Lecture 7
Quantum Mechanical Measurements.
Symmetries, conserved quantities, and the labeling of states

Today's Program:

1. Expectation values

2. Finding the momentum eigenfunctions and the dispersion relations for free particle.

3. Commutator and observables that commute

4. Symmetries and conserved quantities – labeling of states

Questions you will by able to answer by the end of today's lecture

1. What is the significance of commuting and non-commuting operators?

2. How are constants of motion used to label states?

3. What is the connection between symmetries and constant of motion?

4. What are the properties of "conservative systems"?

5. What is the dispersion relation for a free particle, why are E and k used as labels?

References:

1. Introductory Quantum and Statistical Mechanics, Hagelstein, Senturia, Orlando.

2. Principles of Quantum Mechanics, Shankar.

Now let's find out what happens when we try to take a measurement of a physical quantity.

Consider a system whose state is characterized at a given time by the wavefunction $\psi(\vec{r}, t)$. We want to predict the result of a measurement at this time of a physical quantity a associated with the observable $\hat{A}$. The prediction of a possible outcome will be in terms of probabilities. We will now give a set of rules that will allow us to predict the probability of obtaining any eigenvalue of $\hat{A}$ in a measurement.

Let us first assume that the spectrum of $\hat{A}$ is entirely discrete. If all the eigenvalues a_n of A are non-degenerate there is associated with each of them a unique eigenvector $u_n(x)$:

$$\hat{A}u_n(x) = a_n u_n(x)$$

Since A is Hermitian the set of $u_n(x)$ is a complete basis for the wavefunction space. That means that any wave function can be represented as a linear combination of $u_n(x)$:

$$\psi(x) = \sum_n C_n u_n(x)$$

Where the coefficients of the expansion are just as they are in the geometrical analogy projections of the function $|\psi\rangle$ onto the $|u_n\rangle$ direction given by the inner products between the function $|\psi\rangle$ and the normalized basis function $|u_n\rangle$:

$$C_n = \langle u_n | \psi \rangle$$

As you already know what the definition of an inner product between vectors is we now define the inner product between functions.

An inner product between two functions was

$$\langle u(x) | \psi(x) \rangle = \int u(x)^* \psi(x) dx$$

Remind ourselves of the geometrical interpretation (in 2D for simplicity). For two vectors ψ, u_n the inner product is in a number (which can be complex), which is the projection of one vector onto the other vector. $\langle u | \psi \rangle = C$

How do we represent a vector ψ in a particular basis?

Choose a particular set of vectors, which span the vector space u_1, u_2,.... Usually we choose basis set to be orthonormal (i.e. the basis vectors are of length 1 and are orthogonal to each other). Then we find the projection of ψ onto the direction of each basis vector.

$$\langle u_1 | \psi \rangle = C_1$$
$$\langle u_2 | \psi \rangle = C_2$$

Write the original function as a linear combination of the basis vector: $\psi = C_1 u_1 + C_2 u_2$.

In general: $\psi = \sum_{i=1}^{N} C_i u_i$.

Finding the eigenvectors and eigenvalues of operators, discuss the geometrical interpretation of eigenvectors and eigenvalues – scaling.

Fourth Postulate (discrete non-degenerate): When the physical quantity a is measured on a system in the normalized state $|\psi(t)\rangle$ the probability $P(a_n)$ of obtaining the non-degenerate eigenvalue a_n of the corresponding observable is:

$$P(a_n) = |\langle \psi | u_n \rangle|^2 = \left| \int \left(\sum_s C_s^* u_s^*(x) \right) u_n(x) dx \right|^2 = \left| \sum_s C_s^* \int u_s^*(x) u_n(x) dx \right|^2 = |C_n|^2$$

where $u_n(x)$ is the normalized eigenvector of A associated with the eigenvalue a_n.

Expectation values:
What is the average value we expect to get from a series of experiments?

For quantum mechanical system described by a wavefunction $\psi(x,t)$ the average value of a physical quantity described by an observable $\hat{A}$ is:

$$\langle \hat{A} \rangle = \langle \psi(x,t) | \hat{A} | \psi(x,t) \rangle = \int \psi(x)^* \hat{A} \psi(x) dx$$

At any given moment t_0 we can represent $\psi(x,t_0)$ as a linear combination of eigenfunctions of observable $\hat{A}$: $\psi(x,t_0) = \sum_n C_n u_n(x)$, where $C_n = \langle u_n | \psi(x,t_0) \rangle = \int u_n^*(x) \psi(x,t_0) dx$.

Substituting this into the equation above we get:

$$\langle \hat{A} \rangle = \langle \psi(x,t) | \hat{A} | \psi(x,t) \rangle = \int \psi(x)^* \hat{A} \psi(x) dx = \int \sum_n C_n^* u_n^*(x) \left[\hat{A} \sum_n C_n u_n(x) \right] dx =$$

$$= \int \sum_n C_n^* u_n^*(x) \left[\sum_n C_n \hat{A} u_n(x) \right] dx = \int \sum_n C_n^* u_n^*(x) \left[\sum_n C_n a_n u_n(x) \right] dx =$$

$$= \sum_n \sum_s C_n^* C_s a_s \int u_n^*(x) u_s(x) dx = \sum_n |C_n|^2 a_n$$

Let's consider an example: Particle flying in free space.
We have previously approximated particles in free space with plane waves but in reality they are more like a linear superposition of multiple plane waves.
Let's consider a particle described by a wavefunction:

$$\psi(x,t) = \frac{1}{2} e^{ik_0 x - i\omega_0 t} + \frac{1}{2} e^{2ik_0 x - 4i\omega_0 t} + \frac{1}{\sqrt{2}} e^{-ik_0 x - i\omega_0 t}$$

What is the average momentum of this particle?
Using a definition of the expectation value we can write:

$$\langle \hat{p} \rangle = \langle \psi(x,t) | \hat{p} | \psi(x,t) \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) \, \hat{p} \psi(x,t) \, dx =$$

$$= \int_{-\infty}^{\infty} \left[\frac{1}{2} e^{-ik_0 x + i\omega_0 t} + \frac{1}{2} e^{-2ik_0 x + 4i\omega_0 t} + \frac{1}{\sqrt{2}} e^{ik_0 x + i\omega_0 t} \right] - i\hbar \frac{\partial}{\partial x} \left[\frac{1}{2} e^{ik_0 x - i\omega_0 t} + \frac{1}{2} e^{2ik_0 x - 4i\omega_0 t} + \frac{1}{\sqrt{2}} e^{-ik_0 x - i\omega_0 t} \right] dx =$$

$$= \int_{-\infty}^{\infty} \left[\frac{1}{2} e^{-ik_0 x + i\omega_0 t} + \frac{1}{2} e^{-2ik_0 x + 4i\omega_0 t} + \frac{1}{\sqrt{2}} e^{ik_0 x + i\omega_0 t} \right] \left[\frac{1}{2} \hbar k_0 e^{ik_0 x - i\omega_0 t} + \frac{1}{2} 2\hbar k_0 e^{2ik_0 x - 4i\omega_0 t} - \frac{1}{\sqrt{2}} \hbar k_0 e^{-ik_0 x - i\omega_0 t} \right] dx =$$

$$= \frac{1}{4} \hbar k_0 + \frac{1}{4} 2\hbar k_0 - \frac{1}{2} \hbar k_0 +$$

$$+ \int_{-\infty}^{\infty} \left[\frac{1}{4} 2\hbar k_0 e^{ik_0 x - 3i\omega_0 t} - \frac{1}{2\sqrt{2}} \hbar k_0 e^{-2ik_0 x} + \frac{1}{4} \hbar k_0 e^{-ik_0 x + 3i\omega_0 t} - \frac{1}{2\sqrt{2}} \hbar k_0 e^{-3ik_0 x + 3i\omega_0 t} + \frac{1}{2\sqrt{2}} \hbar k_0 e^{2ik_0 x} + \frac{1}{2\sqrt{2}} 2\hbar k_0 e^{3ik_0 x - 3i\omega_0 t} \right] dx =$$

$$= \frac{1}{4} \hbar k_0 + \frac{1}{4} 2\hbar k_0 - \frac{1}{2} \hbar k_0 = \frac{1}{4} \hbar k_0$$

So on average the momentum is equal to: $\frac{1}{4} \hbar k_0$

What is the probability for this particle to be flying left (in the opposite direction of x axis)?
Here we need to find the probability that particle has negative momentum. Indeed from plane wave expansion we find that our particle can have momentum of $-\hbar k_0$ since it has a plane wave

component $e^{-ik_0 x - i\omega_0 k}$. The coefficient in front of this plane wave is $\frac{1}{\sqrt{2}}$ and consequently the

probability of our particle to move backwards is $\left| \frac{1}{\sqrt{2}} \right|^2 = \frac{1}{2}$.

Fifth Postulate (discrete non-degenerate):

If the measurement of a physical quantity a on the system in the state $\psi(\vec{r},t)$ gives the result a_n
the state of the system immediately after the measurement is $u_n(x)$.

$$\psi(x,0) \longrightarrow \psi(x,t_0) \; \boxed{\text{MEASUREMENT}} \; u_n(x,t_0) \longrightarrow \psi'(x,t_1)$$
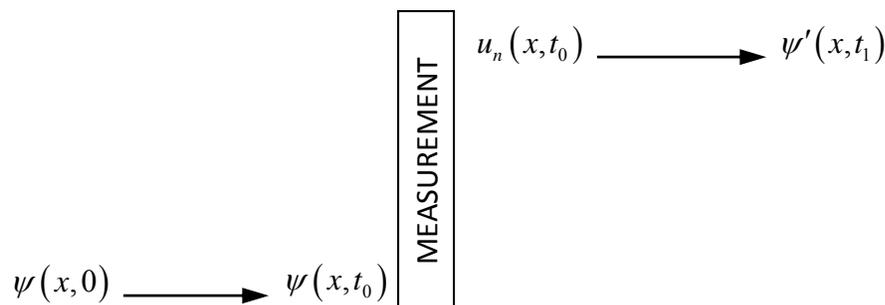
Consequences:

(1) The state of the system right after a measurement is always an eigenvector corresponding to the specific eigenvalue, which was the result of the measurement.

(2) The state of the system is fundamentally perturbed by the measurement process.

How precisely can we measure a physical quantity? – Before we can answer this question let's consider a helpful mathematical concept:

The Commutator operator and commutation relations

The *Commutator* operator is defined as: $\left[\hat{A}, \hat{B} \right] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$

Two observables $\hat{A}$ and $\hat{B}$ are said to commute if: $\hat{A}\hat{B} = \hat{B}\hat{A} \Rightarrow \left[\hat{A}, \hat{B} \right] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} = 0$

Geometrical interpretation: Recall from your linear algebra recitation and the problem set 1. When two matrices commute they share eigenvectors.

Example: Free space Hamiltonian and momentum: $\hat{H} = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}$ and $\hat{p} = -i\hbar\dfrac{\partial}{\partial x}$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}, -i\hbar\frac{\partial}{\partial x} \right]\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(-i\hbar\frac{\partial \psi(x)}{\partial x} \right) + i\hbar\frac{\partial}{\partial x}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} \right) = i\frac{\hbar^3}{2m}\frac{\partial^3 \psi(x)}{\partial x^3} - i\frac{\hbar^3}{2m}\frac{\partial^3 \psi(x)}{\partial x^3} = 0$$

Do $\hat{H} = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}$ and $\hat{p} = -i\hbar\dfrac{\partial}{\partial x}$ share eigenfunctions?

The eigenfunctions for momentum are plane waves e^{ikx}: $-i\hbar\dfrac{\partial}{\partial x}e^{ikx} = \hbar k \cdot e^{ikx}$

And from the previous lectures we remember that the plane waves are also eigenfunctions for the free space Hamiltonian: $-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}e^{ikx} = \dfrac{\hbar^2 k^2}{2m}e^{ikx}$

Fundamental theorem of algebra: If two operators A and B commute one can construct a basis of the state space with eigenfunctions common to A and B, conversely if a basis set is found of eigenfunctions common to both A and B then A and B commute.

How about position and momentum? Do $\hat{x}$ and $\hat{p}$ commute?

$$[\hat{x}, \hat{p}]\,\psi(x) = x\left(-i\hbar\frac{\partial \psi(x)}{\partial x} \right) - \left(-i\hbar\frac{\partial}{\partial x}\left(x\psi(x) \right) \right) = -i\hbar x\frac{\partial \psi(x)}{\partial x} + i\hbar x\frac{\partial \psi(x)}{\partial x} + i\hbar\,\psi(x) = i\hbar\,\psi(x)$$

Then: $[\hat{x}, \hat{p}] = i\hbar$

It turns out that this relationship is very significant as it Mathematics it means that x and p cannot be measured with absolute precision at the same time. In fact their uncertainties (or measurement error) must obey the following relationship:

$$\Delta x \cdot \Delta p \geq \frac{\left|\left[\hat{x}, \hat{p}\right]\right|}{2} \Rightarrow \Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

This relationship is called **Heisenberg's Uncertainty Principle**. In fact it also holds for the uncertainties of energy and time:

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$$

Symmetries, conserved quantities and constants of motion – how do we identify and label states (good quantum numbers)

The connection between symmetries and conserved quantities:

In the previous section we showed that the Hamiltonian function plays a major role in our understanding of quantum mechanics using it we could find both the eigenfunctions of the Hamiltonian and the time evolution of the system.

What do we mean by when we say an object is symmetric? What we mean is that if we take the object perform a particular operation on it and then compare the result to the initial situation they are indistinguishable. When one speaks of a symmetry it is critical to state symmetric with respect to which *operation.*

How do symmetries manifest themselves in equations? Let us suppose that your system is symmetric with respect to translations in *x* that would imply that any physical property could not have an *x* dependence. In particular the energy would not have an explicit dependence on *x* thus:

$$\frac{\partial H(x, p)}{\partial x} = 0 = -\frac{dp}{dt} \Rightarrow p = const$$

The momentum in this case is called a constant of motion. **This illustrates a fundamental connection between symmetries and conserved quantities. In fact, every symmetry in a physical system implies an associated conserved quantity.**

In quantum mechanics the time evolution of an observable is describe by the following equation:

Ehrenfest Theorem:

$$\frac{d}{dt}\left\langle \hat{A} \right\rangle = \frac{1}{i\hbar}\left\langle \left[\hat{A}, \hat{H}\right] \right\rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle$$

$$\frac{d}{dt}\left\langle \psi(x) \middle| \hat{A} \middle| \psi(x) \right\rangle = \frac{1}{i\hbar}\left\langle \psi(x) \middle| \left[\hat{A}, \hat{H}\right] \middle| \psi(x) \right\rangle + \left\langle \psi(x) \middle| \frac{\partial \hat{A}}{\partial t} \middle| \psi(x) \right\rangle$$

Consequently in order for a physical quantity to be a constant of motion the corresponding observable has to obey the following relationships:

$$\begin{cases} \dfrac{\partial \hat{A}}{\partial t} = 0 \\ \left[\hat{A}, \hat{H} \right] = 0 \end{cases} \Rightarrow \dfrac{d}{dt}\left\langle \hat{A} \right\rangle = 0$$

States are labeled by specific values of their properties, which do not change with time – these properties are called constants of motion. We learned that in QM physical properties are represented by operators and that the values of properties obtained in measurements are eigenvalues of the corresponding operators. **Hence the eigenvalues are used as the labels.**

Conserved Quantities Example 0: Conservative Systems

The simplest example of a conserved quantity is Energy. Two lectures ago we have considered systems, where Hamiltonian does not depend on time explicitly. Obviously Hamiltonian commutes with itself and consequently energy is conserved and can be used as a label for a state.

$$\left. \begin{array}{l} \dfrac{\partial \hat{H}}{\partial t} = 0 \\ \left[\hat{H}, \hat{H} \right] = 0 \end{array} \right\} \Rightarrow \dfrac{d}{dt}\left\langle \hat{H} \right\rangle = 0 \Rightarrow E = const \Rightarrow u_E(x) \Rightarrow \psi(x,t) = \sum_E u_E(x)e^{-i\frac{E}{\hbar}t}$$

Reminder:

Schrodinger's equation: $\left[-\dfrac{\hbar^2}{2m}\vec{\nabla} + V(\vec{r}) \right]\psi(\vec{r},t) = i\hbar\dfrac{\partial}{\partial t}\psi(\vec{r},t)$

This type of differential equation is separable, i.e. we can look for a solution in the following form: $\psi(\vec{r},t) = \varphi(\vec{r})\xi(t)$. Let's substitute it into the Schrodinger's equation above:

$$\left[-\dfrac{\hbar^2}{2m}\vec{\nabla} + V(\vec{r}) \right]\varphi(\vec{r})\xi(t) = i\hbar\dfrac{\partial}{\partial t}\varphi(\vec{r})\xi(t)$$

$$\dfrac{1}{\varphi(\vec{r})}\left\{ \left[-\dfrac{\hbar^2}{2m}\vec{\nabla} + V(\vec{r}) \right]\varphi(\vec{r}) \right\} = \dfrac{1}{\xi(t)}i\hbar\dfrac{\partial}{\partial t}\xi(t)$$

Note that the left side of the equation only depends on position $\vec{r}$ and the right side of the equation only depends on time t. This can only be true when both sides of the equation are constant E – for energy. Then the equation above splits into the following two equations:

$$(I) \quad i\hbar\dfrac{d}{dt}\xi(t) = E\xi(t) \Rightarrow \xi(t) = e^{-i\frac{E}{\hbar}}$$

$$(II) \quad \left[-\dfrac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r}) \right]\varphi(\vec{r}) = E\varphi(\vec{r}) \Rightarrow u_E(x), \ E$$

Then the solutions to time-dependent Schrodinger's equation will have a form:

$$\psi_E(\vec{r},t) = u_E(\vec{r})\xi_E(t) = u_E(\vec{r})e^{-i\frac{E}{\hbar}t}$$

In general, since the Hamiltonian may have many eigenvalues and corresponding eigenfunctions, the solution for this system is a linear combination of all the possible solutions corresponding to different energies:

$$\Psi(\vec{r},t) = \sum_E C_E u_E(\vec{r})e^{-i\frac{E}{\hbar}t}, \text{ where } C_E \text{ are the coefficients that can be determined from the initial}$$

and boundary conditions.

This is a very important result: If we know the special wavefunctions (Hamiltonian eigenfunctions) we can easily find time evolution of this conserveative system.
If we know E and $u_E(\vec{r})$ then we know $\Psi(\vec{r},t)$ at any time!

Conserved Quantities Example I: Particle in free space

Labeling of states is particularly important when the energy eigenvalues are degenerate such as in the case of the particle in free space:

$$\hat{H}\psi(x) = E\psi(x) \Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x) \Rightarrow u_E(x) = \begin{cases} e^{i\sqrt{\frac{2mE}{\hbar^2}}x} \\ \\ e^{-i\sqrt{\frac{2mE}{\hbar^2}}x} \end{cases}$$

Using the energy as a "label" doesn't completely and uniquely specify a state.

What about momentum? – If momentum is a constant of motion then we can use it as an additional label to uniquely specify the eigenstate. We have shown earlier that the momentum operator commutes with free space Hamiltonian, and since it does not explicitly depend on time then momentum is indeed a constant of motion.
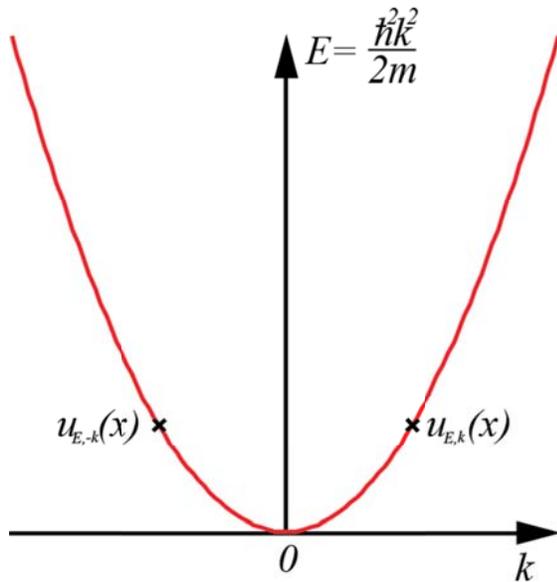
$$\left.\begin{array}{c} \hat{p} = -i\hbar\frac{\partial}{\partial x} \Rightarrow \frac{\partial\hat{p}}{\partial t} = 0 \\ \\ \left[\hat{p},\hat{H}\right] = 0 \end{array}\right\} \Rightarrow \frac{d}{dt}\langle\hat{p}\rangle = 0$$

Therefore the momentum is a conserved quantity and its eigenvalues can be used to label the states. Then the unique labels for the eigenfunctions above would be:

$$u_{E,k}(x) = e^{ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$u_{E,-k}(x) = e^{-ikx}$$

In fact we represent all the eigenfunctions (eigenstates) of the free space Hamiltonian and the momentum on the E vs k plot. Every point on this plot uniquely and completely specifies the state.

Graph with vertical axis $E = \dfrac{\hbar^2 k^2}{2m}$ and horizontal axis k, with parabola. Points marked $u_{E,-k}(x)$ on left and $u_{E,k}(x)$ on right, origin labeled 0.

Conserved Quantities Example II: Parity operator and symmetric potentials

Definition of a parity operator: $\hat{\Pi}\psi(x) = \psi(-x)$

What are the eigenfunctions and eigenvalues of the parity operator:

$$\hat{\Pi}u(x) = \lambda u(x) \Rightarrow \hat{\Pi}\hat{\Pi}u(x) = \hat{\Pi}\lambda u(x) \Rightarrow \hat{\Pi}\hat{\Pi}u(x) = \lambda\hat{\Pi}u(x) \Rightarrow u(x) = \lambda^2 u(x) \Rightarrow \lambda = \pm 1$$

The eigenfunctions of the parity operator all are either odd or even.

$f(-x) = f(x)$ even

$f(-x) -= f(x)$ odd□

Does Hamiltonian for Simple Harmonic Oscillator commute with the parity operator?

$$\hat{H}(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 \Rightarrow \hat{H}(-x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial(-x)^2} + \frac{1}{2}m\omega^2(-x)^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2 = \hat{H}(x)$$

Let's check the commutator:

$$\left[\hat{\Pi}, \hat{H}\right]\psi(x) = \hat{\Pi}\hat{H}\psi(x) - \hat{H}\hat{\Pi}\psi(x) = \hat{\Pi}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right)\psi(x) - \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right)\psi(-x) =$$

$$= \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial(-x)^2} + \frac{1}{2}m\omega^2(-x)^2\right)\psi(-x) - \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right)\psi(-x) = 0$$

This means that one can always find a set of eigenfunctions common to $\hat{H}$ and $\hat{\Pi}$. In fact, last lecture we have shown that SHO eigenfunctions are always even or odd.

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