Advanced Quantum Physics
Week 1

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Principles of quantum mechanics

Hilbert space

A Hilbert space $\mathcal{E}_H$ is a complex vector space with a Hermitian scalar product. The state of a quantum system is described by a *ket* $|\Psi\rangle \in \mathcal{E}_H$. The scalar product is written $\langle\Psi_2|\Psi_1\rangle$. It is linear in $|\Psi_1\rangle$ and antilinear in $|\Psi_2\rangle$ and $(\langle\Psi_2|\Psi_1\rangle)^* = \langle\Psi_1|\Psi_2\rangle$. We have that $\langle\Psi|\Psi\rangle = 1$ for physical states. $\langle\Psi|$ is called a *bra*. It is a linear form on the Hilbert space.

We will only consider separable Hilbert spaces. Those admit an orthonormal countable basis $\{\Psi_1, \Psi_2, \ldots\}$.

The object $|\Psi_n\rangle\langle\Psi_n|$ is a projector on the ket $|\Psi_n\rangle$. If the $|\Psi_n\rangle$'s form a basis of the Hilbert space, then we have the closure relation $\sum_n |\Psi_n\rangle\langle\Psi_n| = 1$.

Superposition principle

A linear combination $\alpha|\Psi_1\rangle + \beta|\Psi_2\rangle$ is a ket in the same Hilbert space and therefore describes a quantum state.

Measurements

To every physical quantity a there is a corresponding operator $\hat{A}$, called observable. The adjoint $\hat{A}^\dagger$ of $\hat{A}$ is defined by $\langle\Psi_2|\hat{A}^\dagger|\Psi_1\rangle = (\langle\Psi_1|\hat{A}|\Psi_2\rangle)^*$. Physical observables are Hermitian, i.e. $\hat{A} = \hat{A}^\dagger$.

Let a_α and $|\alpha, r\rangle$ be the eigenvalue and (possibly) degenerate eigenvectors of $\hat{A}$. As a consequence of the spectral theorem:

- The set $\{|\alpha, r\rangle\}$ is a Hilbertian basis
- The observable can be written as
$$\hat{A} = \sum_{\alpha} \sum_{r} a_{\alpha} |\alpha, r\rangle\langle\alpha, r| = \sum_{\alpha} a_{\alpha} \hat{P}_{\alpha},$$
where $\hat{P}_{\alpha}$ is the projector onto the eigensubspace $\mathcal{E}_{\alpha}$ associated with the eigenvalue a_{α}.

If we perform a measurement on a quantum state $|\Psi\rangle$:

- The result of a measurement of $\hat{A}$ is one of its eigenvalues a_{α}
- The probability to measure a_{α} is $p(a_{\alpha}) = \langle\Psi|\hat{P}_{\alpha}|\Psi\rangle$
- This means that the average value of a measurement of $\hat{A}$ is
$$\langle a\rangle = \langle\Psi|\hat{A}|\Psi\rangle = \sum_{\alpha} a_{\alpha} p(a_{\alpha})$$
- Just after the measurement the system will be in the state
$$|\Psi'\rangle = \frac{\hat{P}_{\alpha}|\Psi\rangle}{\|\hat{P}_{\alpha}|\Psi\rangle\|}$$

Some examples of physical observables:

- Position operator: $\hat{x}$
- Momentum operator: $\hat{p} = -i\hbar\frac{d}{dx}$
- Energy operator: $\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(\hat{x})$

Time evolution

The time evolution of a (non-relativistic) quantum system is given by the Schrödinger equation
$$i\hbar\frac{d}{dt}|\Psi(r,t)\rangle = \hat{\mathcal{H}}(t)|\Psi(r,t)\rangle$$
It is easy to check that this equation ensures that the norm of $|\Psi(r,t)\rangle$ is conserved.

When the Hamiltonian is time-independent, it is useful to look for the eigenvectors and eigenvalues of $\hat{\mathcal{H}}$. This is the stationary Schrödinger equation
$$\hat{\mathcal{H}}|\phi_n\rangle = E_n|\phi_n\rangle$$
Then, if $|\Psi(t=0)\rangle = \sum_n c_n|\phi_n\rangle$, then
$$|\Psi(t)\rangle = \sum_n c_n e^{-iE_n t/\hbar}|\phi_n\rangle,$$
where $c_n = \langle\phi_n|\Psi(t=0)\rangle$. It is clear that an eigenstate of $\hat{\mathcal{H}}$ will just evolve with a phase and any measurement will yield a constant result. The state is stationary.

Commuting observables

Here we consider two observables $\hat{A}$, $\hat{B}$ that commute, i.e.

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0.$$

In this situation, there exist a basis $|\Psi_{m,n,p}\rangle$ of the Hilbert space such that

$$\hat{A}|\Psi_{m,n,p}\rangle = a_m|\Psi_{m,n,p}\rangle$$
$$\hat{B}|\Psi_{m,n,p}\rangle = b_n|\Psi_{m,n,p}\rangle$$

In other words, both operators can be diagonalized at the same time. They can then also be measured at the same time without interfering with each other.

Non-commuting observables

What happens when the two observables $\hat{A}$, $\hat{B}$ do not commute

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \neq 0?$$

Heisenberg uncertainty principle

We consider the mean-square deviations of the observables Δa and Δb. They satisfy this inequality

$$\Delta a \Delta b \geq \frac{1}{2}\left|\langle\Psi|[\hat{A}, \hat{B}]|\Psi\rangle\right|$$

Ehrenfest theorem

Let us consider a quantum system described by $\hat{\mathcal{H}}(t)$ and an observable $\hat{A}(t)$. The evolution of the expectation value of $\hat{A}(t)$ is governed by

$$\frac{d}{dt}\langle a\rangle(t) = \frac{1}{i\hbar}\langle\Psi(t)|[\hat{A}, \hat{\mathcal{H}}]|\Psi(t)\rangle + \langle\Psi(t)|\frac{\partial\hat{A}}{\partial t}|\Psi(t)\rangle$$

As a consequence, if $[\hat{\mathcal{H}}, \hat{A}] = 0$ we conclude that $\hat{A}$ is a conserved quantity. For an isolated system, the Hamiltonian is time-independent and the energy is a conserved quantity.

A couple of one-dimensional examples

General considerations

Let us consider a potential $V(x)$ that goes to zero at $\pm\infty$. There are two kinds of solutions. A continuum of solutions with $E > 0$. These are delocalized scattering states. They are twice degenerate. When $E < 0$, the condition that the wavefunction be zero at $\pm\infty$ implies that only some energies are allowed. The corresponding *bound states* have an exponential decay and are localized. As a result of the Sturm-Liouville theorem the bound state associated to the n^{th} excited state has n nodes in its wavefunction.

Infinite potential well

The eigenvectors and eigenvalues are given by

$$\Psi_n(x) = A\sin(k_n x) \qquad E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2},$$

where n take integer values ≥ 1.

Harmonic oscillator

We consider a harmonic oscillator

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

Introducing

$$\hat{X} = \hat{x}\sqrt{\frac{m\omega}{\hbar}} \qquad \hat{P} = \frac{\hat{p}}{\sqrt{m\hbar\omega}}$$

we have that

$$\hat{\mathcal{H}} = \frac{1}{2}\big(\hat{X}^2 + \hat{P}^2\big) \qquad \big[\hat{X}, \hat{P}\big] = i$$

We then define the ladder operators

$$\hat{a} = \frac{1}{\sqrt{2}}\big(\hat{X} + i\hat{P}\big) \qquad \hat{a}^\dagger = \frac{1}{\sqrt{2}}\big(\hat{X} - i\hat{P}\big) \qquad [\hat{a}, \hat{a}^\dagger] = 1$$

The Hamiltonian reads

$$\hat{\mathcal{H}} = \hbar\omega\big(\hat{N} + \frac{1}{2}\big) \qquad \hat{N} = \hat{a}^\dagger\hat{a}$$

Its eigenvectors are $|n\rangle$

$$\hat{\mathcal{H}}|n\rangle = \hbar\omega(n + \frac{1}{2})|n\rangle,$$

with n an integer ≥ 0. The ladder operators have the properties

$$a|n\rangle = \sqrt{n}|n-1\rangle$$
$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

Mathematical tools

Fourier transforms

The Fourier transform of $\Psi(x)$ is given by

$$\varphi(p) = \int \frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}} \Psi(x) dx$$

The inverse transform is

$$\Psi(x) = \int \varphi(p) \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} dp$$

The physical interpretation of $\varphi(p)$ is that it is the probability amplitude of the momentum. We define $|p\rangle = e^{ipx/\hbar}/\sqrt{2\pi\hbar}$. It is clearly an eigenstate of the momentum operator $\hat{p} = -i\hbar d/dx$. Therefore we can write

$$|\Psi\rangle = \int \varphi(p)|p\rangle dp$$

and we have

$$\varphi(p) = \langle p|\Psi\rangle$$

The Dirac δ function

In a similar way as for the Fourier transform, we would like to write

$$\Psi(x) = \langle \delta_x|\Psi\rangle$$

It turns out that the "function" associated to the ket $|\delta_x\rangle$ is the Dirac δ function $\delta(x' - x)$. This function has the property that

$$f(x) = \int \delta(x - y) f(y) dy$$

The Dirac δ function is not a proper function. One must use the distribution theory to give it a mathematically correct meaning. In practice we can nevertheless think of it as a function that vanishes everywhere except at zero where it is infinite. We will in general use the notation $|x\rangle = |\delta_x\rangle$ so that

$$\Psi(x) = \langle x|\Psi\rangle$$

Representation of a quantum state

Here are three different ways to represent a one-dimensional quantum state

- Hilbertian basis

$$|\Psi\rangle = \sum_n c_n |\Psi_n\rangle \qquad c_n = \langle \Psi_n | \Psi \rangle$$

- Fourier basis

$$|\Psi\rangle = \int \varphi(p) |p\rangle dp \qquad \varphi(p) = \langle p | \Psi \rangle$$

- Dirac delta function basis

$$|\Psi\rangle = \int \Psi(x) |x\rangle dx \qquad \Psi(x) = \langle x | \Psi \rangle$$