Lecture 17
Example: Quantum mechanics

- wave function and Schrodinger equation
- discretization
- preservation of probability
- eigenvalues & eigenstates
- example

Quantum mechanics

- single particle in interval $[0,1]$, mass m
- potential $V : [0,1] \to \mathbf{R}$

$\Psi : [0,1] \times \mathbf{R}_+ \to \mathbf{C}$ is (complex-valued) *wave function*

interpretation: $|\Psi(x,t)|^2$ is probability density of particle at position x, time t

(so $\int_0^1 |\Psi(x,t)|^2 \, dx = 1$ for all t)

evolution of Ψ governed by *Schrodinger* equation:

$$i\hbar\dot{\Psi} = \left(V - \frac{\hbar^2}{2m}\nabla_x^2 \right) \Psi = H\Psi$$

where H is *Hamiltonian* operator, $i = \sqrt{-1}$

Discretization

let's discretize position x into N discrete points, k/N, $k = 1, \ldots, N$

wave function is approximated as *vector* $\Psi(t) \in \mathbf{C}^N$

∇_x^2 operator is approximated as *matrix*

$$\nabla^2 = N^2 \begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & & 1 & -2 \end{bmatrix}$$

so $w = \nabla^2 v$ means

$$w_k = \frac{(v_{k+1} - v_k)/(1/N) - (v_k - v_{k-1})(1/N)}{1/N}$$

(which approximates $w = \partial^2 v / \partial x^2$)

discretized Schrodinger equation is (complex) linear dynamical system

$$\dot{\Psi} = (-i/\hbar)(V - (\hbar/2m)\nabla^2)\Psi = (-i/\hbar)H\Psi$$

where V is a diagonal matrix with $V_{kk} = V(k/N)$

hence we analyze using linear dynamical system theory (with complex vectors & matrices):

$$\dot{\Psi} = (-i/\hbar)H\Psi$$

solution of Shrodinger equation: $\Psi(t) = e^{(-i/\hbar)tH}\Psi(0)$

matrix $e^{(-i/\hbar)tH}$ propogates wave function forward in time t seconds (backward if $t < 0$)

Preservation of probability

$$\begin{aligned}\frac{d}{dt}\|\Psi\|^2 &= \frac{d}{dt}\Psi^*\Psi \\ &= \dot{\Psi}^*\Psi + \Psi^*\dot{\Psi} \\ &= ((-i/\hbar)H\Psi)^*\Psi + \Psi^*((-i/\hbar)H\Psi) \\ &= (i/\hbar)\Psi^*H\Psi + (-i/\hbar)\Psi^*H\Psi \\ &= 0\end{aligned}$$

(using $H = H^T \in \mathbf{R}^{N\times N}$)

hence, $\|\Psi(t)\|^2$ is constant; our discretization preserves probability *exactly*

$U = e^{-(i/\hbar)tH}$ is *unitary*, meaning $U^*U = I$

unitary is extension of *orthogonal* for complex matrix: if $U \in \mathbf{C}^{N\times N}$ is unitary and $z \in \mathbf{C}^N$, then

$$\|Uz\|^2 = (Uz)^*(Uz) = z^*U^*Uz = z^*z = \|z\|^2$$

Eigenvalues & eigenstates

H is symmetric, so

- its eigenvalues $\lambda_1, \ldots, \lambda_N$ are real ($\lambda_1 \leq \cdots \leq \lambda_N$)
- its eigenvectors $v_1, \ldots, v_N$ can be chosen to be orthogonal (and real)

from $Hv = \lambda v \;\Leftrightarrow\; (-i/\hbar)Hv = (-i/\hbar)\lambda v$ we see:

- eigenvectors of $(-i/\hbar)H$ are same as eigenvectors of H, $i.e.$, $v_1, \ldots, v_N$
- eigenvalues of $(-i/\hbar)H$ are $(-i/\hbar)\lambda_1, \ldots, (-i/\hbar)\lambda_N$ (which are pure imaginary)

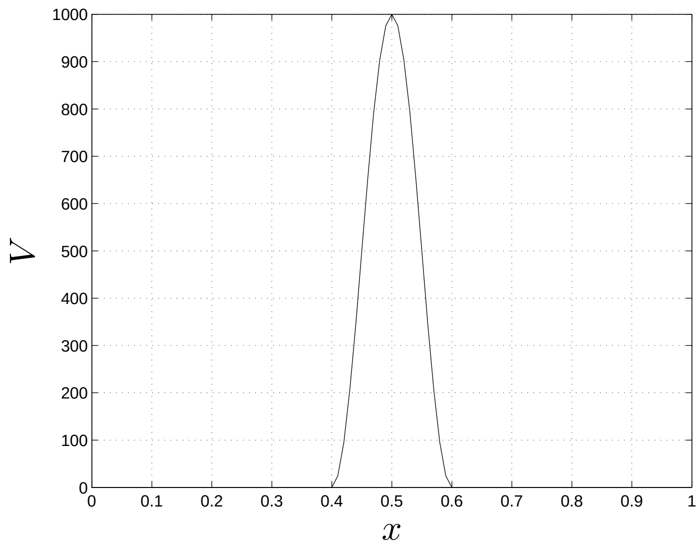
- eigenvectors v_k are called *eigenstates* of system
- eigenvalue λ_k is *energy* of eigenstate v_k
- for mode $\Psi(t) = e^{(-i/\hbar)\lambda_k t} v_k$, probability density

$$|\Psi_m(t)|^2 = \left| e^{(-i/\hbar)\lambda_k t} v_k \right|^2 = |v_{mk}|^2$$

  doesn't change with time (v_{mk} is mth entry of v_k)

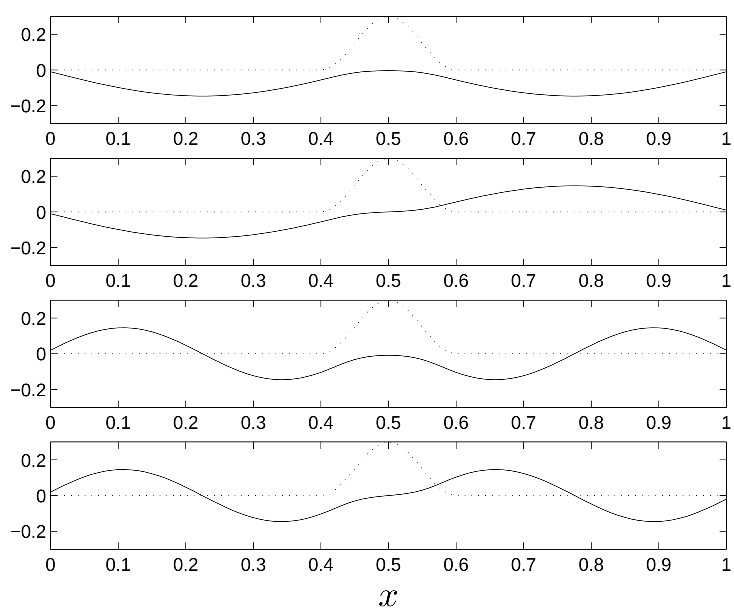
Example

Potential Function $V(x)$



- potential bump in middle of infinite potential well
- (for this example, we set $\hbar = 1$, $m = 1$ . . .)

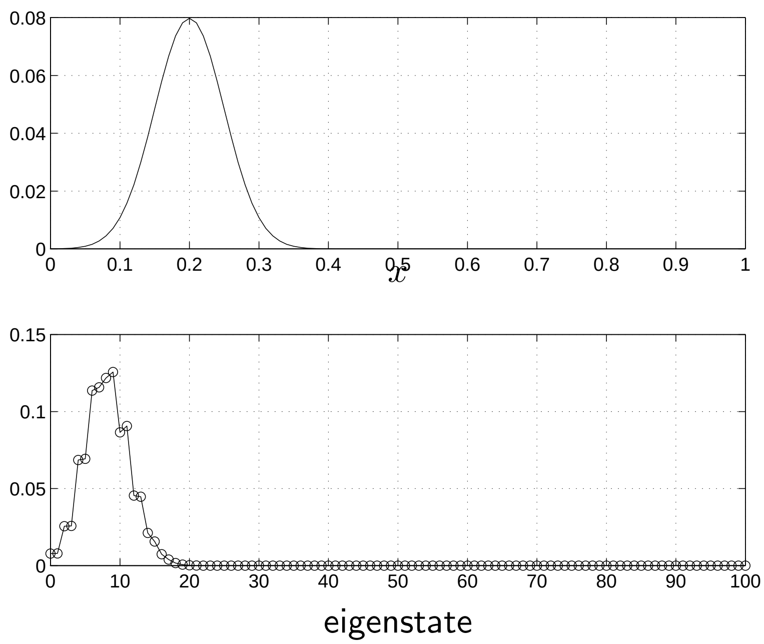
lowest energy eigenfunctions



- potential V shown as dotted line (scaled to fit plot)
- four eigenstates with lowest energy shown ($i.e.$, v_1, v_2, v_3, v_4)

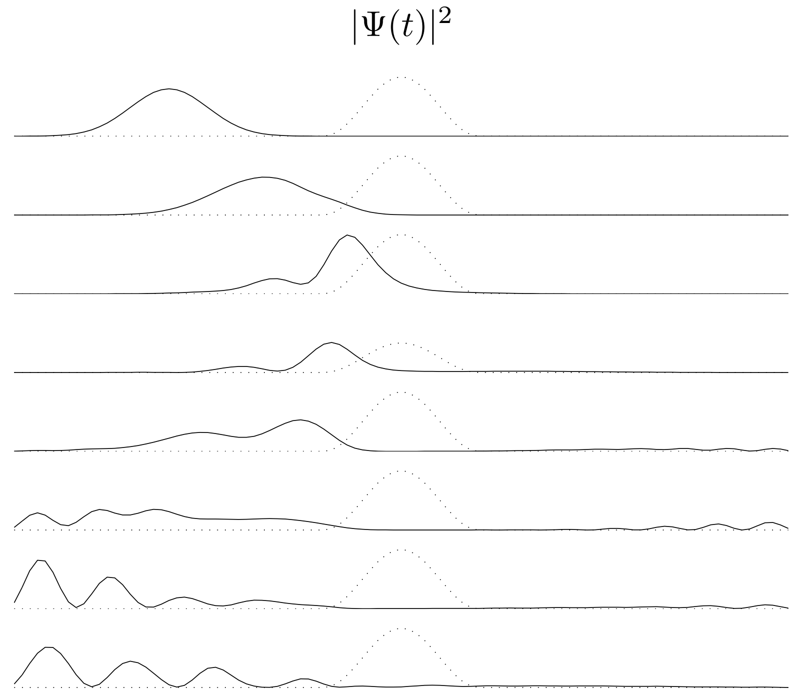
now let's look at a trajectory of Ψ, with initial wave function $\Psi(0)$

- particle near $x = 0.2$
- with momentum to right (can't see in plot of $|\Psi|^2$)
- (expected) kinetic energy half potential bump height



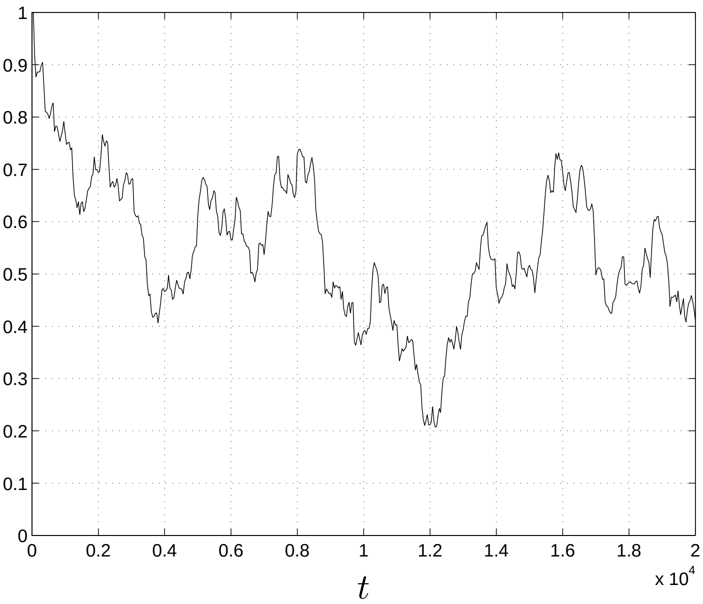
- top plot shows initial probability density $|\Psi(0)|^2$
- bottom plot shows $|v_k^*\Psi(0)|^2$, *i.e.*, resolution of $\Psi(0)$ into eigenstates

time evolution, for $t = 0, 40, 80, \ldots, 320$:



cf. classical solution:

- particle rolls half way up potential bump, stops, then rolls back down
- reverses velocity when it hits the wall at left
  (perfectly elastic collision)
- then repeats



plot shows probability that particle is in left half of well, $i.e.$, $\sum_{k=1}^{N/2} |\Psi_k(t)|^2$, versus time t