Quantum mechanics

Phys 750 Lecture 14

Route to quantum mechanics

- Basic postulate of quantum mechanics: a particle can be described by its classical Hamiltonian with the additional requirement that its conjugate variables do not commute

kinetic energy

$$H = \frac{p^2}{2m} + V(x)$$

potential energy

- Impose the commutation relation

$$[x, p] \equiv xp - px = i\hbar$$

Planck constant

Route to quantum mechanics

- The coordinates and momenta of the system are promoted from mere numbers to differential operators

$$x_{\mathrm{cl}} \to x, \quad p_{\mathrm{cl}} \to p = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

- Verify that this definition of momentum works:

$$\begin{aligned} xpF(x) &= -i\hbar x F'(x) \\ pxF(x) &= -i\hbar \frac{\partial}{\partial x}\big(xF(x)\big) \\ &= -i\hbar\big(F(x) + xF'(x)\big) \end{aligned} \quad \longrightarrow \quad [x,p]F(x) = i\hbar F(x) \quad \forall F(x)$$

Schrödinger equation

- Evolution of a single quantum particle is governed by the time-dependent Schrödinger equation (TDSE)

1st order in time

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t)$$

2nd order in space

- Describes a field $\psi(x,t)$ rather than a trajectory $x(t)$

- Takes the form of a heat equation with sources/sinks but in imaginary time:

$$\left(\frac{\partial}{\partial(it)} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\psi = 0$$

Wavefunction

- $\psi(x,t)$ is complex-valued and represents the “probability amplitude” of a particle in space and time
- The conventional probability distribution $\sim |\psi(x,t)|^2$ must be (at all times) normalizable:

$$\int dx\, |\psi(x,t)|^2 = 1$$

- Despite the probabilistic interpretation, the evolution of the wavefunction is completely deterministic

Time evolution

- TDSE is a PDE of the form $i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t)$

quantum Hamiltonian

- Has a formal solution

$$\psi(x,t_2) = e^{-i(t_2-t_1)\hat{H}/\hbar}\psi(x,t_1) = \hat{U}(t_2,t_1)\psi(x,t_1)$$

evolution operator

- Evolution is unitary

$$\hat{U}^\dagger\hat{U} = \hat{U}\hat{U}^\dagger = \hat{1}$$

$$\hat{U}^{-1} = \hat{U}^\dagger$$

and hence time-reversible and norm-preserving

Energy eigenstates

- Analogue of classical “normal modes” (Fourier transformed in time) are the energy eigenstates
- Substitution of $\psi(x,t) = \psi_E(x)e^{-iEt/\hbar}$ into

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t)$$

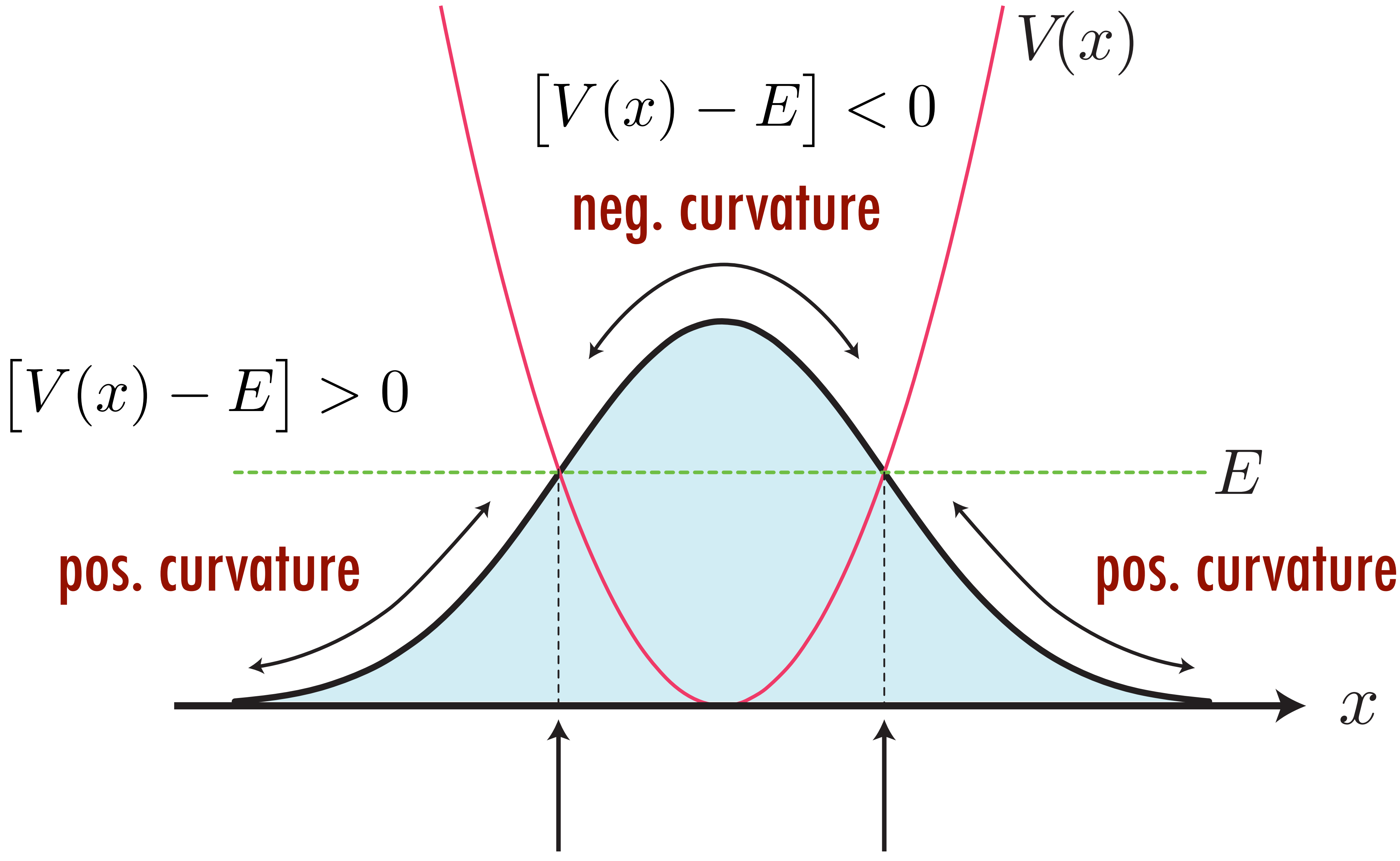
yields the time-independent Schrödinger equation

$$E\psi_E(x) = -\frac{\hbar^2}{2m}\psi_E''(x) + V(x)\psi_E(x)$$

Energy eigenstates

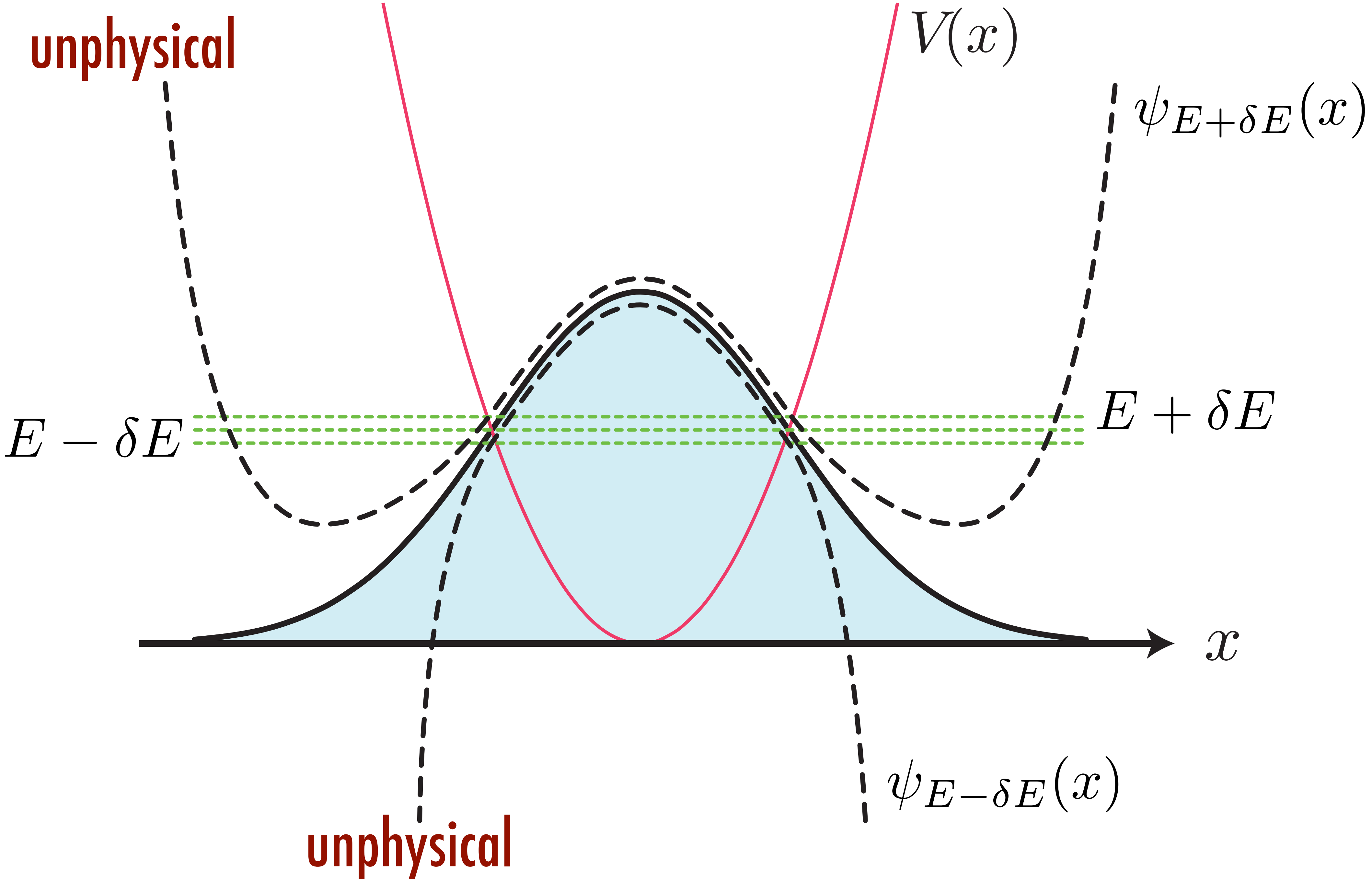
- Rewrite as $\nabla^2 \psi_E(x) = \frac{2m}{\hbar^2}\left[V(x) - E\right]\psi_E(x)$
- Reminiscent of the Poisson equation (cf. $\nabla^2 \phi = \rho$), but with a complicated source term:
  - sign of $V(x) - E$ (the curvature) is spatially varying
  - proportional to the wavefunction itself (which amounts to an additional self-consistency condition)

Energy eigenstates



classical turning points

Energy eigenstates



Energy eigenstates

- The eigenfunctions must be solved in conjunction with appropriate boundary conditions and/or asymptotic behaviour; e.g.,

  $|V\psi| < \infty$ requires that $\psi \to 0$ wherever $V \to \infty$

- "Quantization" arises when only discrete values of E lead to normalizable solutions

- Spectrum of eigenergies is generally discrete when the particle is contained and continuous otherwise

Spectral decomposition

- Energy eigenstates $\{\phi_n(x)\}$ form a complete basis
- Orthonormal with respect to overlaps (L^2 inner products)

$$\langle \phi_n | \phi_{n'} \rangle = \int dx \, \phi_n(x)^* \phi_{n'}(x) = \delta_{n,n'}$$

$$\sum_n \phi_n(x)^* \phi_n(x') = \delta(x - x')$$

- Any valid wave function can be expanded in this basis

Spectral decomposition

- Snapshot at time $t = 0$:

$$\psi(x,0) = \sum_n c_n \phi_n(x)$$

- Characterized by components along each basis function

$$c_n = \langle \phi_n | \psi(t=0) \rangle = \int dx\, \phi_n(x)^* \psi(x,0)$$

Spectral decomposition

- Since, $\hat{H}\phi_n = E_n\phi_n$ the complete time evolution enters as an additional set of phase factors

$$\begin{aligned}\phi(x,t) &= e^{-it\hat{H}/\hbar}\sum_n c_n\phi_n(x)\\ &= \sum_n c_n e^{-itE_n/\hbar}\phi_n(x)\end{aligned}$$

- Introducing an upper cutoff to the summation discards physics on time scales shorter than $\Delta t \lesssim \frac{\hbar}{E_{\text{cutoff}}}$