C/CS/Phys 191 Quantum Mechanics in a Nutshell I 10/04/05
Fall 2005 Lecture 11

In this and the next lecture we summarize the essential physical and mathematical aspects of quantum mechanics relevant to this course. Topics in this set of notes: Planck-Einstein, postulates, operators, representations.

Planck-Einstein Relation $E = h\nu$

This is the equation relating energy to frequency. It was the earliest equation of quantum mechanics, implying that energy comes in multiples ("quanta") of a fundamental constant h. It is written as either

$$E = h\nu$$

or

$$E = \hbar\omega$$

where $\hbar = h/2\pi$. ν is linear frequency and ω is angular frequency. The fundamental constant h is called Planck's constant and is equal to 6.62608×10^{-34} Js ($\hbar = 1.05457 \times 10^{-34}$ Js, or 1.05457×10^{-27} erg s).

This relation was first proposed by Planck in 1900 to explain the properties of black body radiation. The interpretation was that matter energy levels are quantized. At the time this appeared compatible with the notion that matter is composed of particles that oscillate. The discovery that the energy of electrons in atoms is given by discrete levels also fitted well with the Planck relation. In 1905 Einstein proposed that the same equation should hold also for photons, in his explanation of the photoelectric effect. The light incident on a metal plate gives rise to a current of electrons only when the frequency of the light is greater than a certain value. This value is associated with the energy required to remove an electron from the metal (the "work function"). The electron is ejected only when the light energy matches the discrete electron binding energy. Einstein's proposal that the light energy is quantized just like the electron energy was more radical at the time: light quantization was harder for people to accept than quantization of energy levels of matter particles. (The word "photon" for these quantized packets of light energy came later, given by G. N. Lewis, of Lewis Hall!)

1 Fundamental physical postulates

Why do quantum state evolve in time according to this particular operator, and what is the meaning of this operator? To answer this we have to look at quantum mechanics from a more physical perspective. The physical basis of quantum mechanics rests on three fundamental postulates. These are given below in the wording of K. Gottfried and T. M. Yan (Quantum Mechanics: Fundamental, Springer 2003).

I. States, superposition The most complete description of the *state* of any physical system S at any time is provided by some vector $|v\rangle$ in the Hilbert space H appropriate to the system. Every linear combination of such state vectors $|\Psi\rangle$ represents a possible physical state of S.

This last sentence is the *superposition principle* that we have been using from the very beginning. Note the difference between a quantum and a classical description of a physical system. A classical description is complete with specification of the positions and momenta of all particles, each of which can be precisely measured at any time. In contrast, the quantum description is specified by the wave function $|\Psi\rangle$ that lives in an abstract Hilbert space that has no direct connection to the physical world. Classical mechanics is deterministic - particle positions and momenta can be specified for all times using the classical equations of motion. In contrast, quantum mechanics provides a statistical prediction of the outcomes of all observables on the system as the wave function $\left|\Psi\right\rangle$ evolves. Both descriptions are "complete" but they differ in the information that can be obtained. The uncertainty principle fundamentally changes the relation between coordinates and momenta in quantum mechanics.

II. Observables The physically meaningful entities of classical mechanics, such as position (q or x), momentum (p), etc. are represented by Hermitian operators. Following Dirac, we refer to these as "observables". We generalize these today to any physical meaningful entities, i.e., including those observables that have no classical correspondence (e.g., intrinsic spin).

III. Probabilistic interpretation and Measurement A set of N replicas of a quantum system S described by a state $\left|\Psi\right\rangle$ when subjected to measurements for a physical observable A, will yield in each measurement one of the eigenvalues $\{a_1, a_2, ...\}$ of $\hat{A}$ and as $N \to \infty$ this eigenvalue will appear with probability $P_\Psi(a_1), P_\Psi(a_2), ...$ where

$$P_\Psi(a_i) = |\left\langle a_i \middle| \Psi \right\rangle|^2$$

and $\left|a_i\right\rangle$ is the eigenvector corresponding to the eigenvalue a_i.

This is precisely the definition of probability in terms of specific outcomes in a sequence of identical tests on copies of S, provided that

$$\sum_i P_\Psi(a_i) = \sum_i |\left\langle a_i \middle| \Psi \right\rangle|^2 = \left\langle \Psi \middle| \Psi \right\rangle = 1.$$

This is automatically satisfied for states that are normalized to unity.

The expectation value of an observable A in an arbitrary state $\left|\Psi\right\rangle$ also looks like an average over a probability distribution:

$$\begin{aligned} \langle A \rangle_\Psi &= \left\langle \Psi \middle| \hat{A} \middle| \Psi \right\rangle \\ &= \sum_i \left\langle \Psi \middle| a_i \right\rangle a_i \left\langle a_i \middle| \Psi \right\rangle \\ &= \sum_i a_i P_\Psi(a_i). \end{aligned}$$

Note that if the state Ψ is an eigenstate of A, then

$$\left\langle \Psi \middle| A \middle| \Psi \right\rangle = a_j$$

where a_j is the corresponding eigenvalue, i.e., only a single term contributes.

We can generalize this procedure from projection onto eigenstates to projection onto an arbitrary state $\left|\phi\right\rangle$. Thus, the probability to find a quantum system S that is in state $\left|\Psi\right\rangle$ in another state $\left|\phi\right\rangle$ is equal to

$$P_\Psi(\phi) = |\left\langle \phi \right| \left| \Psi \right\rangle|^2.$$

This projection of the ket $\left|\Psi\right\rangle$ onto another state, be it an eigenfunction of some operator $\left|a_i\right\rangle$, a basis function for the Hilbert space $\left|v_i\right\rangle$, or an arbitrary state $\left|\phi\right\rangle$, is referred to as a "probability amplitude", since its square modulus is a probability. Note that the probability amplitude is specified both by $\left|\Psi\right\rangle$ *and* the other state: the latter specifies the "representation" of $\left|\Psi\right\rangle$ which realizes the quantum state in a measurable basis. The probability amplitude is also referred to as the "wave function" in the specified "representation".

A single measurement of th observable A on a state $\left|\Psi\right\rangle$ in the basis (representation) of eigenstates of $\hat{A}$ will yield the value a_i, with probability $P_\Psi(a_i) = |\left\langle a_i\right| \Psi\rangle|^2$. This defines the measurement operator

$$\hat{M}_i = \left|a_i\right\rangle \left\langle a_i\right|$$

that acts on the state $\left|\Psi\right\rangle$. The normalized state after measurement is then easily seen to be equal to

$$\frac{\hat{M}_i\left|\Psi\right\rangle}{\sqrt{\left\langle\Psi\right| M_i^\dagger M_i\left|\Psi\right\rangle}}.$$

For a measurement in the $\left|a_i\right\rangle$ basis this is given by

$$\left|i\right\rangle \frac{\left\langle i\right| \left|\Psi\right\rangle}{\sqrt{\left\langle\Psi\right| M_i^\dagger M_i\left|\Psi\right\rangle}},$$

where we have abbreviated

$$\left|a_i\right\rangle \equiv \left|i\right\rangle.$$

For example, suppose we have the linear superposition

$$\left|\Psi\right\rangle = \alpha_1\left|1\right\rangle + \alpha_2\left|2\right\rangle + \alpha_3\left|3\right\rangle + ... + \alpha_k\left|k\right\rangle.$$

Making a single measurement of the observable A on $\left|\Psi\right\rangle$ will result in the outcome a_i with probability

$$P_\Psi(a_i) = |\alpha_i|^2$$

and the resulting state after the measurement is equal to

$$\left|i\right\rangle \left(\frac{\alpha_i}{|\alpha_i|}\right).$$

The measurement of the observable has "collapsed" the state $\left|\Psi\right\rangle$ to a single eigenstate $\left|i\right\rangle \equiv \left|a_i\right\rangle$ of $\hat{A}$ (recall these constitute an orthonormal basis).

2 Operators

In an earlier lecture we defined the operator $P = |\nu\rangle\langle\nu|$ which projects an arbitrary state onto the state $|\nu\rangle$. For an orthonormal basis $\{|j\rangle\}$ we can define the set of projection operators $P_j = |j\rangle\langle j|$ which obey the so-called "completeness relation" $\sum_{j=1}^k P_j = \sum_j |j\rangle\langle j| = 1$.

A linear operator maps states (kets) onto linear combinations of other states (kets). Suppose a ket $|b\rangle$ is mapped to a ket $|a\rangle$: the operator for this is denoted by the outer product $|a\rangle\langle b|$. So the action of linear operators can easily be written in our bra-ket language, e.g.,

$$\begin{aligned} X|\psi\rangle &= |a\rangle\langle b|\psi\rangle \\ Y|\psi\rangle &= |c\rangle\langle d|\psi\rangle \\ XY|\psi\rangle &= |a\rangle\langle b|c\rangle\langle d|\psi\rangle. \end{aligned}$$

If one these kets is a superposition of states, e.g., $|a\rangle = \alpha|0\rangle + \beta|1\rangle$, then the resulting state is also a superposition, i.e.,

$$X|\psi\rangle = (\langle b|\psi\rangle\alpha)|0\rangle + (\langle b|\psi\rangle\beta)|1\rangle.$$

So the bra-ket notation is naturally suited to the linear nature of quantum mechanical operators.

The inner product in the center of the last equation is a number, so clearly the "product" XY is also an operator. We often denote operators by the notation $\hat{X}$. Note that the order of these operators matters: applying $\hat{X}\hat{Y}$ to $|\psi\rangle$ results in a state proportional to $|a\rangle$, while applying $\hat{Y}\hat{X}$ results in a state proportional to $|c\rangle$.

Now lets consider how to express an operator that acts on states in a Hilbert space spanned by an orthonormal set $|j\rangle$. We can write the operator in terms of its action on these basis states, by making use of the completeness relation:

$$\begin{aligned}\hat{X}|j\rangle &= \hat{I}\hat{X}|j\rangle \\ &= \sum_{j'} |j'\rangle\langle j'|\hat{X}|j\rangle \\ &= \sum_{j'} X_{j'j}|j'\rangle,\end{aligned}$$

where $X_{j'j}$ is the $j'j$th element of the matrix representing the linear action of $\hat{X}$ on the basis. Furthermore,

$$\begin{aligned}\hat{X} &= \hat{I}\hat{X}\hat{I} \\ &= \sum_{j,j'} |j\rangle\langle j|\hat{X}|j'\rangle\langle`j'| \\ &= \sum_{j,j'} X_{jj'}|j\rangle\langle j'|.\end{aligned}$$

The diagonal matrix element X_{jj} is often referred to as the "expectation value" of $\hat{X}$ on state $|j\rangle$.

An important global characteristic of operators is their trace:

$$Tr\hat{X} = \sum_j X_{jj}.$$

For finite dimensional spaces the trace is easy to evaluate and is easily seen to be independent of basis (hint: insert the unit operator in above equation).

From now on we will drop the "$\hat{X}$" notation, unless essential to avoid misunderstanding, and simply refer to the operator as X.

A general operator A has a number of related operators that have their analogs in matrix algebra. The operator transpose A^T is defined by

$$A^T = \sum_{jj'} |j\rangle\langle j'|A|j\rangle\langle j'|$$

and the operator complex conjugate A^* by

$$A^* = \sum_{jj'} |j\rangle\langle j|A|j'\rangle^*\langle j'|$$

If $A = A^T$, then A is a symmetric operator, while if $A = -A^T$ it is skew-symmetric. A very important related operator is the Hermitian adjoint

$$A^\dagger = (A^*)^T = \sum jj'|j\rangle\langle j'|Aj\rangle^*\langle j'|$$

If $A = A^\dagger$, then A is Hermitian.

Hermitian operators are essential to quantum mechanics. A basic postulate of quantum mechanics is that physically meaningful entities of classical mechanics, such as momentum, energy, position, etc., are represented by Hermitian operators. Dirac called these entities "observables". Hermitian operators have some useful properties that again have their analog in matrix algebra. Thus, starting from the basic definition of Hermitian adjoint

$$\langle k|A|k'\rangle^* = \langle k'|A^\dagger|k\rangle$$

which means that if

$$A|\psi\rangle = |\psi'\rangle$$

that

$$\langle\psi'| = \langle\psi|A^\dagger,$$

one can easily show that

$$(BA)^\dagger = A^\dagger B^\dagger.$$

Now if both A and B are Hermitian operators, $A^\dagger B^\dagger = BA$, whence

$$(BA)^\dagger = AB.$$

For this product operator to be also Hermitian, we require $AB = BA$ and this is only true if A and B commute. This commutation property is so important in quantum mechanics that we define a special notation for it. The commutator of two operators is defined as the operator

$$C = AB - BA = [A, B]$$

and the operators A and B commute if $C = [A, B] = 0$. Note that this result implies that if the commutator $[A, B] \neq 0$ and A, B are both observables, then the product AB is not an observable. We say that "A and B are incompatible observables".

Eigenvalues/Eigenvectors

Since linear operators can be represented by matrices (on finite dimensional complex vector spaces), all the relevant properties of such matrices follow also for operators. Thus,

- any single Hermitian operator A can be diagonalized by a unitary transformation

  $$U^\dagger AU = a,$$

  where $a_{ij} = a\delta_{ij}$.

- elements of the diagonalized form are real eigenvalues $a_1, a_2, ...a_d$ where d is the dimension of the complex vector space. They may be degenerate, i.e., several having the same value. The set $\{a_i\}$ is called the "spectrum" of $\hat{A}$.
- the eigenvalues are the roots of the secular equation

  $$det(A - aI) = 0,$$

  i.e., the roots of an algebraic equation of degree d.
- the basis vectors $|1\rangle, |2\rangle, ...|d\rangle$ that diagonalize A are the eigenvectors (eigenkets) and satisfy

  $$A|n\rangle = a_n|n\rangle.$$

  Hence we may write A in terms of its eigenvectors/eigenvalues as

  $$A = \sum_n |n\rangle a_n \langle n|.$$

  This is known as the spectral decomposition of A.
- eigenvectors with different eigenvalues are orthogonal.
- If $A_i, i = 1, 2, ...K$ is a set of commuting Hermitian operators, i.e.,

  $$[A_i, A_j] = 0$$

  then one can simultaneously diagonalize the operators with the same unitary transformation. The eigenvalues are $a_n^{(i)}$ and the eigenvectors satisfy

  $$\{A_i - a_n^{(i)}\}|a_n^{(1)} a_n^{(2)} ... a_n^{(K)}\rangle = 0$$

  where the ket is labelled by all of its eigenvalues.
- If A, B are Hermitian and do not commute, they cannot be simultaneously diagonalized.

Hermitian operators and unitary evolution (once again)

Unitary matrices are related to Hermitian matrices, as

$$U = e^i A,$$

since $U^\dagger = exp(-iA^\dagger) = exp(-iA)$ and hence $UU^\dagger = 1$.

What do we mean by the exponential of a linear operator? Think matrix representation:

$$e^{iAt} = 1 + (iAt) + \frac{(iAt)^2}{2} + \frac{(iAt)^3}{3} + ...$$

with

$$A^n = AA...A$$

the n-fold product. This is fine as long as the operator A is not dependent on time itself, in which case we need to be more careful.

The unitary time evolution of quantum systems is determined by the Hermitian operator H which corresponds to the observable of the system energy, according to

$$U(t) = e^{-(i/\hbar)Ht}$$

where t is the time and $\hbar$ a fundamental constant, Planck's constant, which has units of energy-time (Joule-sec). The Hermitian operator H is called the "Hamiltonian" and the above equation is a solution of the time dependent Schrodinger equation. We shall give a heuristic derivation of this below by combining some physical reasoning with the abstract framework of quantum states and operators.

3 Time evolution of real quantum systems

Given the three postulates relating the mathematical framework of quantum to physical systems, together with the Planck-Einstein relation, we can now make a heuristic derivation of the time dependent Schrodinger equation. One simple but critical leap of "analogy" to classical mechanics will be required.

Time evolution is characterized by a continuous parameter t. Because of superposition (postulate I) , this time evolution must be characterized by a linear transformation in the Hilbert space:

$$|\Psi;t\rangle = L_t|\Psi;0\rangle$$

Conservation of probability tells us that

$$\langle\Psi;t|\Psi;t\rangle = \langle\Psi;0|\Psi;0\rangle$$

Hence we conclude that $L_t^\dagger L_t = 1$, i.e., L_t is unitary, so write as $U(t)$. More precisely then,

$$|\Psi;t'\rangle = U(t',t)|\Psi;t\rangle$$

If the time origin is not important, U depends only the the time difference, i.e., $U(t'-t)$. We also want U to obey the composition law

$$U(t_2)U(t_1) = U(t_2+t_1).$$

Then we obtain

$$U(t) = [U(t/N)]^N.$$

Now consider what happens as we make the time interval infinitesimal. As $\delta t = t/N \to 0$, $U(\delta t) \to 1$. We can write an expression for this that is unitary to first order as

$$U(\delta t) = 1 - i\Delta(\delta t),$$

where the operator Δ is Hermitian. What physical operator might Δ correspond to? Here comes the physical leap of analogy. First look at what the units of Δ are; they are time^{-1}, i.e., the units of frequency. What physical observable has units of frequency? The Planck-Einstein relation says that $E = \hbar\omega$ where ω is frequency and $\hbar = h/2\pi$, with h the fundamental Planck constant. So lets choose our operator Δ to correspond to energy divided by $\hbar$. Now we know that in classical mechanics that the energy is given by the Hamiltonian operator $H = KE + PE$ and that this operator generates the time evolution. So in a simple leap of analogy, lets take $\hbar\Delta$ to be equal to the quantum mechanical Hamiltonian operator that corresponds to the total energy of the quantum system, i.e., a sum of kinetic and potential energy operators. Then we have

$$U(\delta t) = 1 - \frac{i}{\hbar}H\delta t.$$

The rest is plain sailing. We can either take the limit as $N \to \infty$ to derive the exponential form $exp[-iHt/\hbar]$ or, more simply, we use the composition law to write

$$\begin{aligned} U(t+\delta t) - U(t) &= [U(\delta t) - 1]U(t) \\ &= -i\frac{\delta t H}{\hbar}U(t). \end{aligned}$$

Rewriting and taking the limit $\delta \to 0$, we obtain

$$i\hbar\frac{\partial U}{\partial t} = HU(t).$$

This is the Schrodinger equation for the time evolution operator $U(t)$. Rewriting the evolution operator in its full form as $U(t,t_0)$ and multiplying on the right by $|\Psi;t_0\rangle$, we find

$$i\hbar\frac{\partial U(t,t_0)}{\partial t}|\Psi;t_0\rangle = HU(t,t_0)|\Psi;t_0\rangle,$$

which is equivalent to

$$i\hbar\frac{\partial|\Psi;t\rangle}{\partial t} = H|\Psi;t\rangle.$$

So we have arrived at the time dependent Schrodinger equation for the time evolution of the wave function of a quantum system.

4 Position Representation of Quantum State Function

We will motivate this using the framework of measurements. Consider first the simpler example of a photon. The polarization of the photon can be either horizontal (H) or vertical (V), from which we have a discrete basis of two states $|H\rangle$ and $|V\rangle$. We can measure the polarization by passing the photon through a polarizer crystal, which passes either H or V light depending on its orientation. The measurement operators for this simple 2-state basis are

$$M_H = |H\rangle\langle H|, M_V = |V\rangle\langle V|.$$

A single measurement on an arbitrary state $|\psi\rangle$ will collapse $|\psi\rangle$ onto one of the two orthonormal basis vectors. For example, if the H measurement is made, the state after measurement will be

$$|H\rangle\left(\frac{\langle H|\psi\rangle}{\sqrt{\langle\psi|H\rangle\langle H|\psi\rangle}}\right).$$

If the measurement is repeated many times, this state will be obtained with probability

$$P_H = |\langle H|\psi\rangle|^2.$$

Now consider a particle in a quantum state, e.g., the energy level of a hydrogen atom. The hydrogen atom consists of 1 positively charged proton in the nucleus and 1 negatively charged electron. The electron is ~ 1800 times lighter than the proton, so to a first approximation the electron can be regarded as moving around a stationnary proton. The possible energy levels for this electronic motion form a discrete, infinite set of levels of negative total energy (indicating overall binding to the proton), and are given by the relation $E_n \sim -1/n^2$, $n = 1,2,3,\ldots\ldots$ The energy eigenvectors $|n\rangle$ formed by these energy levels form an infinite dimensional Hilbert space. Now what if we want to observe the electron? It is moving in configuration space, so lets consider the effect of the measurement operator corresponding to a location $\mathbf{r}$ in configuration space. The measurement operator is

$$P_{\mathbf{r}} = |\mathbf{r}\rangle\langle\mathbf{r}|$$

and a measurement on the ket $|\psi\rangle$ collapses this onto the state $|\mathbf{r}\rangle\langle\mathbf{r}|\psi\rangle$, with probability

$$|\langle\mathbf{r}|\psi\rangle|^{\mathbf{2}} = |\psi(\mathbf{r})|^{\mathbf{2}}.$$

So $|\psi(\mathbf{r})|$ is the probability amplitude of finding an electron at $\mathbf{r}$, i.e., "the wave function in the position representation". Note that the state after measurement is the position ket $|\mathbf{r}\rangle$.

We can understand this in a pictorial manner by imagining a basis consisting of a very densely spread set of delta functions: the wave function is the amplitude of the the expansion of the quantum state in this basis.

$$\begin{aligned}
|\psi\rangle &= \sum_i \alpha_i |\mathbf{r}_i\rangle \\
\langle\mathbf{r}|\psi\rangle &= \sum_i \alpha_i \langle\mathbf{r}|\mathbf{r_i}\rangle \\
&= \alpha_i \delta(\mathbf{r}-\mathbf{r}_i) \\
&= \psi(\mathbf{r}).
\end{aligned}$$

The position representation is defined by the continuous set of basis vectors $|\mathbf{r}\rangle$, satisfying

$$\begin{aligned}
\int d\mathbf{r}|\mathbf{r}\rangle\langle\mathbf{r}| &= 1 \ (completeness) \\
\langle\mathbf{r}|\mathbf{r}'\rangle &= \delta(\mathbf{r}-\mathbf{r}'),
\end{aligned}$$

where $\delta(\mathbf{r}-\mathbf{r}')$ is the Dirac delta function. This is defined by the relation (shown here for 1D)

$$\int_{-\infty}^{+\infty} dx\delta(x-x')f(x')dx' = f(x).$$

Setting $f(x) = 1$ shows that the integral under the delta function is equal to unity. The three dimensional delta function is given by

$$\delta(\mathbf{r}-\mathbf{r}') = \delta(x-x')\delta(y-y')\delta(z-z').$$

We can regard the Dirac delta function as the limit of a sequence of functions possessing unit norm, e.g., a sequence of Gausssians with variable width λ:

$$f_\lambda = \frac{1}{\lambda\sqrt{2\pi}} exp^{-(x-x')^2/2\lambda^2}.$$

Note that the norm of the basis states $|r\rangle$ is ill-defined, unless one agrees to implicitly integrate over the position coordinate and make use of the delta function property.

To summarize, the ket $|\psi\rangle$ can be expanded in the position representation as

$$|\psi\rangle = \int d\mathbf{r}' |\mathbf{r}'\rangle \langle \mathbf{r}'| |\psi\rangle$$

The inner product between two state $|\psi\rangle$ and $|\phi\rangle$ can be expressed in terms of the corresponding wave functions in the position representation:

$$\begin{aligned}\langle \phi | \psi \rangle &= \int d\mathbf{r} \langle \phi | \mathbf{r} \rangle \langle \mathbf{r} | \psi \rangle \\ &= \int d\mathbf{r} \phi^*(\mathbf{r}) \psi(\mathbf{r}).\end{aligned}$$

Now the norm is well-behaved

$$\langle \psi | \psi \rangle = \int \psi^*(\mathbf{r}) \psi(\mathbf{r}) d\mathbf{r} = 1.$$

This implies we can choose a set of functions $\phi_n(\mathbf{r})$ satisfying

$$\int \phi_n^*(\mathbf{r}) \phi_m(\mathbf{r}) d\mathbf{r} = \delta_{mn}$$

which is just the orthonormality condition between $|\phi_n\rangle$ and $|\phi_m\rangle$. We can make this set of functions a basis for the Hilbert space spanned by the energy eigenstates $|n\rangle$. This basis of wave functions in position representation has a well behaved norm

$$||\phi_n||^2 = \int |\phi_n(\mathbf{r})|^2 d\mathbf{r} = 1.$$

These functions are therefore a set of square integrable functions, often also called L^2 functions.

Similar arguments lead to the definition of the momentum representation. The ket $|\psi\rangle$ can be expanded in the momentum representation as

$$|\psi\rangle = \int d\mathbf{p}' |\mathbf{p}'\rangle \langle \mathbf{p}' | \psi\rangle$$

where $\langle \mathbf{p}' | \psi \rangle = \psi(\mathbf{p}')$ is the probability amplitude to find the particle with momentum $\mathbf{p}'$. It is the wave function in the momentum representation. Note that equivalently, it can be understood as the expansion coefficient in the expansion in momentum eigenstates $|\mathbf{p}'\rangle$.

Projecting this expansion into the position representation yields the basic equation relating position and momentum representations of a quantum state $|\psi\rangle$:

$$\psi(\mathbf{r}) = \langle \mathbf{r} | \psi \rangle = \int \mathbf{dp}' \langle \mathbf{r} | \mathbf{p}' \rangle \psi(\mathbf{p}').$$

Note that using the Dirac notation we are correct in writing ψ on both right and left hand sides of this equation. However, the two functions may have very different dependence on their respective variables $\mathbf{r}$ and $\mathbf{p}$. To avoid confusion, one usually gives these different names, e.g., $\psi(\mathbf{r})$ and $\tilde{\psi}(\mathbf{p})$.

Transformation between position and momentum representations

What is the transformation element $\langle \mathbf{r} | \mathbf{p}' \rangle$ in the above equation? If we set this equal to $e^{i\mathbf{p}\cdot\mathbf{r}}$ then the equation looks like a Fourier transform of the wave function in momentum space, $\tilde{\psi}(\mathbf{p})$, i.e.,

$$\psi(\mathbf{r}) = \int d\mathbf{p} e^{i\mathbf{p}\cdot\mathbf{r}} \tilde{\psi}(\mathbf{p}).$$

This is not quite a Fourier transform, since we have momentum p rather than wave vector k in the integral. However, p and k satisfy the *de Broglie* relation,

$$\mathbf{p} = \hbar \mathbf{k}$$

which leads to the Fourier transform relation

$$\psi(\mathbf{r}) = \int d\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{r}} \tilde{\psi}(\mathbf{k})$$

where we have omitted factors of $\hbar$ and 2π.