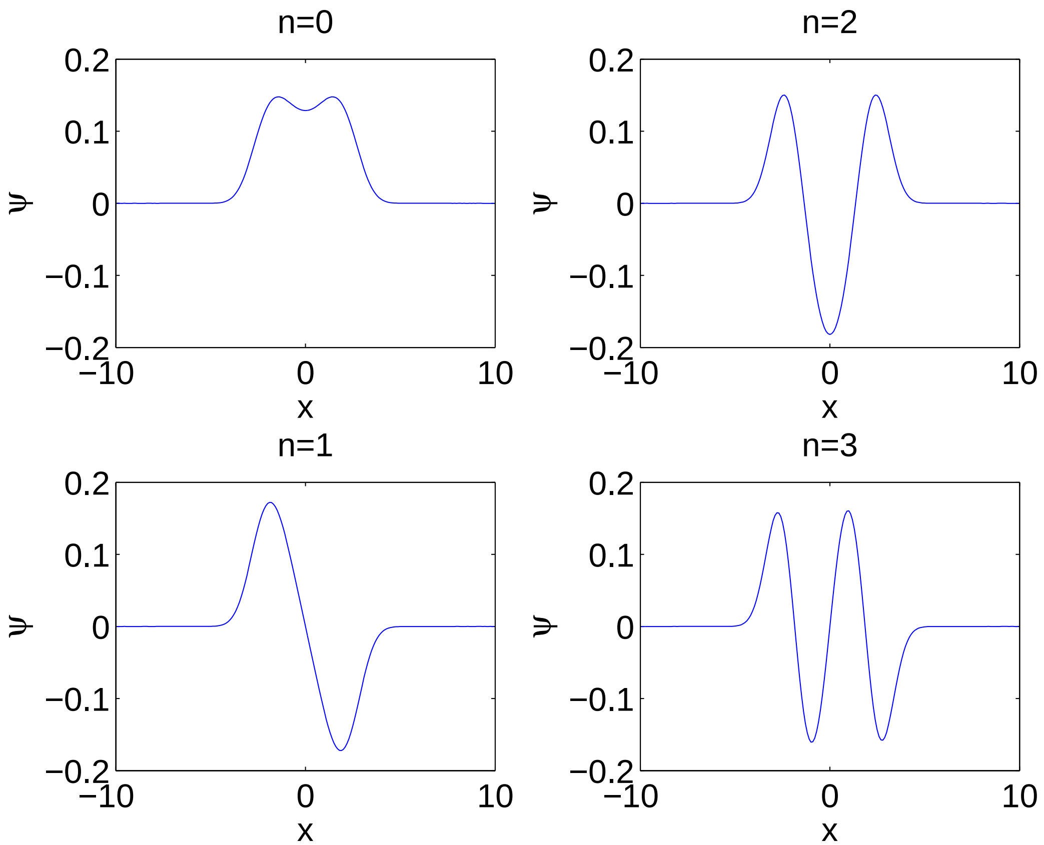


$$E_{0\ldots3} = 0.4604\ \ 0.4739\ \ 1.1328\ \ 1.3692$$

Application: [no more] tunneling

$$V(x) = \frac{1}{8\overline{x}^{\,2}}(x-\overline{x}\,)^2(x+\overline{x}\,)^2\,[\Rightarrow V''(\pm\overline{x}\,)=1], \qquad N=201, L=20$$





$$E_{0\ldots3} = 0.3502\ 0.5232\ 1.1140\ 1.7299$$

Why it works well but not perfectly

- if L is big enough: $\left|\psi(\pm L/2) \sim \mathrm{e}^{-L/l_{\mathrm{phys}}}\right| \Rightarrow$forced periodicity is an exponentially small distortion
- for cutoff $1/a$ there is a dual argument in momentum space
- or make connection with the sampling theorem:
    - a continuous time signal with frequencies $\nu < \nu_{\mathrm{max}}$ can be reconstructed exactly from sampling at a rate $\nu_{\mathrm{Nyquist}} = \tau^{-1} = 2\nu_{\mathrm{max}}$ [44 kHz in CD players]
    - translate time $\to x$, $2\pi\nu_{\mathrm{max}} = p_{\mathrm{max}}$, sampling $\tau \to a$
    - in oscillator type states no exact p_{max}, but only exponentially small violations...

A puzzle

For any pair of finite matrices:

$$\mathrm{tr}[\hat{p},\hat{x}] = \mathrm{tr}(\hat{p}\hat{x}) - \mathrm{tr}(\hat{x}\hat{p}) = 0 \quad \text{but} \quad \mathrm{tr}\left(\frac{\hbar}{i}\right) \overbrace{=}^{?} \frac{\hbar}{i} N$$

$\Rightarrow$ no finite dim reps of Heisenberg algebra ('anomaly'), but

$$\text{partial trace } d(k) = \frac{1}{N} \sum_{n=0}^{k-1} \langle n | (1 - i(\hat{p}\hat{x} - \hat{x}\hat{p})) | n \rangle \qquad (|n\rangle \leftrightarrow \text{har. osc.})$$

$$\rightarrow \text{full trace: } d(N) = \frac{1}{N}\mathrm{tr}(1 - i(\hat{p}\hat{x} - \hat{x}\hat{p})) = \begin{cases} 0 & \text{for Heisenberg} \\ 1 & \text{for finite matrices} \end{cases}$$