Quantum Harmonic Oscillator

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Quantisation paradigms

- **First quantisation:** particles are described by wave-functions obeying the Schrödinger equation.
- **Second quantisation:** fields are quantised; particles appear as excitations of the fields.

Classical system: a particle of mass m attached to a spring of constant k.

$$p = m\dot{x}, \qquad E = \frac{p^2}{2m} + \frac{1}{2}kx^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \quad \omega \equiv \sqrt{\frac{k}{m}}.$$

Quantisation: promote

$$x \to \hat{x} = x, \qquad p \to \hat{p} = -\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}x},$$

leading to the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2} m\omega^2 x^2 \right) \psi(x) = E\, \psi(x).$$

Solutions

Define the dimensionless variable

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}}\, x.$$

The normalised eigenfunctions are

$$\psi_n(\xi) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} H_n(\xi)\, \mathrm{e}^{-\xi^2/2}, \qquad n = 0, 1, 2, \ldots$$

where H_n are the Hermite polynomials and the energies are

$$E_n = \hbar\omega \left(n + \frac{1}{2}\right).$$

The ground-state energy is non-zero:

$$E_0 = \frac{1}{2}\hbar\omega \quad \text{(zero-point energy)}.$$

Classical expectation: minimum at $x = 0$, $p = 0$ gives $E = 0$.

Why is the ground-state energy non-zero?

Heisenberg uncertainty:

$$\Delta x \, \Delta p \geq \frac{\hbar}{2}.$$

Estimate the energy in terms of typical fluctuations:

$$E \sim \frac{(\Delta p)^2}{2m} + \frac{1}{2} m\omega^2 (\Delta x)^2.$$

Using the saturated bound $\Delta p \sim \hbar/(2\Delta x)$:

$$E(\Delta x) \sim \frac{\hbar^2}{8m(\Delta x)^2} + \frac{1}{2} m\omega^2 (\Delta x)^2.$$

Minimization and zero-point energy

Minimize

$$E(\Delta x) = \frac{\hbar^2}{8m(\Delta x)^2} + \frac{1}{2}m\omega^2(\Delta x)^2.$$

Let $u = (\Delta x)^2$. Then

$$E(u) = \frac{\hbar^2}{8m}\frac{1}{u} + \frac{1}{2}m\omega^2 u, \qquad \frac{\mathrm{d}E}{\mathrm{d}u} = -\frac{\hbar^2}{8m}\frac{1}{u^2} + \frac{1}{2}m\omega^2 = 0.$$

Hence

$$(\Delta x)^2 = u = \frac{\hbar}{2m\omega},$$

and the minimum energy is

$$E_{\min} = \frac{1}{2}\hbar\omega.$$

Interpretation: the ground state has irreducible quantum fluctuations (zero-point motion).

Ladder operators

The Hamiltonian operator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2, \qquad [\hat{x}, \hat{p}] = \mathrm{i}\hbar.$$

Define annihilation and creation operators

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{\mathrm{i}}{m\omega} \hat{p} \right), \qquad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{\mathrm{i}}{m\omega} \hat{p} \right),$$

which satisfy

$$[\hat{a}, \hat{a}^\dagger] = 1.$$

Inverse relations and Hamiltonian

Invert the definitions:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right), \qquad \hat{p} = -\mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a} - \hat{a}^\dagger\right).$$

Define the number operator

$$\hat{n} \equiv \hat{a}^\dagger \hat{a}.$$

Then the Hamiltonian becomes

$$\hat{H} = \hbar\omega\left(\hat{n} + \frac{1}{2}\right).$$

If $|n\rangle$ is an eigenstate of $\hat{n}$ with eigenvalue $n \geq 0$, then

$$\hat{H}\,|n\rangle = E_n\,|n\rangle, \qquad E_n = \hbar\omega\left(n + \frac{1}{2}\right).$$

Action of ladder operators

Let $\hat{n}\,|n\rangle = n\,|n\rangle$.

Lowering. Using $\hat{n}\hat{a} = \hat{a}(\hat{n}-1)$:

$$\hat{a}\,|n\rangle = \sqrt{n}\;|n-1\rangle\,.$$

Raising. Using $\hat{n}\hat{a}^\dagger = \hat{a}^\dagger(\hat{n}+1)$:

$$\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\;|n+1\rangle\,.$$

Ground state and spectrum

The ground state $|0\rangle$ is defined by

$$\hat{a}\,|0\rangle = 0.$$

Then

$$\hat{H}\,|0\rangle = \hbar\omega\left(\hat{n} + \frac{1}{2}\right)|0\rangle = \frac{1}{2}\hbar\omega\;|0\rangle\,.$$

All excited states are generated algebraically:

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\,|0\rangle\,.$$

Interpretation: $\hat{a}^\dagger$ creates one quantum of energy $\hbar\omega$; $\hat{a}$ annihilates one quantum.

Many oscillators and Fock space

Consider N independent oscillators labeled by k:

$$\hat{H} = \sum_{k=1}^{N} \hat{H}_k = \sum_{k=1}^{N} \left(\frac{\hat{p}_k^2}{2m_k} + \frac{1}{2} m_k \omega_k^2 \hat{x}_k^2 \right).$$

Each mode has operators $\hat{a}_k, \hat{a}_k^\dagger$ with

$$[\hat{a}_k, \hat{a}_q] = 0, \qquad [\hat{a}_k^\dagger, \hat{a}_q^\dagger] = 0, \qquad [\hat{a}_k, \hat{a}_q^\dagger] = \delta_{kq}.$$

Hamiltonian:

$$\hat{H} = \sum_{k=1}^{N} \hbar\omega_k \left(\hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right), \qquad \hat{a}_k \left|0\right\rangle = 0 \ \forall k.$$

Fock states

Define occupation-number (Fock) states

$$|n_1, n_2, \ldots, n_N\rangle = \prod_{k=1}^{N} \frac{(\hat{a}_k^\dagger)^{n_k}}{\sqrt{n_k!}} |0\rangle \, .$$

They satisfy

$$\hat{a}_k^\dagger \hat{a}_k |n_1, \ldots, n_k, \ldots, n_N\rangle = n_k \, |n_1, \ldots, n_k, \ldots, n_N\rangle \, .$$

Indistinguishability and quantum statistics

Exchange symmetry for identical quanta is encoded in the algebra of creation/annihilation operators.

Bosons:

$$[\hat{a}_i, \hat{a}_j] = 0, \qquad [\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij},$$

so multiple quanta can occupy the same state.

Fermions: use operators $\hat{c}_i, \hat{c}_i^\dagger$ with

$$\{\hat{c}_i, \hat{c}_j\} = 0, \qquad \{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij}.$$

In particular,

$$(\hat{c}_i^\dagger)^2 = 0 \quad \Rightarrow \quad \text{Pauli exclusion principle.}$$

Fermionic number operator check

Define the fermionic number operator for mode 1:

$$\hat{n}_1 = \hat{c}_1^\dagger \hat{c}_1.$$

On a state with mode 1 occupied, $|11\rangle$ (schematically),

$$\hat{n}_1 |11\rangle = |11\rangle ,$$

as expected (eigenvalue 1).

One-particle states and normalization

Define one-particle momentum eigenstates

$$|\boldsymbol{p}\rangle = \hat{a}^{\dagger}_{\boldsymbol{p}}\,|0\rangle\,.$$

Normalization:

$$\langle \boldsymbol{p}|\boldsymbol{p}'\rangle = (2\pi)^3\delta^{(3)}(\boldsymbol{p}-\boldsymbol{p}').$$

Resolution of the identity (one-particle subspace):

$$\mathbf{1} = \int \frac{\mathrm{d}^3 p}{(2\pi)^3}\,|\boldsymbol{p}\rangle\,\langle \boldsymbol{p}|\,.$$

Position space and wave-functions

Plane-wave overlap:

$$\langle \boldsymbol{x} | \boldsymbol{p} \rangle = \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}}.$$

Define position eigenstates by Fourier transform:

$$|\boldsymbol{x}\rangle = \int \frac{\mathrm{d}^3 p}{(2\pi)^3}\, \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}}\, |\boldsymbol{p}\rangle\,.$$

Wave-function of a state $|\psi\rangle$:

$$\psi(\boldsymbol{x}) = \langle \boldsymbol{x} | \psi \rangle\,.$$

Two-particle states and exchange

For identical particles, the two-particle momentum wave-function satisfies

$$\langle \boldsymbol{p}, \boldsymbol{q} | \boldsymbol{r}, \boldsymbol{s} \rangle = \delta^{(3)}(\boldsymbol{p} - \boldsymbol{r})\delta^{(3)}(\boldsymbol{q} - \boldsymbol{s}) \pm \delta^{(3)}(\boldsymbol{p} - \boldsymbol{s})\delta^{(3)}(\boldsymbol{q} - \boldsymbol{r}),$$

with $+$ for bosons and $-$ for fermions.

Dirac delta identities

One-dimensional Fourier representation:

$$\delta(x-y) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{e}^{\mathrm{i}p(x-y)}\,\mathrm{d}p.$$

Change of variables:

$$\delta(g(x)) = \sum_i \frac{\delta(x-x_i)}{|g'(x_i)|}, \qquad g(x_i) = 0.$$

Time evolution: Schrödinger picture

States evolve in time; operators are (usually) time-independent:

$$\mathrm{i}\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \,.$$

Time-evolution operator:

$$|\psi(t_2)\rangle = \hat{U}(t_2, t_1) |\psi(t_1)\rangle \,, \qquad \hat{U}(t_2, t_1) = \exp\left[-\frac{\mathrm{i}}{\hbar} \hat{H}(t_2 - t_1)\right] .$$

Time evolution: Heisenberg picture

States are time-independent; operators evolve:

$$\hat{O}_H(t) = \hat{U}^\dagger(t,0)\,\hat{O}_S\,\hat{U}(t,0), \qquad \left\langle \hat{O}(t) \right\rangle = \langle\psi(0)|\,\hat{O}_H(t)\,|\psi(0)\rangle\,.$$

Equation of motion:

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}_H(t) = \frac{\mathrm{i}}{\hbar}\,[\hat{H},\hat{O}_H(t)].$$

Question: Is relativistic quantum mechanics causal?

We will:

- Solve relativistic time evolution
- Start from a localized state
- Show spreading outside the light cone

Relativistic Wave Equation

Consider the Klein–Gordon equation:

$$(\Box + m^2)\psi = 0$$

Plane wave solutions:

$$\psi \sim e^{i(\mathbf{p}\cdot\mathbf{x} - E_p t)}$$

with:

$$E_p = \sqrt{\mathbf{p}^2 + m^2}$$

General Solution

General positive-energy solution:

$$\psi(\mathbf{x}, t) = \int \frac{d^3p}{(2\pi)^3} \tilde{\psi}(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x}} e^{-iE_p t}$$

This defines time evolution.

Localised Initial State

Take a sharply localised state:

$$\psi(\mathbf{x}, 0) = \delta^{(3)}(\mathbf{x})$$

Then:

$$\tilde{\psi}(\mathbf{p}) = 1$$

So:

$$\psi(\mathbf{x}, t) = \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{x}} e^{-i\sqrt{\mathbf{p}^2+m^2}\,t}$$

What happens for space-like separation?

$$|\mathbf{x}| > t$$

If causal:

$$\psi(\mathbf{x}, t) = 0$$

Let's evaluate the integral.
The integral gives (asymptotically):

$$\psi(\mathbf{x}, t) \sim \frac{1}{\sqrt{|\mathbf{x}|^2 - t^2}} \, e^{-m\sqrt{|\mathbf{x}|^2 - t^2}}$$

valid for:

$$|\mathbf{x}| > t$$

Nonzero outside the light cone!

Interpretation

Even if initially localised:

$$\psi(\mathbf{x}, 0) = \delta(\mathbf{x})$$

At any $t > 0$:

$$\psi(\mathbf{x}, t) \neq 0 \quad \text{for all } \mathbf{x}$$

- Instantaneous spreading
- Apparent violation of causality

Resolution: Quantum Field Theory

In QFT, use fields instead of wave-functions.
Key condition:

$$[\phi(x), \phi(y)] = 0 \quad \text{for space-like separation}$$

- Observables commute
- No faster-than-light signalling

Conclusion

- Relativistic wave-functions spread outside light cone
- Single-particle interpretation breaks down
- Causality restored in quantum field theory

Microcausality in QFT

In quantum field theory, causality is imposed at the level of fields:

$$(x-y)^2 < 0 \quad \Longrightarrow \quad [\hat{\mathcal{O}}(x), \hat{\mathcal{O}}(y)] = 0.$$

In particular, for a real scalar field,

$$[\hat{\phi}(x), \hat{\phi}(y)] = 0 \qquad \text{for space-like separation.}$$

Observables at space-like separated points commute, so no measurable signal propagates faster than light.
More later.