

Position and the Free Particle

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The Position Operator

Preamble

- For a free particle, the Hamiltonian commutes with the momentum operator, i.e $[p, H] = 0$ as a result momentum is conserved and under time evolution eigenstates do not change.
- Under Fourier transformations position and momentum can be interchanged. Even more, position eigenstates will be δ functions (distributions), and now $[q, H] \neq 0$

The Position Operator

Given a Hilbert Space \mathcal{H} , we define the position operator by the eigenvalue problem

$$Q\psi(q) = q\psi(q)$$

- It has the same issues as $P \implies$ we need to relax the space of admissible functions (distributions)

Interdude 1: Distributions

Also known as Schwartz distributions or generalized functions, which are defined as continuous linear functionals on a space of infinitely differentiable test functions.

- PDE & Weak Solutions: enable the discovery of solutions that wouldn't exist in the classical sense, known as weak solutions.
- Enable construction of Sobolev Spaces: useful for analyzing the regularity of PDEs and their solutions.
- Physical motivation: singular initial conditions, problems dealing with discontinuous functions (etc).

The Position Operator

By the following relationship

$$\int_{-\infty}^{\infty} q \delta(q - q') f(q) dq = \int_{-\infty}^{\infty} q' \delta(q - q') f(q) dq,$$

it follows that

$$q \delta(q - q') = q' \delta(q - q'),$$

in the sense of distributions. Thus; $\delta(q - q')$ is eigenfunction of Q with eigenvalue q' .

The Position Operator

Q and P do not commute, in fact

$$[Q, P] = i\hbar,$$

And even more; H commutes with P , but P does not commute with $Q \implies Q$ does not commute with H , thus Q is not conserved.

Interlude 2: Spectral theorem

Finite-Dimensional Case: for a Hermitian matrix, this theorem states that it is unitarily diagonalizable.

This is: \exists unitary matrix U such that

$$A = U\Lambda U^\dagger,$$

where Λ is a diagonal matrix containing the real eigenvalues of A , and the columns of U are the orthonormal eigenvectors of A .

Or in other words: every symmetric matrix can be diagonalized using orthogonal eigenvectors

Interlude 2: Spectral theorem

Infinite-Dimensional Case: for a self-adjoint operator on a Hilbert space, the spectral theorem generalizes by stating that A is unitarily equivalent to a multiplication operator.

This is: \exists an isometry U and a measure space such that

$$(U^{-1}AUf)(x) = \lambda(x)f(x),$$

where $\lambda(x)$ is the spectrum of A , and the operator acts like multiplication by $\lambda(x)$.

The Position Operator

Thus, by the spectral theorem; any state can be written as a linear combination of eigenvectors of the given operator.

Thus we can interpret

$$\psi(q) = \int_{-\infty}^{\infty} \delta(q - q') \psi(q') dq'$$

as the expansion of an arbitrary state in terms of a continuous linear combination of eigenvectors of Q with eigenvalue q' .

The Momentum Space Representation

Momentum Representation

Let \mathcal{H} be a Hilbert space. Going back to the Hamiltonian of the free particle, by taking states to be wavefunctions $\psi(q)$, we can Fourier transform them, as

$$\tilde{\psi}(k) = \mathcal{F}\psi = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp(-ikq) \psi(q) dq.$$

And even more, we can consider \mathcal{H} to be a space of functions $\tilde{\psi}(k)$ on momentum space.

Momentum Operator

Given a Hilbert space \mathcal{H} with the momentum operator

$$P\tilde{\psi}(k) = k\tilde{\psi}(k),$$

we will call them momentum space representation.

Note: By the Plancherel theorem, momentum and space representations are unitarily equivalent representations of the group \mathbb{R} .

Eigenfunctions of P

In this representation, the eigenfunctions of P are distributions $\delta(k - k')$, with eigenvalue k' , and the expansion of any state reads

$$\tilde{\psi}(k) = \int_{-\infty}^{\infty} \delta(k - k') \tilde{\psi}(k') dk'.$$

And even more, the position operator is

$$Q = i \frac{d}{dk},$$

with eigenfunctions

$$\frac{1}{\sqrt{2\pi}} \exp(-ikq')$$

Dirac Notation

Dirac Notation

In Dirac notation, Q and P are

$$Q|q\rangle = q|q\rangle, P|k\rangle = k|k\rangle,$$

and arbitrary states

$$\langle q|\psi\rangle = \psi(q), \langle k|\psi\rangle = \psi(k).$$

Proper interpretation of relations

$$\langle q|q'\rangle = \delta(q - q'), \langle k|k'\rangle = \delta(k - k')$$

Dirac Notation

We have

$$|\psi\rangle = \int_{-\infty}^{\infty} |q\rangle \langle q|\psi\rangle dq,$$

$$|\psi\rangle = \int_{-\infty}^{\infty} |k\rangle \langle k|\psi\rangle dk,$$

with identity

$$1 = \int_{-\infty}^{\infty} |q\rangle \langle q| dq = \int_{-\infty}^{\infty} |k\rangle \langle k| dk$$

Dirac Notation: Switching representations 1

Transformation between both bases/representations is done by Fourier transform

$$\langle k|\psi\rangle = \int_{-\infty}^{\infty} \langle k|q\rangle \langle q|\psi\rangle dq$$

and

$$\langle k|q\rangle = \frac{1}{\sqrt{2\pi}} \exp(-ikq).$$

Dirac Notation: Switching representations 2

Transformation between both bases/representations is done by Fourier transform

$$\langle q|\psi\rangle = \int_{-\infty}^{\infty} \langle q|k\rangle \langle k|\psi\rangle dk$$

and

$$\langle q|k\rangle = \frac{1}{\sqrt{2\pi}} \exp(ikq).$$

Interlude 3: Bra-Ket Notation and Dual Spaces

- A state vector $|\psi\rangle$ (ket) lives in \mathcal{H}
- Its dual $\langle\psi|$ (bra) lives in \mathcal{H}^* (the dual space)
- When we write $\langle\psi|\phi\rangle$, we're actually applying a linear functional from \mathcal{H}^* to the complex numbers.
- Every observable corresponds to a linear operator A that acts on states.
- When we measure an observable, we're essentially using elements of the dual space

Heisenberg uncertainty

Theorem

$$\frac{\langle \psi | Q^2 | \psi \rangle}{\langle \psi | \psi \rangle} \frac{\langle \psi | P^2 | \psi \rangle}{\langle \psi | \psi \rangle} \geq \frac{1}{4}$$

The proof relies on using self-adjointness of P and Q together with commutation relations between Q and P .

The Propagator in Position Space

Time Evolution

For any quantum system, time evolution is given by the unitary operator

$$U(t) = \exp(-itH),$$

considering that H is independent of time.

- Momentum Space: just the multiplication operator.
- Position Space: given by an integral kernel called the propagator.

Interlude 4: Time Evolution

If H is time dependent but the commutes at different times, then the time evolution is given by

$$U(t) = \exp\left[-\frac{1}{\hbar} \int_0^t dt' H(t')\right]$$

If H is time dependent and at different times do not commute, then the time evolution is given by

$$U(t) = 1 + \sum_{n=1}^{\infty} \left(\frac{-i}{\hbar}\right)^n \int_0^{t_1} dt_1 \cdots \int_0^{t_{n-1}} dt_n H(t_1) \cdots H(t_n)$$

Propagator

Definition: The position space propagator is the kernel $U(t, q_t, q_0)$ of the time evolution operator acting on position space wavefunctions. Determines the time evolution of wavefunctions for all times t by

$$\psi(q_t, t) = \int_{-\infty}^{\infty} U(t, q_t, q_0) \psi(q_0, 0) dq_0,$$

where $\psi(q_0, 0)$ is the initial value of the wavefunction at time 0.

Propagator: Dirac Notation

Using Dirac notation we have

$$\begin{aligned}\psi(q_t, t) &= \langle q_t | \psi(t) \rangle = \langle q_t | \exp(-itH) | \psi(0) \rangle, \\ \implies \psi(q_t, t) &= \langle q_t | \exp(-itH) \int_{-\infty}^{\infty} |q_0\rangle \langle q_0 | \psi(0) \rangle dq_0,\end{aligned}$$

and the propagator can be written as

$$U(t, q_t, q_0) = \langle q_t | \exp(-itH) | q_0 \rangle$$

Propagator for the Free Particle

For the free particle we can compute the propagator, which is

$$U(t, q_t, q_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(-ik(q_t - q_0)) \exp(-\frac{ik^2 t}{2m}) dk,$$

and $U(t, q_t, q_0) = U(t, q_t - q_0)$. due to translation invariance of H , the propagator only depends on the difference $q_t - q_0$.

Tricks from Complex Analysis

Let's consider $it \rightarrow z = \tau + it$, then the propagator is well defined when $\tau = \text{Re}(z) > 0$, which defined a holomorphic function in z . Then we can find

$$U(z, q_t - q_0) = \sqrt{\frac{m}{2\pi z}} \exp\left(-\frac{m}{2z}(q_t - q_0)^2\right)$$

Relation with Heat Equation (Diffusion Equation)

If $z = \tau$ is real and positive, then this is the kernel function for solutions to the partial differential equation

$$\frac{\partial}{\partial \tau} \psi(q, t) = \frac{1}{2m} \frac{\partial^2}{\partial q^2} \psi(q, \tau),$$

which models the way temperature diffuses in a medium, it also models the way probability of a given position diffuses in a random walk.

Interlude 5: Fokker-Planck Equation

The FP equation is a classical PDE that describes the time evolution of a probability density function:

$$\frac{\partial}{\partial t}p(x, t) = -\frac{\partial}{\partial x}(\mu(x, t)p(x, t)) + \frac{\partial^2}{\partial x^2}(D(x, t)p(x, t))$$

- Solving certain FPEs using quantum mechanical methods.
- The quantum extensions of the FPE help describe phenomena like decoherence, thermalization, and energy relaxation in quantum systems interacting with their environment.

Propagators in frequency-momentum space

Causality

The propagator as defined before works for positive and negative times, let's define a version that takes into account causality

Definition(Retarded Propagator): The retarded propagator $U_+(t, q_t - q_0)$ is given by 0 if $t < 0$ and $U_+(t, q_t - q_0) = U(t, q_t, q_0)$ if $t > 0$.

It can also be wrtitten in terms of a step function θ

Integral Representation of θ

A useful representation of θ is given by

$$\theta(t) = \lim_{\epsilon \rightarrow 0^+} \frac{i}{2\pi} \int_{-\infty}^{\infty} \frac{1}{\omega + i\epsilon} \exp(-i\omega t) d\omega.$$

Propagator in frequency domain

The Fourier transform of the previously computed propagator is

$$\hat{U}(\omega, k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left(\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{ik^2 t}{2m}\right) \exp(i\omega t) \right) dt,$$

\Rightarrow

$$\hat{U}(\omega, k) = \delta\left(\omega - \frac{1}{2m} k^2\right)$$

Retarded Propagator in position space

The retarded propagator in position space is given by

$$U_+(t, q_t - q_0) = \lim_{\epsilon \rightarrow 0^+} \left(\frac{1}{2\pi}\right)^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{i}{\omega + i\epsilon} f(\omega, k, t, q_t - q_0) d\omega dk,$$

where

$$f(\omega, k, t, q_t - q_0) = \exp(-i(\omega + \frac{1}{2m}k^2)t) \exp(ik(q_t - q_0))$$

Retarded Propagator in position space

Doing the change of variables $\omega \rightarrow \omega' = \omega + \frac{1}{2m}k^2$, we can find

$$U_+(t, q_t - q_0) = \lim_{\epsilon \rightarrow 0^+} \left(\frac{1}{2\pi}\right)^2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g d\omega' dk$$

where

$$g = \frac{\exp(-i\omega' t) \exp(ik(q_t - q_0))}{\omega' - \frac{1}{2m}k^2 + i\epsilon}$$

Retarded Propagator in position space

Which is the Fourier transform

$$U_+(t, q_t - q_0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \hat{U}_+(\omega, k) h d\omega dk,$$

where

$$\hat{U}_+(\omega, k) = \lim_{\epsilon \rightarrow 0^+} \frac{i}{2\pi} \frac{1}{\omega - \frac{1}{2m}k^2 + i\epsilon}$$

and

$$h = \exp(-i\omega t) \exp(ik(q_t - q_0))$$

Green's Functions and Solutions to the Schrodinger Equation

Green's Function

- Act as an integral kernel that transforms differential equations into more manageable algebraic forms.
- In position basis, the Green's function acts as a propagator, describing how quantum particles move between different positions

Given the PDE

$$D\psi = J,$$

We define the Green's function of D to be the distribution with Fourier transform

$$\hat{G} = \frac{1}{\hat{D}}$$

Schrodinger Equation

Let D be given by

$$D = i \frac{\partial}{\partial t} + \frac{1}{2m} \frac{\partial^2}{\partial q^2},$$

then, it's Fourier transform will be

$$\hat{D} = \omega - \frac{k^2}{2m},$$

ans thus, it's Green function will be

$$\hat{G} = \frac{1}{\omega - \frac{k^2}{2m}}$$

Schrodinger Equation

And then, solutions of $D\psi = J$, are found by computing the inverse Fourier transform of $\hat{G}\hat{J}$

$$\psi(q, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{\omega - \frac{k^2}{2m}} \hat{J}(\omega, k) \exp(-i\omega t) \exp(ikq) d\omega dk$$

Final Words: P and Q Representations

Complementary Descriptions of Quantum Systems linked by Fourier transformations;

- Q representation describes the system using a wavefunction, which gives the probability amplitude for finding the particle at a specific position.
- P representation describes the system using a wavefunction, that provides the probability amplitude for the particle having a specific momentum.
- In Q representation Q is multiplicative and P is a differential operator.
- in P representation P is multiplicative and Q is a differential operator.