PHYS-454

The Quantum Harmonic Oscillator

The simple harmonic motion

- The SHM is produced when the particle moves on a straight line around an equilibrium point and the **resultant** force on it is given by:

$$F = -Dx$$

- Here with x we denote the displacement from the equilibrium position. D is called restoring constant (unit: N/m).
- The force given above is a **conservative force**. The minus sign indicates that the force always tends to restore the particle to its equilibrium position. To this **restoring force** we associate the following potential:

$$U = \frac{1}{2} D x^2$$

- The two formulae above satisfy the well-known relation:

$$F = -\frac{dU}{dx}$$

Why SHM is important-a?

- Consider a single dimensional potential V(x) with a minimum, or stable equilibrium point, say at x=0. Following a Taylor expansion around x=0 we get:

$$V(x) = V(0) + V'(0)x + \frac{1}{2}V''(0)x^2 + ...$$

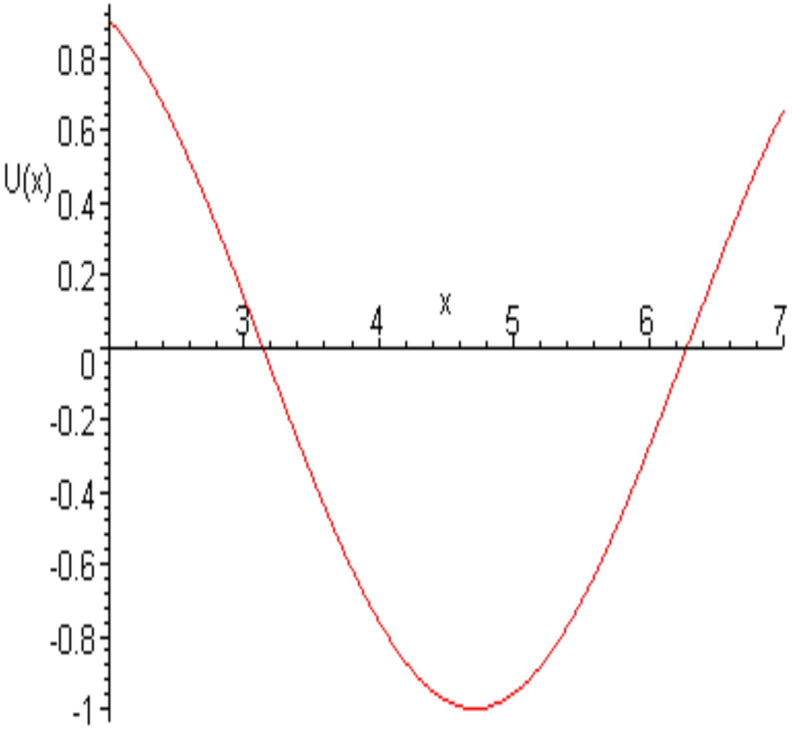
- Since x=0 is a minimum we have:

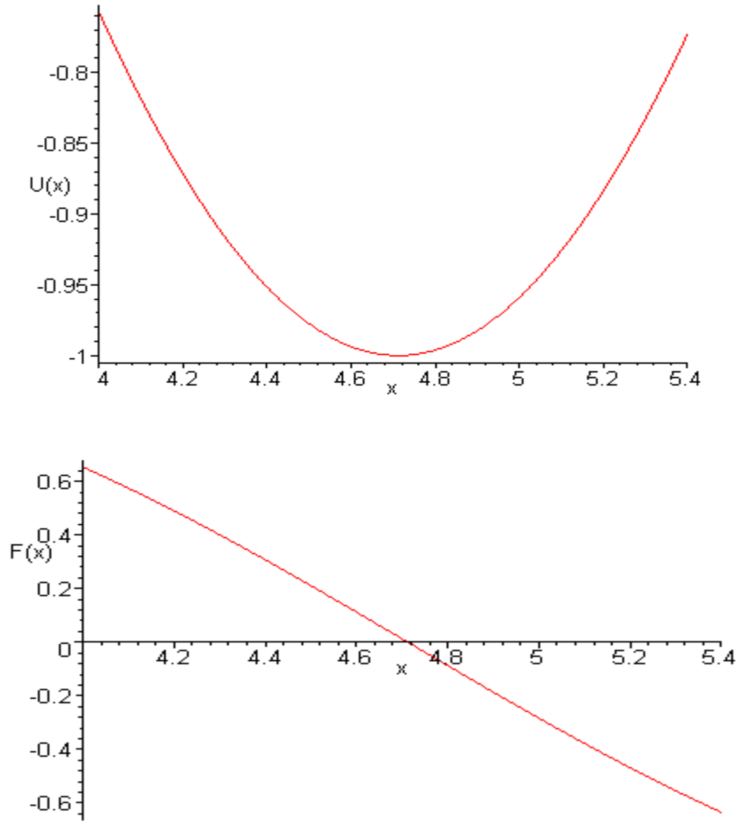
$$V'(0) = 0 \qquad V''(0) = D > 0$$

- Then $V(x) - V(0) = \frac{1}{2}Dx^2$

- Any potential around a stable equilibrium point can be approximated by a simple harmonic oscillator

Why SHM is important-b?





The quantum mechanical SHO-a

- **The quantum mechanical Hamiltonian of a simple harmonic oscillator gets the form:**

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 \equiv \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

$$x \to x, \quad p \to -i\hbar \frac{d}{dx}$$

$$H \to -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

The quantum mechanical SHO -b

- We can show that the Schrödinger eq. takes the form:

$$\psi'' + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}m\omega^2 x^2\right)\psi = 0$$

- By introducing the dimensionless parameters:

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x, \qquad K \equiv \frac{2E}{\hbar\omega}$$

- We get

$$\frac{d^2\psi}{d\xi^2} = \left(\xi^2 - K\right)\psi$$

The quantum mechanical SHO -c

- Solving the above differential eq. we can get the eigenfunctions and eigenvalues of the s.h.o. Hamiltonian:

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2} \qquad E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

- Where the functions $H_n(\xi)$ are the so called **Hermite polynomials**. Some of them are given below

Hermite polynomials -properties

$$H_0 = 1$$
$$H_1 = 2\xi$$
$$H_2 = 4\xi^2 - 2$$
$$H_3 = 8\xi^3 - 12\xi$$
$$H_4 = 16\xi^4 - 48\xi^2 + 12$$
$$H_5 = 32\xi^5 - 160\xi^3 + 120\xi$$

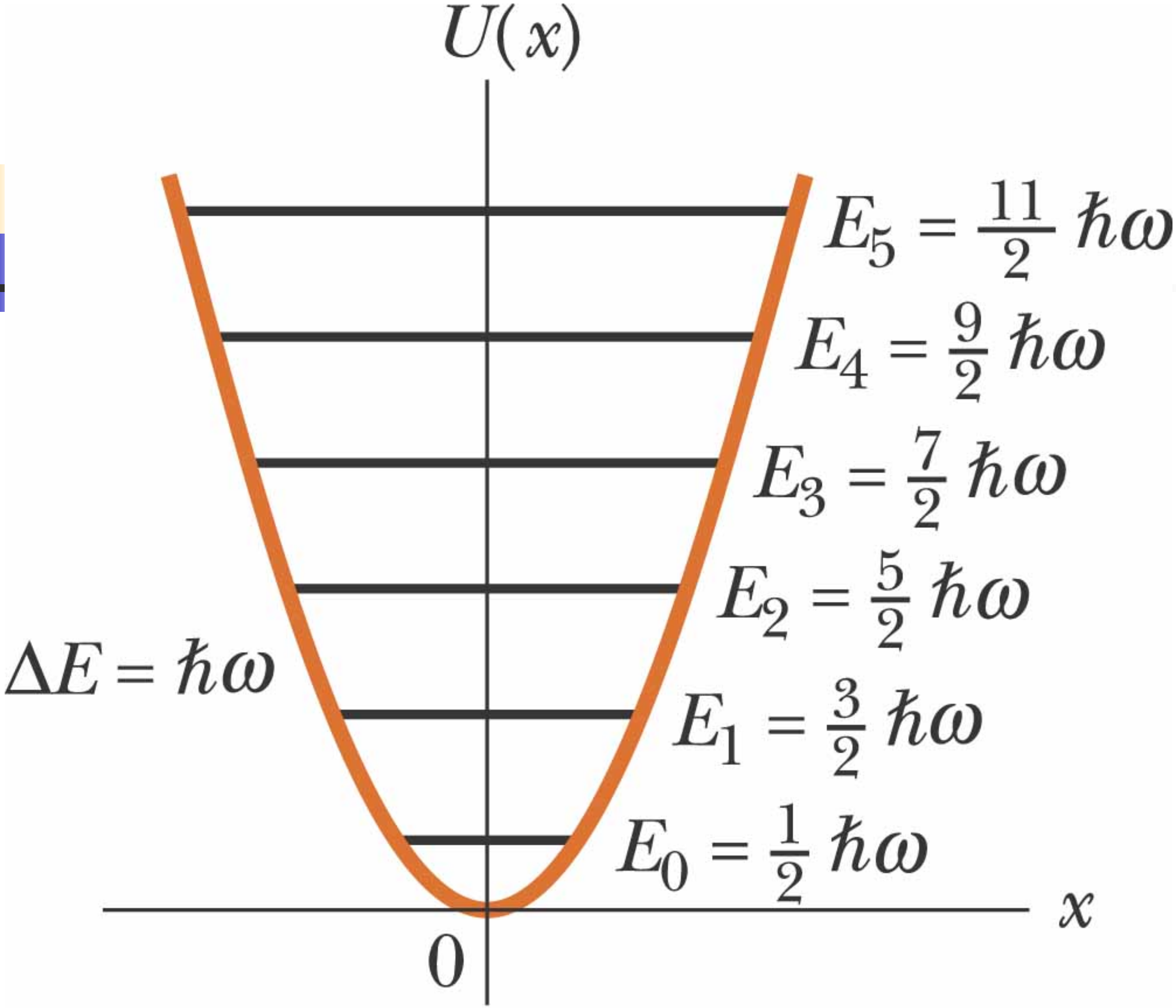
$$H_n(\xi) = (-1)^n e^{\xi^2} \left(\frac{d}{d\xi}\right)^n e^{-\xi^2}$$

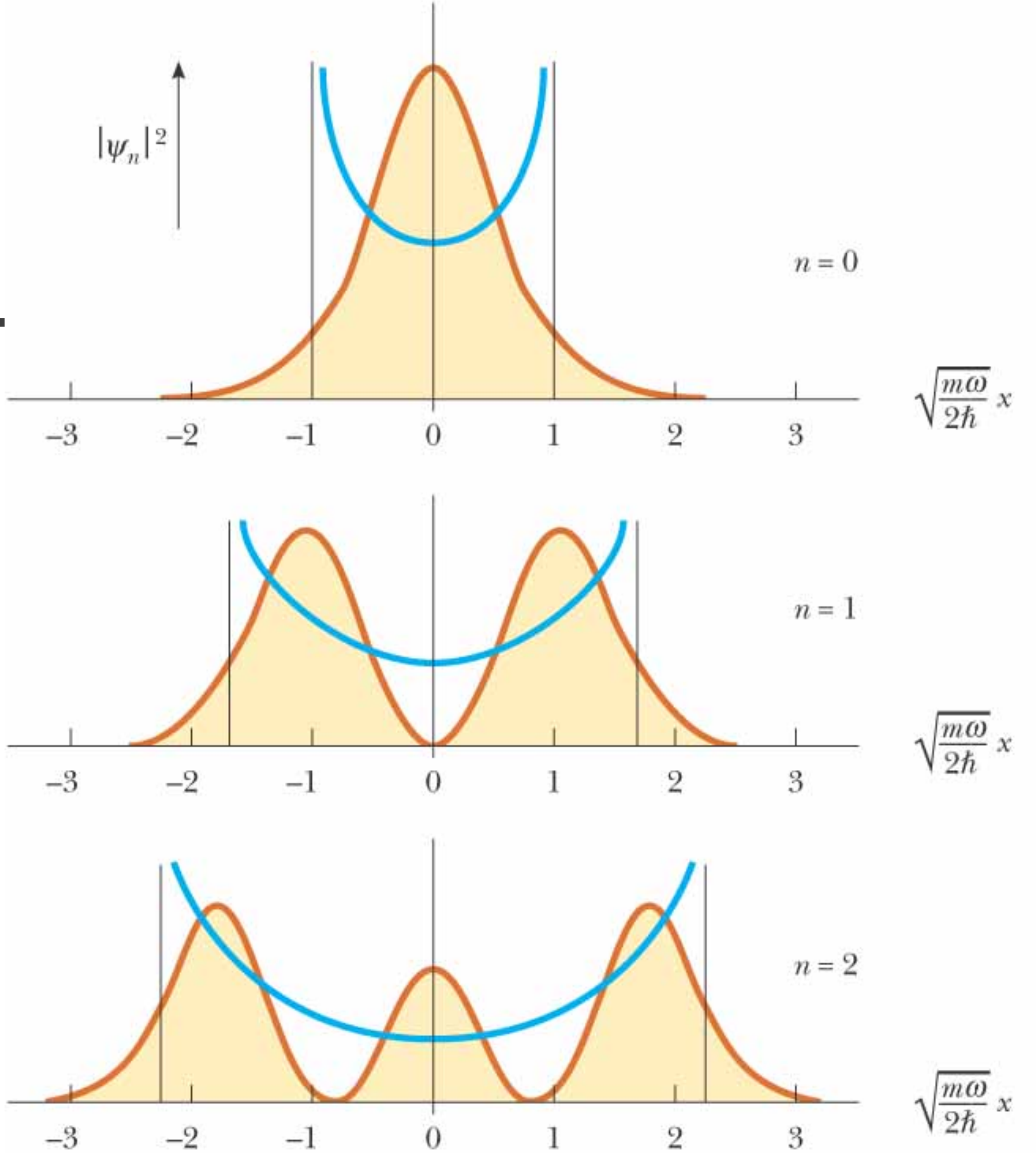
$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2nH_{n-1}(\xi)$$

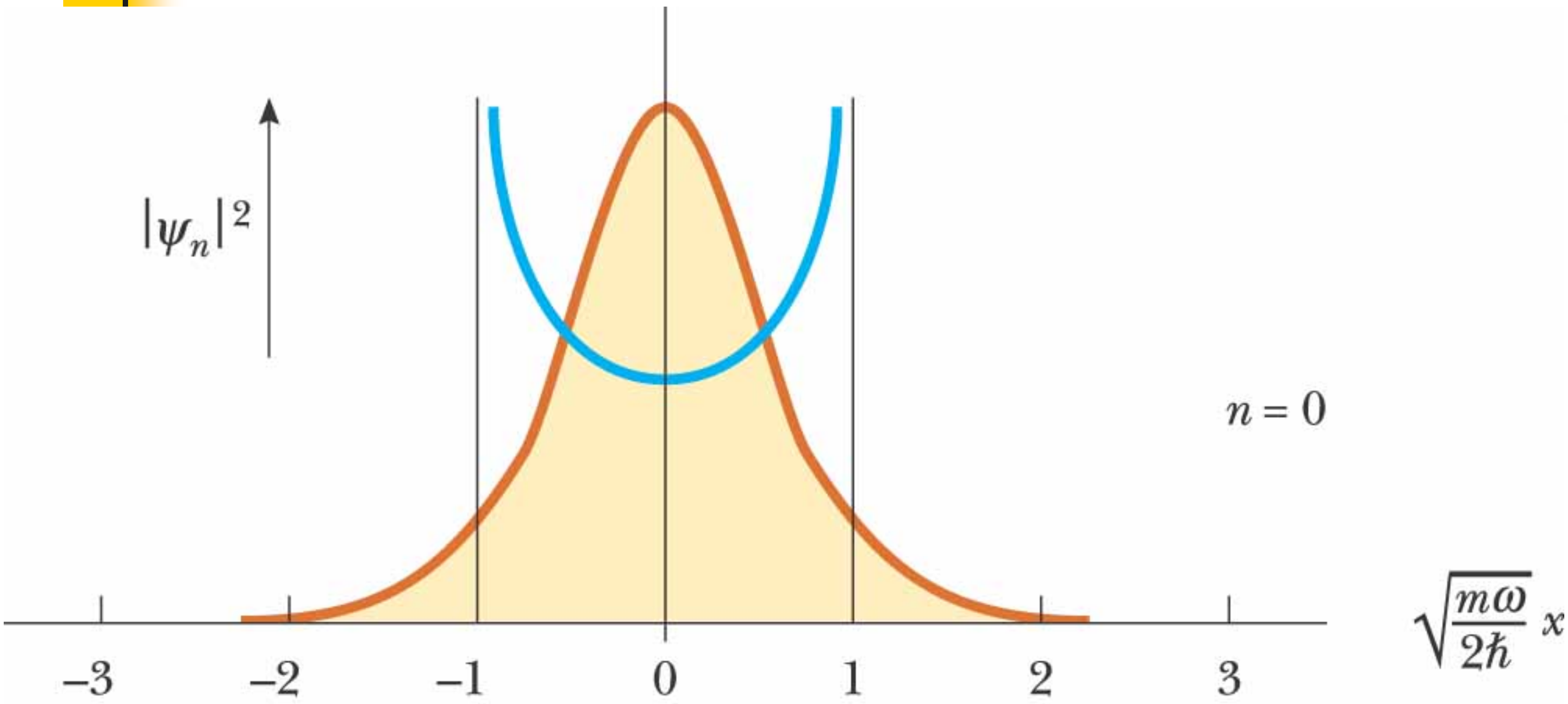
$$\frac{dH_n}{d\xi} = 2nH_{n-1}(\xi)$$

$$H_n(x) = \sum_{s=0}^{[n/2]} (-1)^s (2x)^{n-2s} \frac{n!}{(n-2s)!s!}$$

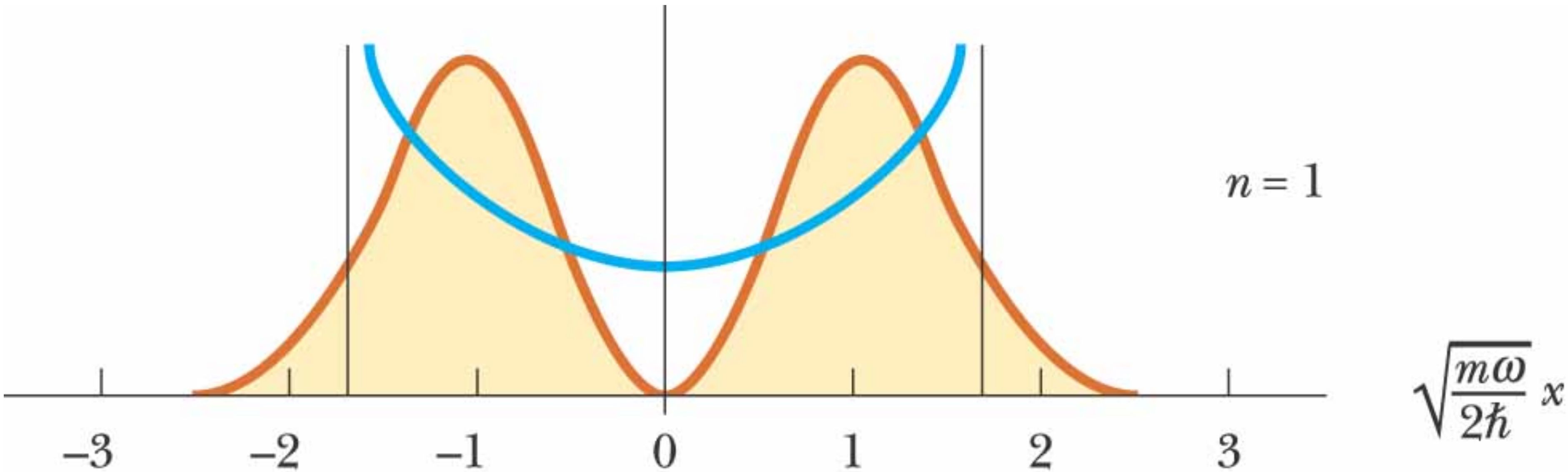
$$\int_{-\infty}^{\infty} H_m(x) H_n(x) e^{-x^2/2} dx = 0$$


U(x)
E5 = 11/2 ħω
E4 = 9/2 ħω
E3 = 7/2 ħω
E2 = 5/2 ħω
ΔE = ħω
E1 = 3/2 ħω
E0 = 1/2 ħω
x
0


$|\psi_n|^2$
$n = 0$
$n = 1$
$n = 2$
$\sqrt{\frac{m\omega}{2\hbar}}\,x$
–3
–2
–1
0
1
2
3



$|\psi_n|^2$
$n = 0$
$\sqrt{\frac{m\omega}{2\hbar}}\,x$
–3
–2
–1
0
1
2
3



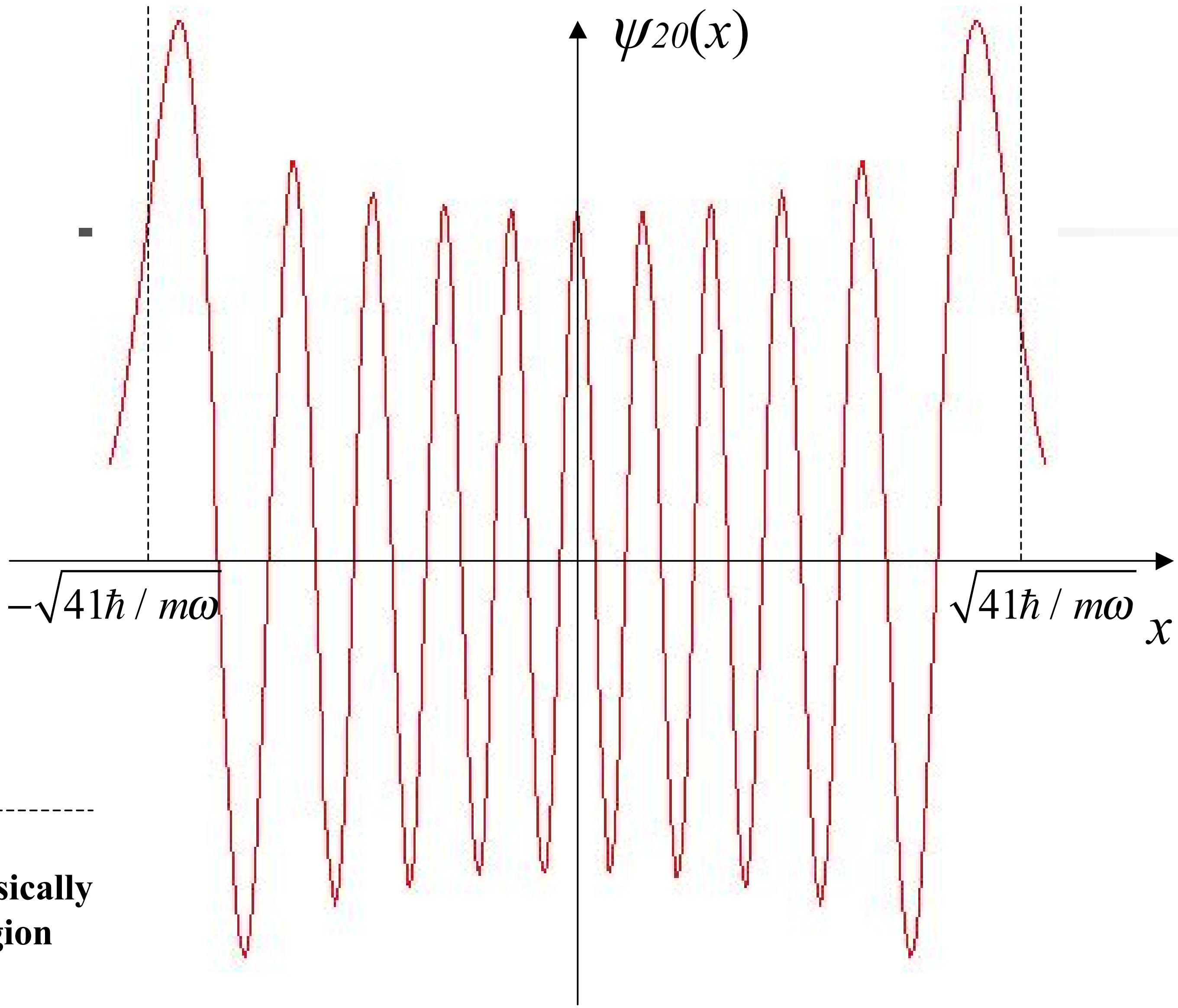
n = 1
−3
−2
−1
0
1
2
3
$\sqrt{\frac{m\omega}{2\hbar}}\,x$

Discussion-a
The shape of the wave functions

- The wave functions are alternatively even and odd due to the symmetry of the potential.
- The number of nodes of the wavefunction ψ_n is equal to n.
- The eigenfuctions do not terminate in the classically allowed region.

Discussion -b
Behavior for large n

- As *n* becomes higher the quantum wave function must reproduce the classical behavior.
- Classically the particle “spends” more of its time at regions where the velocity is small. That is, near the extreme points of the oscillation.



Limits of classically allowed region

Discussion -c
Penetration in the forbidden region

State	Probability
n=0	15.7%
n=1	11.2%
n=2	9.5%
n=3	8.5%
n=4	7.9%

State	Probability
n=5	7.4%
n=6	7.0%
n=7	6.7%
n=8	6.4%
n=9	6.2%

Discussion -c
Penetration in the forbidden region

- As we expect the probability of penetration in the forbidden region becomes smaller and smaller as n gets larger. The particle behaves more classically as we go to higher levels.
- The probabilities do not depend on the mass, Planck's constant or ω.

Discussion-d
Radiation emitted by a quantum SHO

- The fact that the energy eigenvalues are equidistant is a characteristic of the parabolic potential.
- In a classical SHO the period (and frequency) does not depend on amplitude. So if the particle is charged it will irradiate with this given frequency.
- In a quantum SHO this imposes that the only transitions that can occur are those for which Δn=1.