All you need to know about QM for this course

$\Psi(q)$

State of particles is described by a complex contiguous wave function $\Psi(q)$ of some coordinates q. Coordinates q could be $(t,\mathbf{x})$ or $(E,\mathbf{p})$, but not both, plus some other coordinates (e.g., particle's spin projection).

$dP=|\Psi(q)|^2 dq$

$dP=|\Psi(q)|^2 dq$ represents probability (or can be just proportional to probability, depending on the choice of normalization) of finding particle with coordinates q in interval dq (assuming that q is contiguous variable, like coordinate x or momentum p). Note: $\Psi(q)$ is not uniquely defined, i.e. $\Psi'(q)=\Psi(q)e^{i\alpha}$ leads to the same probabilities.

$\Psi(q)= \alpha\Psi_1(q)+ \beta\Psi_2(q)$

If $\Psi_1(q)$ describes some physical state 1 and $\Psi_2(q)$ describes a physical state 2, $\Psi(q)= \alpha\Psi_1(q)+ \beta\Psi_2(q)$ describes a new physical state of superposition of the two states 1 and 2.

$\Psi(q_1, q_2)= \Psi_1(q_1)\Psi_2(q_2)$

If $\Psi_1(q_1)$ describes a particle 1, $\Psi_2(q_2)$ describes a particle 2, and these particles do not interact, then their common wave function $\Psi(q_1, q_2)= \Psi_1(q_1)\Psi_2(q_2)$

Fermions and Bosons

Indistinguishable particles should obey either Fermi-Dirac or Bose-Einstein statistics. The general names for these two classes of particles are therefore fermions and bosons

1. Fermions must have their wave functions anti-symmetrical under permutations of any pair of such particles:
$$(1 \leftrightarrow 2) \quad \Rightarrow \quad \Psi(q_1, q_2)= -\Psi(q_2, q_1).$$

    Bosons should have wave functions symmetric under swapping any pair of such particles:
$$(1 \leftrightarrow 2) \quad \Rightarrow \quad \Psi(q_1, q_2)= \Psi(q_2, q_1).$$

2. Two important fermion properties:
    i. It is easy to show that no two fermions can be in the same states. From the opposite, let's assume that there are two fermions with exactly the same wave functions Ψ_0. The combined wave function of two particles is $\Psi_A=\Psi_1(q_1)\Psi_2(q_2) =\Psi_0(q_1)\Psi_0(q_2)$. After switching two fermions, the new function is $\Psi_B=\Psi_0(q_2)\Psi_0(q_1)$. The two functions are required to be different by sign; however, they are clearly identical. This can be true only if $\Psi_0=0$.
    ii. A composite particle made of even number of fermions must be a boson, and a composite particle made of odd number of fermions must be a fermion. Indeed, let's put two identical composite particles next two each other and assume that the number of fermions in each of them is N. Switching one pair of fermions between two composite particles, changes sign of the wave function. After switching all N pairs, we effectively switched the two composite particles, and the new wave function sign is $(-1)^N$. If N is even, the overall sign has not changed and, therefore, the composite particles must have been bosons.

3. Two important boson properties:
    i. There is no limit on the number of boson that can take exactly the same states.
    ii. A composite particle made of bosons must be a boson.

Wave Function Evolution. Measurement.

The notion of an experiment (observation) is the key in the conventional (Copenhagen) interpretation of QM: only by conducting an experiment one can localize a particle with probabilities calculated according to $\Psi(q)$. Before an experiment is conducted, the particle is at neither coordinate (i.e., one should not associate the wave function with some physical smeared distribution of matter). The quantitative role of QM is to give deterministic description of the evolution of $\Psi(q)$, rather than in deterministic predictions for the outcome of experiments. In general, QM can give only probabilistic predictions for the experiment outcome. Equation describing time evolution of Ψ can often be written as

$$i\frac{\partial}{\partial t}\Psi = \hat{H}\Psi, \text{ where } \hat{H} \text{ is some operator acting on function } \Psi.$$

It was shown that the QM probabilistic description could not be reduced to some deterministic, but hidden parameters.

Observable variable and Operator. Eigenstates.

1. Any measurable physical parameter g can be associated with some linear operator $\hat{g}$, such that, if one knows the particle wave function $\Psi(q)$, the average measured value $\overline{g}$ can be calculated according to the integral:

$$\overline{g} = \int \Psi^+ \hat{g}\Psi dq, \text{ where } \Psi^+ \text{ is conjugated and transposed vector } \Psi;$$

    while the spectrum of allowed g-values is found from the following (in general, differential) equation:
$$\hat{g}\Psi = g\Psi .$$

2. This equation may lead to a contiguous or discrete set of solutions of g_m and Ψ_m .

    States Ψ_m and Ψ_n for which $g_m{\neq}g_n$ are orthogonal: $\int \Psi_n^+\Psi_m dq = 0$

    If there are a few wave functions with a common g_k , then any linear combination of them is also a solution. And one can always mix such functions in such a way that their linear combinations also become orthogonal to each other.

3.   Discrete solutions usually result from "bounding" conditions, for example:
    - constraining a particle to be in a potential box of size a → discrete energy levels $\sim n\frac{1}{a}$
    - requirement that $\Psi(\varphi+2\pi)=\Psi(\varphi)$ → discrete values for angular momentum: 0, ±1, ±2, …

Wave function normalization

1.   Any general state of a particle can be represented as a linear combination of eigenstates. It is very instructive to revoke a geometrical analogy of a general unit vector being expressed in terms of base unit vectors.

For a set of discrete eigenstates:

$\Psi(q) = \sum c_m \Psi_m(q)$ where

$P_m = |c_m|^2$ would define a probability of being in state m, all probabilities adding up to 1: $\sum |c_m|^2 = 1$

For a set of contiguous eigentstates

$\Psi(q) = \int c(\nu) \Psi_\nu(q) d\nu$ where

$dP = |c(\nu)|^2 d\nu$ defines a probability for a particle to have ν in an interval $d\nu$,

the integral probability over all states being equal to 1: $\int |c(\nu)|^2 d\nu = 1$

2.   Condition of wave function orthogonality and the total probability normalizations can be combined in one equation as follows:

$\int \Psi_n^+ \Psi_m dq = \delta_{mn}$ for discrete spectrum states, and

$\int \Psi_{\nu'}^+ \Psi_\nu dq = \delta(\nu' - \nu)$ for contiguous spectrum states

The former conditions are obvious. Normalization of contiguous spectrum wave functions on the δ-function insures interpretation of c(ν) coefficients as given above. Indeed,

$$\Delta P = \int_{-\infty}^{+\infty} \Psi^+(q)\Psi(q)dq = \int_{-\infty}^{+\infty} dq \int_{\Delta\nu'} \Psi_{\nu'}^+(q)c^+(\nu')d\nu' \cdot \int_{\Delta\nu} c(\nu)\Psi_\nu(q)d\nu =$$

$$= \iint \left(\int \Psi_{\nu'}^+(q)\Psi_\nu(q)dq \right) \cdot c^+(\nu')c(\nu)d\nu'd\nu =$$

$$= \iint \delta(\nu' - \nu) \cdot c^+(\nu')c(\nu)d\nu'd\nu =$$

$$= \int_{\Delta\nu} |c(\nu)|^2 d\nu$$

A few operators for function Ψ(t,x)

a) coordinates: $\hat{x} = x, \quad \hat{y} = y, \quad \hat{z} = z$

b) momenta: $\hat{p}_x = -i\dfrac{\partial}{\partial x}, \quad \hat{p}_y = -i\dfrac{\partial}{\partial y}, \quad \hat{p}_z = -i\dfrac{\partial}{\partial z}$

c) full energy (Hamiltonian): $\hat{H} = i\dfrac{\partial}{\partial t}$ (i.e., it is Hamiltonian that drives the wave function evolution).

d) kinetic energy (non-relativistic!): $\hat{E} = \dfrac{\hat{p}^2}{2m} = -\left(\dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2}\right)$

e) potential energy: $\hat{V} = V(x, y, z)$

f) angular momentum: $\hat{l}_z = x\hat{p}_y - y\hat{p}_x, \quad \hat{l}_x = y\hat{p}_z - z\hat{p}_y, \quad \hat{l}_y = z\hat{p}_x - x\hat{p}_z, \quad \hat{l}^2 = \hat{l}_x^2 + \hat{l}_y^2 + \hat{l}_z^2$

   or in polar coordinates (R,θ,φ): $\hat{l}_z = -i\dfrac{\partial}{\partial \varphi}$ and $\hat{l}^2 = -\left[\dfrac{1}{\sin^2\theta}\dfrac{\partial^2}{\partial\varphi^2} + \dfrac{1}{\sin\theta}\dfrac{\partial}{\partial\theta}\left(\sin\theta\dfrac{\partial}{\partial\theta}\right)\right]$

Note that coordinate operators (a) follow from the definition of Ψ(t,**x**). Operators (b), (c), (f) can be derived by considering invariance of physics laws under translations in space (b), time (c), and angular rotations (f). Operators (f) also can be easily obtained by substituting QM momentum operators for momenta in the classical mechanics equations for angular momentum. Operators for kinetic and potential energies can also be obtained the same way.

Hamiltonian Eigenstates

Note that Hamiltonian plays the dual role: it drives the wave function evolution and is the operator of the full energy $\hat{H}\Psi = E\Psi$. For an enclosed system Hamiltonian cannot depend on time and it obviously commutates with itself. Therefore, the latter equation should have a set of stationary solutions Ψ_m with conserved energy values of E_m. Combining the two equations, one can easily obtain the explicit form of time dependence of Ψ_m functions:

$$\hat{H}\Psi_m = E_m\Psi_m \quad \text{and} \quad i\frac{\partial}{\partial t}\Psi_m = \hat{H}\Psi_m,$$

from where: $\quad i\dfrac{\partial}{\partial t}\Psi_m = E_m\Psi_m,$

which has factorized solutions: $\Psi_m(t, x, y, z) = e^{-iE_m t}\psi_m(x, y, z).$

Then, any arbitrary state can be written as: $\Psi(t, x, y, z) = \sum_m c_m\, e^{-iE_m t}\, \psi_m(x, y, z).$

Momentum Eigenstates

Eigenstates for momentum operator can be found from the corresponding differential equation:

$$\hat{p}_x\psi(x, y, z) = p_x\psi(x, y, z)$$

$$-i\frac{\partial}{\partial x}\psi(x, y, z) = p_x\psi(x, y, z)$$

which has solutions: $\psi_{p_x}(x, y, z) = e^{ip_x x}\chi(y, z).$

Generalizing for other coordinates: $\psi_{\vec{p}}(\vec{r}) = Ce^{ip_x x + p_y y + p_z z} = Ce^{i\vec{p}\vec{r}}$

Normalization[1] on the δ-function $\int \Psi_{p'}^+\Psi_p\, dxdydz = \delta(p' - p)$ results in $C = 1/(2\pi)^{3/2}$.

A general wave function can be, thus, presented as a superposition of momentum eigenstates:

$$\psi(\vec{r}) = \int c(\vec{p})\psi_{\vec{p}}(\vec{r})d^3p = \frac{1}{(2\pi)^{3/2}}\int c(\vec{p})e^{i\vec{p}\vec{r}}d^3p, \quad \text{where } d^3p = dp_x dp_y dp_z.$$

Therefore, $\psi(\vec{r})$ and $c(\vec{p})$ are Fourier transformations of each other.

Full Wavefunction

1) Combining time- and space-dependent parts, the full wave function of a free particle:

$$\Psi(\text{E,}\vec{\text{p}}) = \frac{1}{(2\pi)^{3/2}}e^{-i(Et - \vec{p}\vec{r})}$$

2) For a particle in a fixed size volume V, the wave function can be written as $\Psi = Ce^{-i(Et - \vec{p}\vec{r})}$, where $C = 1/\sqrt{V}$ and there are only discrete solutions for allowed energy eigenstates. Setting $C = 1/\sqrt{V}$ ensures that the integrated probability of finding the particle in the full volume V equals to one: $\int |\Psi|^2\, dV = 1$.

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[1] Here one should use the property : $\displaystyle\int_{-\infty}^{+\infty} e^{i\alpha x}\, dx = 2\pi\delta(\alpha)$

Angular Momentum Eigenstates

1. Solutions for the operator of l_z can be easily found in polar coordinates:

$$\hat{l}_z \Psi = l_z \Psi, \quad \text{or} \quad -i\frac{\partial}{\partial \varphi}\Psi(R,\theta,\varphi) = m\Psi(R,\theta,\varphi),$$

which has solutions: $\Psi(R,\theta,\varphi) = e^{im\varphi} f(R,\theta)$.

From a natural boundary condition of $\Psi(\varphi+2\pi)=\Psi(\varphi)$, one can see that l_z can be equal only to integer numbers.

2. Since l^2 and l_z operator commutate, there should be solutions with definite l^2 and l_z, or, for short, l and m. These solutions can be written in factorized form (p-functions are not normalized):

$$\Psi(R,\theta,\varphi) = f(R)p_l^m(\theta)e^{im\varphi}, \text{where}$$

$$p_0^0(\theta) = 1$$

$$p_1^0(\theta) = \cos\theta, \quad p_1^{\pm 1}(\theta) = \mp\sin\theta$$

$$p_2^0(\theta) = 3\cos^2\theta - 1, \quad p_2^{\pm 1}(\theta) = \mp\cos\theta\sin\theta, \quad p_2^{\pm 2}(\theta) = \sin^2\theta$$

etc...

For fixed l, there are $2l+1$ possible l_z-projections from l to l and $\Delta l_z = 1$.

In-class exercises:

- Show how a energy/momentum quantization arises for a particle constrained to be between two walls.

- Show that extra *finite-size* extra dimensions lead to an apparent (as perceived by an observer in the 3d-space) infinite series of particles with the same properties, but larger and larger masses. Consider "compactified" (circular) or "thin-sheet-like" extra dimensions.

Simultaneously measurable variables

Note that eigenstates for operators $\hat{g}$ and $\hat{f}$ do not necessarily coincide. In this case, we say that values g and f cannot be simultaneously and precisely determined. For two physical parameters to be simultaneously defined, their operators should be commutative, i.e.

$$\hat{g} \cdot \hat{f} = \hat{f} \cdot \hat{g}, \quad \text{or } [\hat{g},\hat{f}] \overset{def}{=} \hat{g} \cdot \hat{f} - \hat{f} \cdot \hat{g} = 0$$

Uncertainty principle

Note that operators of x and p_x do not commutate: $[x, \hat{p}_x] = x\hat{p}_x - \hat{p}_x x = i$. Therefore, they cannot be precisely known at the same time. This leads to the famous Heisenberg's uncertainty principle (1927):

$$\Delta x \cdot \Delta p_x \sim 1$$

This has a number of implications:

- **a particle constrained in space within dx, will have uncertainty in momentum of dp~1/dx**

- **a particle scattered so that its momentum changes by dp can resolve spatial structures of dx~1/dp**

There is a similarly-looking equation for $\Delta t \cdot \Delta E \sim 1$, which, for example, implies that

- **a particle of mass M can pop up into existence for a short time dt~1/M**

- **a particle of mass M and lifetime of τ may be produced with an invariant mass (e.g., judging by its decay products) slightly larger or smaller than its nominal mass, the typical spread being dM~1/τ**

More examples

What can and cannot be measured simultaneously (check commutator):
- YES: x, y, z coordinates
- YES: all momentum components (p_x, p_y, and p_z) and the kinetic energy
- NO: x and p_x
- NO: time and full energy
- YES: x, p_y, and p_z
- NO: L_x and L_y or any other pair ($[L_x,L_y]=iL_z$)
- YES: L_z and L^2 (and similarly for x- and y-components)
- YES: L_z and p_z (and similarly for x- and y-components)
- NO: L_z and p_x or L_z and p_y
- YES: L_z and z (and similarly for x- and y-components)
- YES: L^2, S^2, J^2, and J_z, where vector **J** is a full angular moment **J**=**L**+**S**

Spin

Symmetry of equations with respect to rotations allows introducing a plain <u>internal</u> angular momentum S (called spin) even for point-like particles without requiring anything physically spinning inside. Commutation rules for angular momentum projection operators require that Δl_z or ΔS_z must be an integral number. So the total number of projections for particles with spin S is 2S+1: -S, -S+1, -S+2, …, -1, 0, 1, 2, …, S-1, S, where spin S can take values of only 0, ½, 1, 3/2, 2, etc.

Spin-½ particle z-projection eigenstates can be presented as:

$$\Psi_{up} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \varphi(x) \qquad \Psi_{down} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \chi(x)$$

And a general wave function and its conjugated state become:

$$\Psi(q) = \begin{pmatrix} \chi_1(q) \\ \chi_2(q) \end{pmatrix} \quad \text{and} \quad \Psi^\dagger(q) = \left(\chi_1^*(q),\ \chi_2^*(q) \right)$$

Spin operators are matrices. For spin-½ particles, the operators are:

$$\hat{S}_z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \hat{S}_x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{S}_y = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Pauli proved a theorem that half-integer-spin particles are fermions and integer-spin particles are bosons.