MATH4104: Quantum nonlinear dynamics. Lecture Three. Review of quantum theory.

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Quantum mechanics with particles.

A free particle is one that is not acted on by a force. In one dimension Newtonian physics gives the position as a function of time as

$$x(t) = x_0 + p_0 t/m$$

where x_0, p_0 are initial position and momentum.

The kinetic energy, depends only on momentum

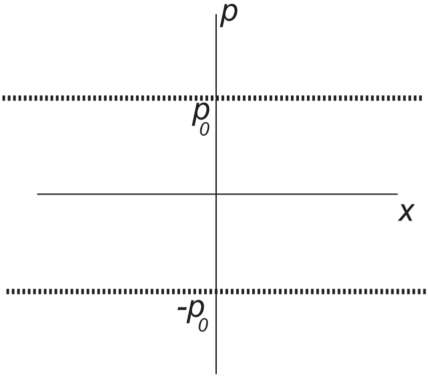
$$E = \frac{p_0^2}{2m}$$

is a constant of the motion

Note: $\pm p_0$ have the same energy.

Quantum mechanics with particles.

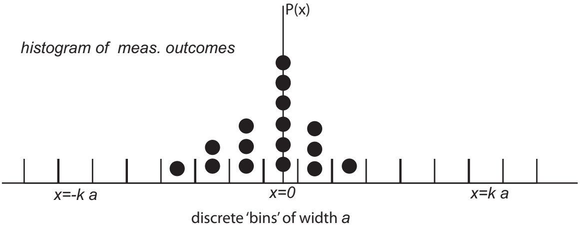
A phase-space picture for free particles of definite energy, E.
A *distribution* of states, all with the same energy,



Note, the position distribution is *uniform*.

Quantum mechanics with particles.

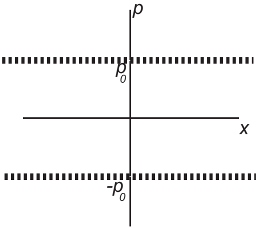
How to describe position measurements?

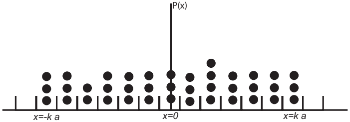


Plot a histograms of number of measurement results that lie in k-th bin.

Can make bin size — a — arbitrarily small.

Classical position distribution for states of definite energy.

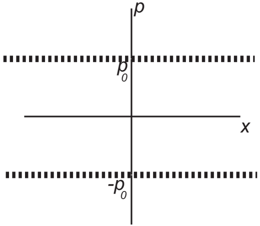




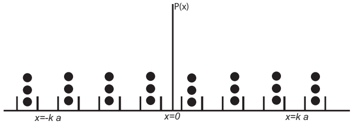
The distribution is uniform (within experimental sampling error).

Quantum position distribution for states of definite energy.

classical phase-space picture



quantum position distribution



The distribution is *oscillatory*.
There are some bins where the particle is *never* seen.

Quantum position distribution for states of definite energy.

Explanation: there are *two* indistinguishable ways to find a particle with definite energy at the $k-$th bin:

- in k and travelling with *positive* momentum and
- in k and travelling with negative momentum.

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$$\begin{aligned} P(k) &= |\mathcal{A}(k : +p_0) + \mathcal{A}(k : -p_0)|^2 \\ &= |\mathcal{A}(k : +p_0)|^2 + |\mathcal{A}(k : -p_0)|^2 + 2\mathrm{Re}\left[\mathcal{A}(k : +p_0)\mathcal{A}(k : -p_0)^*\right] \end{aligned}$$

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The last term is not always positive, so can cancel the first two terms... interference.

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$$\mathcal{A}(n:+p_0) = \frac{1}{\sqrt{N}} e^{-2\pi i n a p_0/h}$$

N is total number of bins and h is Planck's constant.

Note: ap_0 has units of action.

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In continuum limit: $na \to x$

$$\mathcal{A}(x : +p_0) = \frac{1}{\sqrt{N}} e^{-i x p_0 / \hbar}$$

$\hbar = h/2\pi$

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Schrödinger's method for finding the position probability amplitude for states of definite *momentum*.

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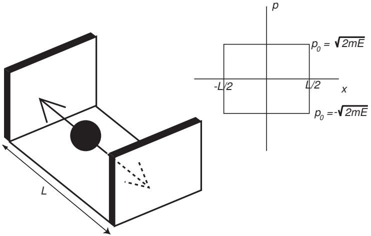
In this case: $\psi(x) \propto e^{-ixp/\hbar}$

Example: particle in a box.

An oscillator, but period depends on energy and motion is not harmonic.



The period,

$$T(E) = \frac{2mL}{p} = L\sqrt{\frac{2m}{E}}$$

The area is given by $2L\sqrt{2mE}$,

$$E_n = \frac{n^2 h^2}{8mL^2}$$

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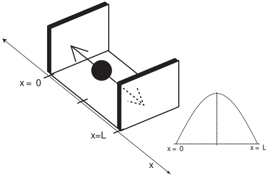

Probability to find particle outside the box is *zero*.

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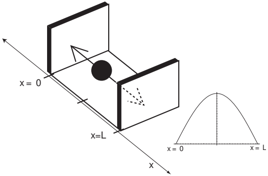

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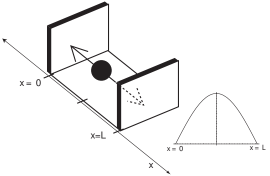

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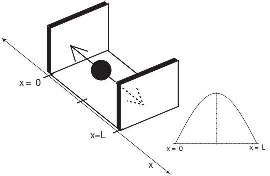

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The minimum allowed energy is $E_{min} = \frac{1}{2m}(p_0)^2_{min} = \frac{h^2}{8mL^2}$

Example: particle in a box.

In general, the allowed momenta are: $\pm\frac{nh}{2L}$.

and allowed energies

$$E_n = \frac{n^2 h^2}{8mL^2} = \frac{n^2 \hbar^2 \pi^2}{2mL^2}$$

and corresponding position probability amplitudes are

$$u_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

Example: simple harmonic oscillator.

Simple harmonic oscillator: period is independent of energy.

$$x(t) = x_0 \cos(2\pi t/T)$$

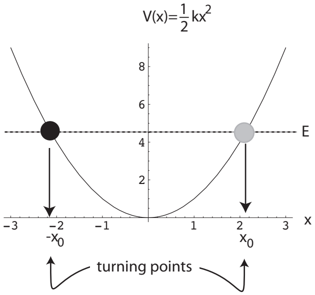
where T is the period of the motion.

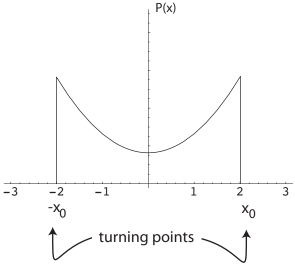
Surfaces of constant energy:

$$E = \frac{p^2}{2m} + \frac{k}{2}x^2 \tag{1}$$

Example: simple harmonic oscillator.

Classical position prob. distribution for a state of definite energy.





Example: simple harmonic oscillator.

Quantum SHO.
Fix energy, then

$$p(x) = \sqrt{2m\left(E - \frac{m\omega^2 x^2}{2}\right)}$$

The momentum is *not fixed*.

Schorödinger equation is required.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{m\omega^2}{2}\, x^2\psi(x) = E\psi(x)$$

In the form $\hat{H}\psi(x) = E\psi(x)$ where formally replace p in Hamiltonian by

$$p \rightarrow \hat{p} = -i\hbar\frac{d}{dx}$$

Example: simple harmonic oscillator.

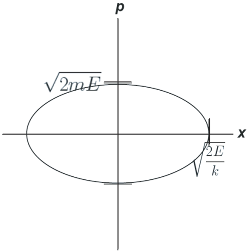
Solution to Schrödinger equation requires restriction on the energy,

$$E_n = \hbar\omega(n + \frac{1}{2}) \qquad n = 0, 1, 2 \ldots$$

the position measurement probability amplitudes are then

$$\psi_n(x) = (2\pi\Delta)^{-1/4} \left(2^n n!\right)^{-1/2} H_n\left(\frac{x}{\sqrt{2\Delta}}\right) e^{-\frac{x^2}{4\Delta}}$$

Quantisation of Sommerfeld-Epstein.



Area of the orbit is $E.T$

Sommerfeld's rule: only those orbits are allowed for which the action is an integer multiple of Planck's constant. The allowed energies are given by

$$E_n = nhf$$

Example: simple harmonic oscillator.

Check some averages

$$P_n(x) = |\psi_n(x)|^2$$

- $\int_{-\infty}^{\infty} dx \; P_n(x) = 1$
- $\int_{-\infty}^{\infty} dx \; x P_n(x) = 0$
- $\int_{-\infty}^{\infty} dx \; x^2 P_n(x) = \Delta(2n+1)$

Prove these results!

Probability for momentum measurements.

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If find a particle between x and $x + dx$, we have *no knowledge* of its momentum

By Feynman's rule, we need to sum over all states of definite momentum which correspond to finding the particle between x and $x + dx$:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp \; \phi(p) e^{-ixp/\hbar}$$

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Momentum probability density is: $P(p) = |\phi(p)|^2$.