

Examples of Bohr-Sommerfeld quantization.

Usual rule:

$$\text{Area} = \oint p dx = (n + \frac{1}{2})(2\pi\hbar).$$

Area of orbit in phase space. This comes from idea that as particle moves in its orbit, it accumulates a phase of $\frac{1}{\hbar} \oint p dx$, but it loses $\pi/2$ phase when passing through turning points. So, if there are 2 turning points, then the total phase accumulated on a single orbit is

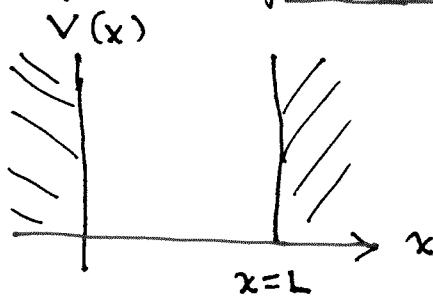
$$\frac{1}{\hbar} \oint p dx - 2\left(\frac{\pi}{2}\right) = 2n\pi$$

which must be an integer multiple of 2π , as indicated. This is the same as the B-S rule above.

(Example of harmonic oscillator done in notes.)

If the wall the particle bounces off is hard, then the phase shift is $-\pi$ at each bounce, instead of $-\pi/2$. That's because $e^{-i\pi} = -1$, so the reflected wave cancels the incident wave at the wall, where boundary conditions require $\psi = 0$.

For example, the ^{1D} particle in a box,

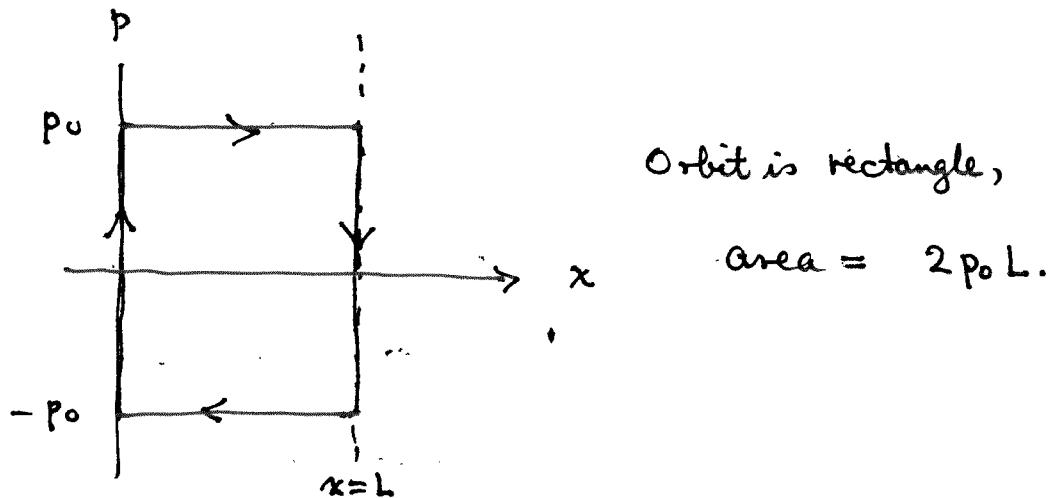


classical

2 hard walls, particle bounces back and forth with momentum p_0 (say) energy $E = p_0^2/2m$.

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Orbit in phase space:



Orbit is rectangle,

$$\text{Area} = 2p_0 L.$$

Quantization condition,

$$\frac{1}{\hbar} \oint p dx - 2(\pi) = 2n\pi,$$

\uparrow
not $\pi/2$, 2 hard walls

or

$$\text{Area} = \oint p dx = (n+1)(2\pi\hbar).$$

$$= 2p_0 L,$$

or

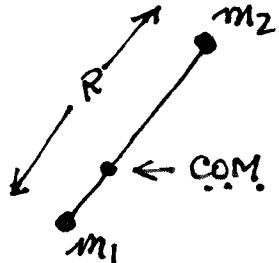
$$p_0 = \frac{(n+1)\pi\hbar}{L}, \quad E = \frac{p_0^2}{2m} = \frac{(n+1)^2 \pi^2 \hbar^2}{2m L^2}.$$

The exact answer, with $n=0, 1, 2, \dots$

$$n+1 = 1, 2, 3, \dots$$

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Another example, the rigid rotor: First we do it classically. Two masses m_1, m_2 are connected by a massless rod of length R .



Reduced mass μ ,

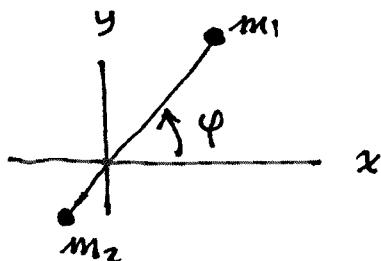
$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

Moment of inertia

$$I = \mu R^2.$$

This is a model of a diatomic molecule.

Rotor rotates about its center of mass in the x-y plane (let's say), with angle φ :



The Lagrangian is just the kinetic energy:

$$L = \frac{1}{2} I \dot{\varphi}^2$$

The momentum conjugate to the angle φ is actually the angular momentum, or, rather, its z-component:

$$p_\varphi = \frac{\partial L}{\partial \dot{\varphi}} = I \dot{\varphi} = L_z.$$

The Hamiltonian is

$$H = p_\varphi \dot{\varphi} - L = \frac{L_z^2}{2I}.$$

This is the classical Hamiltonian. What should the Schrödinger equation be? If we had a Cartesian coordinate x , then we can quantize a classical Hamiltonian $H(x, p)$ by making the replacements, $x \rightarrow$ multiplication by x , $p \rightarrow -i\frac{d}{dx}$. These operators act on wave functions $\psi(x)$. This is called Dirac quantization. We guess we can do the same thing for an angular coordinate like φ . Then $\varphi \rightarrow$ multiplication by φ , $L_z \rightarrow -i\hbar \frac{d}{d\varphi}$ when acting on wave functions $\psi(\varphi)$. Also, since φ is a periodic coordinate, we require

$$\psi(\varphi + 2\pi) = \psi(\varphi).$$

Then if $H = \frac{L_z^2}{2I}$, the Schrödinger equation is

$$-\frac{\hbar^2}{2I} \frac{d^2\psi}{d\varphi^2} = E \psi(\varphi).$$

The normalized solutions are

$$\psi_m(\varphi) = \frac{e^{im\varphi}}{\sqrt{2\pi}}, \quad m=0, \pm 1, \pm 2, \dots$$

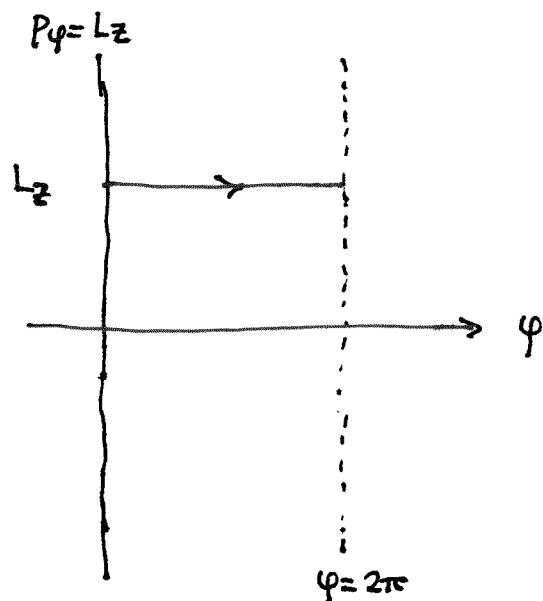
with energies,

$$E_m = \frac{\hbar^2 m^2}{2I}.$$

These are also eigenfunctions of L_z , with eigenvalues

$$L_z = m\hbar.$$

To apply the B-S rules we must look at the orbits in phase space.



The orbits are straight lines at const. L_z . They look something like the orbits of the particle in the box, but they don't bounce since there is no hard wall. There is no soft wall, either; the particle just continues forever with the same $\dot{\varphi}$. Since φ is periodic, the actual motion is a circle. The quantization condition must be

$$\frac{1}{\hbar} \oint L_z d\varphi - 0 = 2m\pi$$

↑ no turning points,

or, Area under curve = $2m\pi\hbar$. This is

$$2\pi L_z = 2m\pi\hbar,$$

or

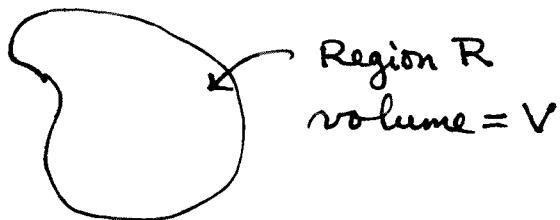
$$L_z = m\hbar,$$

$$E = \frac{L_z^2}{2I} = \frac{m^2\hbar^2}{2I}.$$

The exact answers.

A Planck cell has an area of $2\pi\hbar$ in one-dimensional systems. In higher dimensions it has a volume of $(2\pi\hbar)^n$ in phase space, where n is the number of coordinates in configuration space. The dimension of phase space is $2n$.

Consider, for example, a free particle confined to some region R of 3-dimensional space.



Let $N(E_0)$ = number of energy eigenstates with energy $\leq E_0$. Then by counting Planck cells we have the estimate,

$$N(E_0) = \frac{1}{(2\pi\hbar)^3} \int d^3\vec{x} d^3\vec{p}$$

$H(\vec{x}, \vec{p}) \leq E_0.$

The integral is over a 6-dimensional region of phase space, but it is easy because $H = \frac{\vec{p}^2}{2m}$. Thus:

$$\int_{H \leq E_0} d^3\vec{x} d^3\vec{p} = \int_R d^3\vec{x} \int_{|\vec{p}| \leq p_0} d^3\vec{p} \quad \text{where } p_0 = \sqrt{2mE_0}.$$

But $\int_R d^3\vec{x} = V$

$$\int d^3\vec{p} = \frac{4}{3}\pi p_0^3 = \frac{4}{3}\pi (2mE_0)^{3/2}.$$

$|\vec{p}| \leq p_0$

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Thus,

$$N(E) = \frac{V}{(2\pi\hbar)^3} \frac{4}{3}\pi (2mE)^{3/2}.$$

This is an asymptotic estimate for $N(E)$. It does not take into account any phase shifts at turning points because when E (or N) is large these won't matter. If the particle has spin we should multiply this by 2^{s+1}.

By differentiating we get the density of states:

$$\frac{dN}{dE} = \frac{V}{(2\pi\hbar)^3} 4\pi m \sqrt{2mE}$$

When people talk about the "density of states" they usually mean the number of energy eigenstates per unit ~~per~~ energy interval. But if we ask for the number per unit volume in phase space, the answer is $\frac{1}{(2\pi\hbar)^3}$, independent of the Hamiltonian.