# Position and the Free Particle

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November 22, 2024

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# Contents

# 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 $\delta$ 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 admisible functions (distributions)

# Interdule 1: Distributions

Also known as Schwartz distributions or generalized functions, which are defined as continuous linear functionals on a space of infitely 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 discountinupus 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 $\Lambda$ is a diagonal matrix containing the real eigenvalues of $A$, and the columns of 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

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

# 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 if 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

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

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

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

# 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

$$\psi(q_t, t) = \langle q_t|\psi(t)\rangle = \langle q_t|\exp(-itH)|\psi(0)\rangle,$$

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

and the propgator 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 progator, 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 invarianceo of $H$, the propagator only depends on the difference $q_t - q_0$.

# Tricks from Complex Analysis

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

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

# 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(Retarted Propagator): The retarted 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 wrttitten in terms of a step function $\theta$

# Integral Representation of $\theta$

A useful representation of $\theta$ is given by

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

# Propagator in frequency domain

The Fourier transform of the previously copmuted propagator is

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

$\Longrightarrow$

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

# Retarded Propagator in position space

The retarded propagator in position space is given by

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

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 $\omega \to \omega' = \omega + \frac{1}{2m}k^2$, we can find

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

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

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

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.