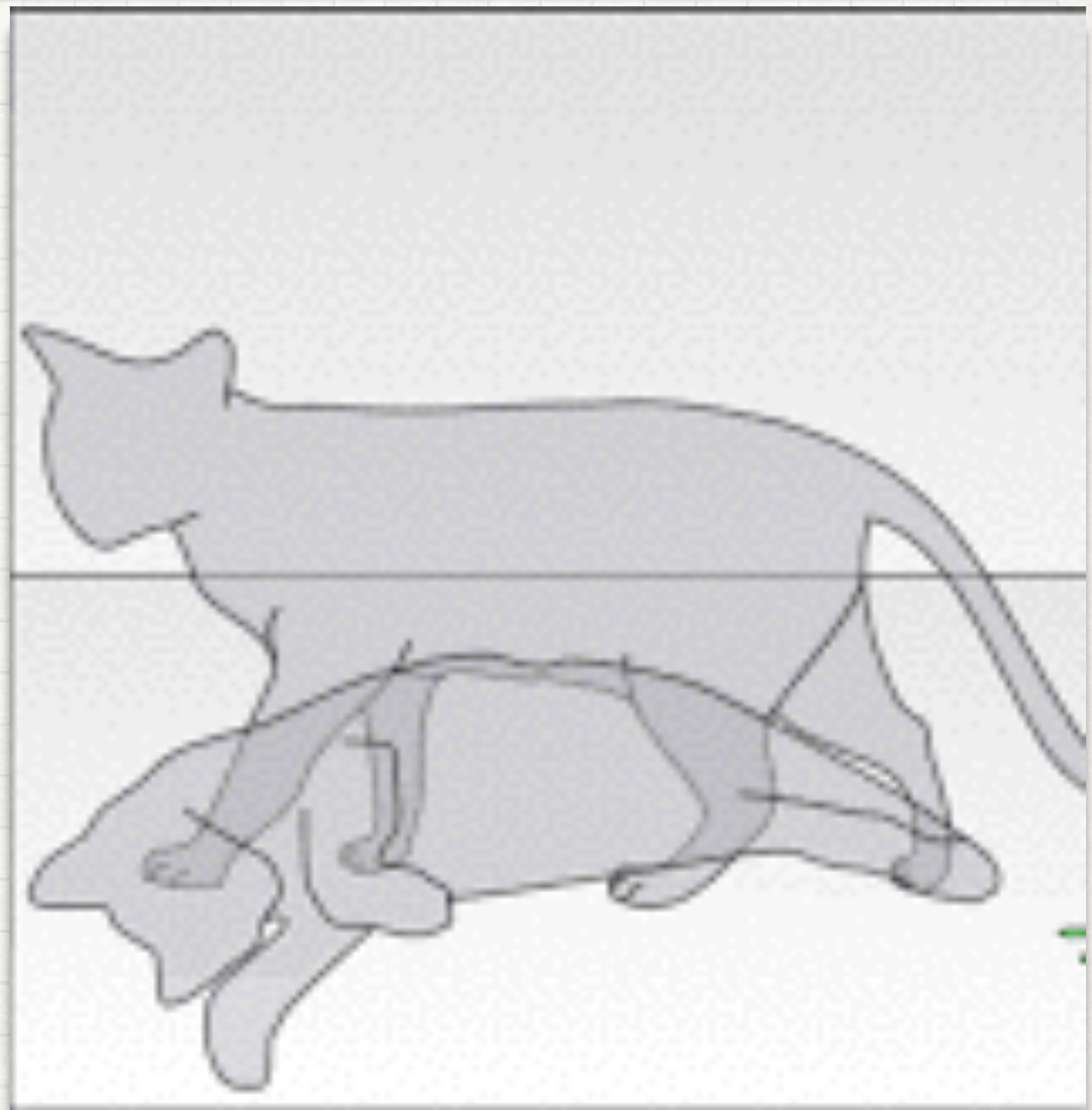
CHAPTER 4

MAKING PREDICTIONS IN QM



Rules of the game of non-relativistic quantum mechanics (Schrödinger picture)

* a physical system at any given time is associated to a "ray" in Hilbert space

$$|\psi(t)\rangle$$

NB: The "ray" reduces to a "vector" when the normalization condition is enforced

* The time evolution of the quantum state is determined by the Schrödinger equation:

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

* Any experimentally observable quantity *O* is associated to an hermitian operator Ô in this Hilbert space

* The possible outcomes of the observation of a quantity *O* associated to the operator Ô are only its eigenvalues o_i. The probability of observing o_i can be calculated by computing the square modulus of the projection on the corresponding eigenstate $|o_i\rangle$: *i.e.*

$$P(o_i) = |\langle o_i|\psi(t)\rangle|^2$$

* After the measurement, leading to a result o_i, the system is collapsed in a quantum state given by the corresponding eigenvector $|o_i\rangle$

Three Important Theorems:

1) Suppose a system is in the quantum state of a system is | **ψ**> , then the **average** outcome of a measurement of an observable Ô is given by the so-called **expectation value:**

$$\langle O \rangle = \langle \psi | \hat{O} | \psi \rangle$$

Corollary 1: if | **ψ**> is an eigenstate of Ô with eigenvalue o then the expectation value trivially leads <O>=o.

Corollary 2: in coordinate representation, the expectation value is written as

$$\langle O \rangle = \frac{\int dx\ \phi^*(x,t)\ \hat{O}_x\ \phi(x,t)}{\int dx \phi^*(x,t)\phi(x,t)}$$

In this equation **φ**(x,t) = < x|**ψ**(t)> is the wave function associated to the state in coordinate representation and Ôx is defined by the projection of Ô:

$$\langle x | \hat{O} | x' \rangle = \delta(x - x')\ \hat{O}_x$$

2) Let us consider a generic hermitian operator O which is an analytic function of momentum and position operators:

$$\hat{O} = f(\hat{P}, \hat{X})$$

Then, the projection of Ô into coordinate representation is built as follows

$$\langle x|\hat{O}|x'\rangle = \delta(x - x')\ \hat{O}_x = \delta(x - x')\ f\left(-i\hbar\frac{\partial}{\partial x}, x\right)$$

3) Two hermitian operators Ô, Ê have the same complete orthonormal set of eigenstates if and only if their **commutator** vanishes:

$$[\hat{O}, \hat{E}] \equiv \hat{O}\hat{E} - \hat{E}\hat{O} = 0$$

What do expectation values mean in practice?

Consider a system in a generic state described by a the wave function $\psi(x)$. The result of performing a measurement of the observable associated to the operator O will yield a different result:

outcome: average:

N independent measurements ⇒ $O_1 = O$, $O_2 = O'$, ..., $O_{N-1} = O''$, $O_N = O'$ ⇒

$$\lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} O_i \equiv \langle O \rangle$$

Now consider the special case in which $\psi(x)$ is an eigenstate of O, with eigenvalue o:

⇒ $O_1 = o$, $O_2 = o$, $O_3 = o$, $O_4 = o$, $O_5 = o$, ... ⇒ All measurements yield the same result!

Examples of construction of operators O(X, P):

Kinetic energy: $$T = \frac{p^2}{2m} \quad \Rightarrow \hat{T} = -\frac{\hbar^2}{2m}\hat{\nabla}^2$$

Potential energy: $$V = V(x) \Rightarrow \hat{V} = V(x)$$

Angular Momentum: $$\vec{L} = \vec{r} \times \vec{p} \qquad \Rightarrow \hat{\vec{L}} = \hat{\vec{r}} \times (-i\hbar\hat{\vec{\nabla}})$$

Assuming normalised wave-functions, the expectation value read:

Average kinetic energy

$$\langle T \rangle = -\frac{\hbar^2}{2m}\int dx \; \psi^*(x)\nabla^2\psi(x)$$

Average potential energy

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

Excercize: Consider the wave function

$$\psi(x) = C\ e^{-\frac{x^2}{4\sigma^2}}$$

1) normalise it by determining C
2) compute <T> and <V>
3) Show that it is an eigenstate of the Harmonic oscillator Hamiltonian!
4) find the corresponding eigenvalue!
5) Is the function

$$\phi(x) = C' \sin(x) e^{-\frac{x^2}{4\sigma^2}}$$

an eigenstate of H?

Example: Consider an eigenstate of the Hamiltonian H

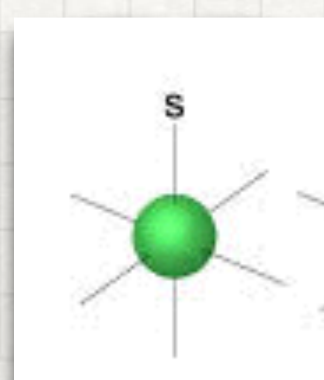
$$\hat{H}\psi_n(x) = E_n\psi_n(x)$$

If my physical system is in the quantum state described by the wave function $\psi_n(x)$ then each measurement of the total energy will give the result E_n !!!!

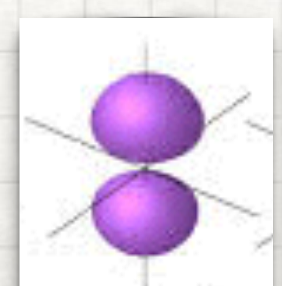
COROLLARY:
an isolated system initially prepared in an eigenstate of H will remain there forever!

NB:
this is not true if the system is <u>not</u> isolated: for example photons can excite the state of molecules:

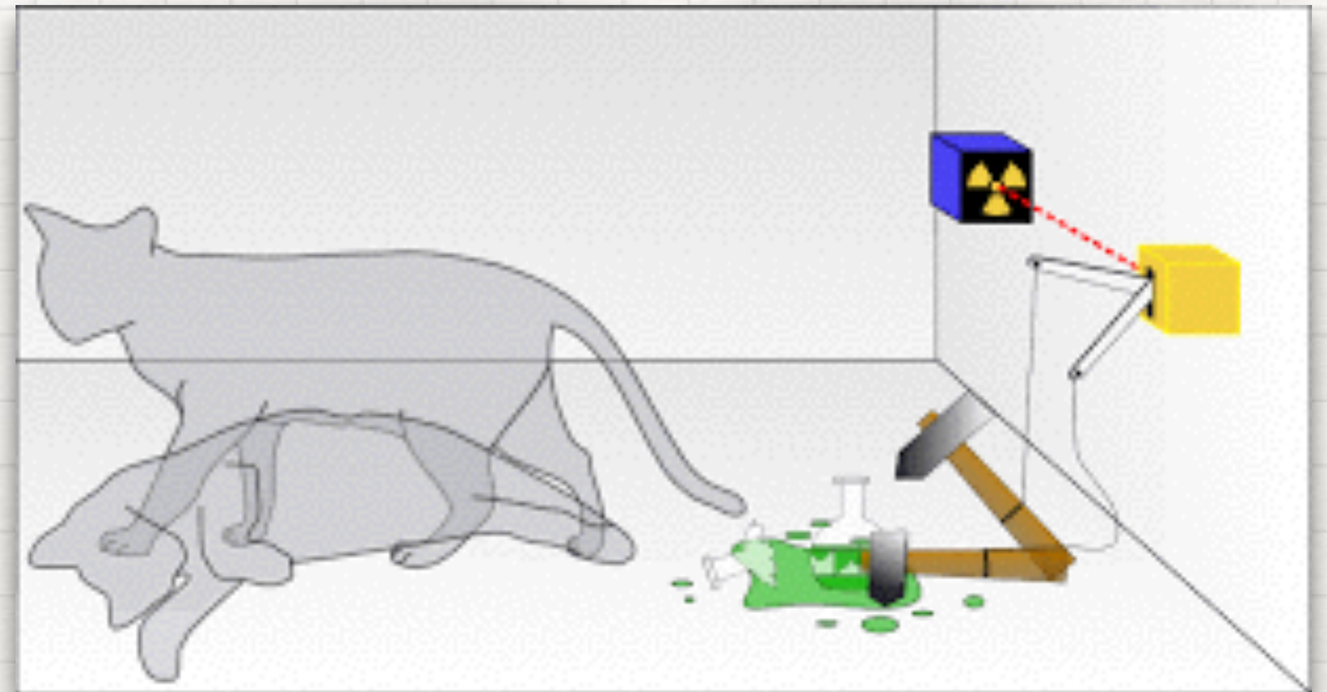
photon



$$\psi_n(x) \rightarrow \psi_m(x)$$



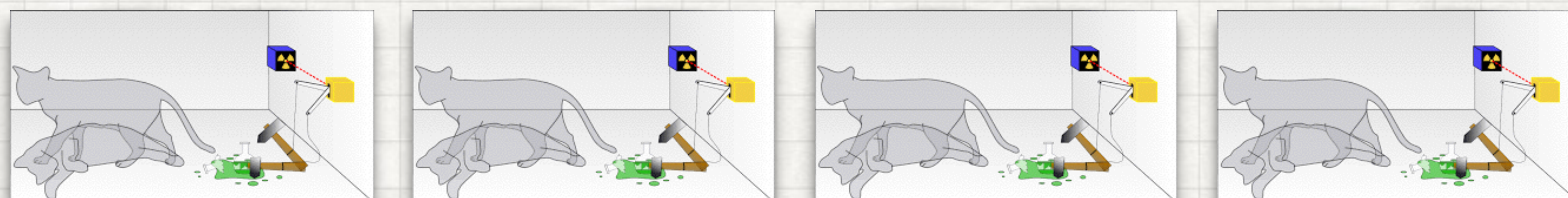
Schrödinger's Cat



The cat is simultaneously dead and alive !

It collapses to either state only upon observation

Expectation value:



=> Average fraction of alive cat at time t <f(t)>