Intermediate Quantum Mechanics
Lectures 14 & 15 Notes (3/9/15 & 3/23/15)

Transformations and Symmetries I

Overview

- Five closely related concepts that play important roles in quantum mechanics are:
  - transformations
  - symmetries
  - invariance
  - conservation laws
  - degeneracy

Transformations

- **Transformations**, as the name implies, are operations that can be done on a system to change it. There are two categories of transformations: discrete and continuous.
- Discrete transformations are ones that you either do or don't do. Examples are:
  - reflection in a mirror
  - interchange of two identical particles
  - charge conjugation (changing particles to anti-particles and vice-versa)
  - time reversal
- Continuous transformations are governed by a parameter that determines (continuously) the size of the transformation. Examples are:
  - translation in time
  - translation in space
  - rotation about an axis
- A general continuous transformation operator is represented by $\hat{U}(\alpha)$ where α is a parameter that indicates by how much to transform.
- When $\hat{U}(\alpha)$ acts on a state it transforms it to another state.

$$\hat{U}(\alpha)\,|\psi\rangle \;=\; |\psi'\rangle$$

Unitarity

- We require that if we transform a physical state of a system, it remain a physical state. That means that its norm must remain one.

$$\langle \psi' \,|\, \psi' \rangle \;=\; \langle \psi \,|\, \psi \rangle \;=\; 1$$

  We then have:

$$\langle \psi' \,|\, \psi' \rangle \;=\; \langle \psi|\hat{U}^\dagger(\alpha)\hat{U}(\alpha)\,|\psi\rangle \;=\; \langle \psi \,|\, \psi \rangle \qquad \Rightarrow \qquad \hat{U}^\dagger(\alpha)\hat{U}(\alpha) \;=\; \hat{I}$$

  That is, $\hat{U}(\alpha)$ must be a unitary operator.

$$\hat{U}^\dagger(\alpha) \;=\; \hat{U}^{-1}(\alpha) \;=\; \hat{U}(-\alpha)$$

- We also require that $\hat{U}(\alpha)$ be a linear operator.

Infinitesimal transformations

- A continuous transformation is completely specified in terms of an infinitesimal transformation. A finite transformation then simply involves applying an infinitesimal transformation an infinite number of times. Let α be the finite amount to transform, $\hat{U}(\alpha)$. This transformation is equivalent to operating with $\hat{U}(\alpha/n)$ n times, $\left[\hat{U}(\alpha/n)\right]^n$. Now let $\alpha/n = \epsilon$ and let $n \to \infty$ while $n\epsilon = \alpha$ a constant.

$$\hat{U}(\alpha) \;=\; \lim_{n\to\infty} \left[\hat{U}(\alpha/n)\right]^n \;=\; \lim_{n\to\infty} \left[\hat{U}(\epsilon)\right]^n$$

- Since $\hat{U}(\epsilon)$ is linear, it must depend linearly upon ϵ.

$$\hat{U}(\epsilon) \;=\; \hat{I} \;-\; \frac{i\epsilon}{\hbar}\,\hat{G}$$

  where the operator $\hat{G}$ must be a Hermitian operator if $\hat{U}(\epsilon)$ is a unitary operator.

- $\hat{G}$ is called the **generator** of the transformation. Since $\hat{G}$ is Hermitian, it must be associated with some observable.

- An example of a continuous transformation and its generator is the time translation operator $\hat{U}_t(\epsilon)$ that we discussed previously.

$$\hat{U}_t(\epsilon) \;=\; \hat{I} \;-\; \frac{i\epsilon}{\hbar}\,\hat{H}$$

  where we found that the generator $\hat{H}$ is the Hamiltonian or energy operator whose observable is what we identify classically as the energy of the system.

Invariance, Symmetry, Conservation

- The physics is **invariant** (unchanged) under a transformation if $\hat{U}$ commutes with the time translation operator.

$$[\hat{U}, \hat{U}_t] \;=\; 0$$

  I'm not indicating a parameter for $\hat{U}$ here since this rule applies to discrete transformations as well as continuous ones.

- This means that if we start with the state $|\psi\rangle$, the transformed state $|\psi'\rangle$ is the same whether we first wait and then transform or if we first transform and the wait.

$$\hat{U}\hat{U}_t(t_0)\,|\psi\rangle \;=\; \hat{U}_t(t_0)\hat{U}\,|\psi\rangle$$

- The Hamiltonian is **symmetric** with respect to a transformation if $\hat{U}$ commutes with the Hamiltonian operator.

$$[\hat{U}, \hat{H}] \;=\; 0$$

  This means, for example, if the Hamiltonian doesn't depend on x, it is symmetric with respect to translations in x or if it doesn't depend on angle, then it is symmetric with respect to rotations.

- The observable associated with the generator $\hat{G}$ is **conserved**, its expectation (average) value doesn't depend on time, if $\hat{G}$ commutes with the Hamiltonian.

$$[\hat{G}, \hat{H}] \;=\; 0$$

- You can easily show that these three conditions are equivalent.

$$[\hat{U}, \hat{U}_t] \;=\; 0 \qquad \Leftrightarrow \qquad [\hat{U}, \hat{H}] \;=\; 0 \qquad \Leftrightarrow \qquad [\hat{G}, \hat{H}] \;=\; 0$$

  That is, under a transformation:

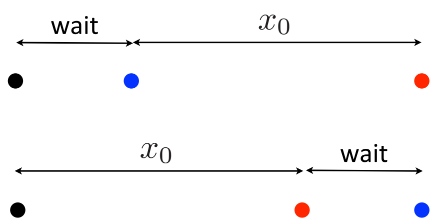
  invariance $\quad\Leftrightarrow\quad$ symmetry $\quad\Leftrightarrow\quad$ conservation

Examples

- Here are a few examples of symmetry and invariance.

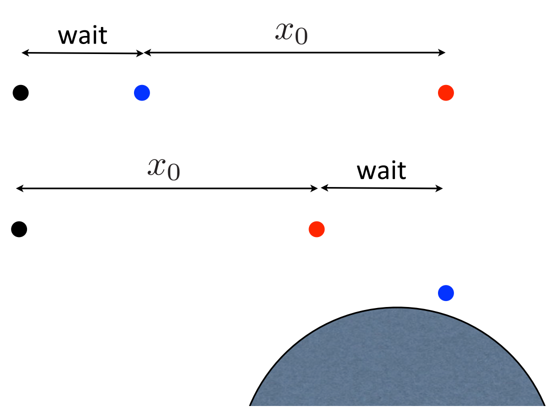
1) A particle in free space: The Hamiltonian $\hat{H} = \hat{p}^2/2m$ is independent of x, so it is symmetric with respect to translations in x, $[\hat{x}, \hat{H}] = 0$. Consider a particle with momentum p. If we wait a while the particle moves from the black point to the blue point in the figure below. Then we translate it in x a distance x_0 to the red point.

   Now reverse the order so that the particle is first translated in x and then we wait. As shown in the figure the particle is in the same position as when the operations were reversed.



2) A particle with a planet nearby: The Hamiltonian depends on x, since in the vicinity of the planet there will be a gravitational potential energy while a long distance way this will be very small. Consider a particle with momentum p. If we wait a while the particle moves from the black point to the blue point in the figure below. Then we translate it in x a distance x_0 to the red point.

   Now reverse the order so that the particle is first translated in x and then we wait. Since now the particle is in the gravitation potential of the planet it is deflected downward. The result is not the same as when the operations are reversed.



3) A particle with spin in free space: The Hamiltonian is spherically symmetric so it is symmetric with respect to rotations. If we wait a while and then rotate we get the same result as when we first rotate and then wait.

4) A particle with spin in a region of uniform magnetic field in the z-direction: The Hamiltonian is not symmetric with respect to rotations about the x or y axes. If we start with an electron with spin-up in the x-direction and wait for one quarter of the precession period, then the state will be spin-up in the y direction. If we then rotate by 90^o about y, it will remain spin-up in the y-direction. If again start with spin-up in the x-direction but first rotate by 90^0 about y, the state will be spin-up in the z-direction. If we now wait for one quarter of the precession period, it will remain spin-up in z. So with one ordering we end up with the state spin-up in y and with the reversed ordering we end up with the state spin-up in z.

Overall symmetries of the universe

- In a couple of the examples above there was a lack of translational or rotational symmetry because the Hamiltonian depended upon position or angle, respectively. That's because we didn't include the source of the Hamiltonian (the planet or the electromagnet) as part of the system. If we include these sources as part of the system, and translate or rotate, then the physics will be invariant.
- It is a basic principle of physics, called the Cosmological Principle, that the universe as a whole is homogeneous (the same from place to place) and is isotropic (has no preferred direction). Under this assumption, if the system is the entire universe, then physics is invariant under translations and rotations. That in turn means that the each component of the net linear moment and net angular momentum of the universe is conserved.

Degeneracy

- As we saw previously, if $[\hat{G}, \hat{H}] = 0$, then the two Hermitian operators $\hat{G}$ and $\hat{H}$ have the same eigenstates. This leads to four possible situations.

  1) Each eigenstate has different eigenvalues of both $\hat{G}$ and $\hat{H}$.

  $$(G_0, E_0) \qquad (G_1, E_1) \qquad (G_2, E_2) \qquad \cdots$$

  2) Some eigenstates have the same eigenvalue of $\hat{G}$. For example,

  $$(G_0, E_0) \qquad (G_0, E_1) \qquad (G_2, E_2) \qquad \cdots$$

  3) Some eigenstates have the same eigenvalue of $\hat{H}$. For example,

  $$(G_0, E_0) \qquad (G_1, E_0) \qquad (G_2, E_2) \qquad \cdots$$

  4) Some eigenstates have the same eigenvalues of both $\hat{G}$ and $\hat{H}$. For example,

  $$(G_0, E_0) \qquad (G_0, E_0) \qquad (G_2, E_2) \qquad \cdots$$

- In the case of 3) and 4), we say that there is **degeneracy**. Two or more distinct eigenstates have the same energy.

- In the case of 4), we know something else. There is a theorem that is fairly easy to prove for finite dimensions but is a bit harder for infinite dimensions, that says that "If there are two or more states for which two commuting Hermitian operators both have the same eigenvalues, then there must be a third Hermitian operator that commutes with the other two and that has different eigenvalues for these states. This makes sense, since if there are two states there must be some way, namely by the value of the observable of the third operator, to distinguish between the two states. For example, if

$$(G_0, E_0) \qquad (G_0, E_0) \qquad (G_2, E_2) \qquad \cdots$$

then there must be another operator $\hat{F}$ such that:

$$(F_0, G_0, E_0) \qquad (F_1, G_0, E_0) \qquad (F_2, G_2, E_2) \qquad \cdots$$

- Note that $[\hat{G}, \hat{H}] = 0$ doesn't necessarily imply degeneracy. In cases 1) and 2) above it doesn't. However degeneracy always implies that there is some Hermitian operator that commutes with $\hat{H}$. So if you find a degeneracy, there must be some symmetry, $[\hat{U}, \hat{H}] = 0$.

Generator of space translations

- We'll now find the generator of space translations: $\hat{U}_x(\epsilon)\,|\psi\rangle \;=\; |\psi'\rangle$.
- Since we know what a space translation does in the position representation, we'll work in that representation.

$$\langle x|\hat{U}_x(\epsilon)\,|\psi\rangle \;=\; \langle x\,|\,\psi'\,\rangle \;=\; \psi'(x) \;=\; \psi(x-\epsilon) \;=\; \psi(x) \;-\; \epsilon\,\frac{\partial}{\partial x}\,\psi(x)$$

$$\Rightarrow \quad \langle x|\hat{U}_x(\epsilon)\,|\psi\rangle \;=\; \left(1 \;-\; \epsilon\,\frac{\partial}{\partial x}\right)\psi(x) \;=\; \left[1 \;-\; \frac{i\epsilon}{\hbar}\left(-i\hbar\,\frac{\partial}{\partial x}\right)\right]\psi(x)$$

$$\Rightarrow \quad \hat{U}_x(\epsilon) \;=\; \hat{I} \;-\; \frac{i\epsilon}{\hbar}\,\hat{p}$$

- The generator of space translations is $\hat{p}$. If $\hat{H}$ is symmetric under space translations, momentum is conserved.

Generator of momentum translations

- Similarly, we find the generator of momentum translations: $\hat{U}_p(\epsilon)\,|\psi\rangle \;=\; |\psi'\rangle$.
- Since we know what a momentum translation does in the momentum representation, we'll work in that representation.

$$\langle p|\hat{U}_p(\epsilon)\,|\psi\rangle \;=\; \langle p\,|\,\psi'\,\rangle \;=\; \tilde{\psi}'(p) \;=\; \tilde{\psi}(p-\epsilon) \;=\; \tilde{\psi}(p) \;-\; \epsilon\,\frac{\partial}{\partial p}\,\tilde{\psi}(p)$$

$$\Rightarrow \quad \langle p|\hat{U}_p(\epsilon)\,|\psi\rangle \;=\; \left(1 \;-\; \epsilon\,\frac{\partial}{\partial p}\right)\tilde{\psi}(p) \;=\; \left[1 \;-\; \frac{i\epsilon}{\hbar}\left(-i\hbar\,\frac{\partial}{\partial p}\right)\right]\tilde{\psi}(p)$$

$$\Rightarrow \quad \hat{U}_p(\epsilon) \;=\; \hat{I} \;-\; \frac{i\epsilon}{\hbar}\,(-\hat{x})$$

- The generator of momentum translations is $-\hat{x}$.

Canonical commutation relations

- Up to now we've been working in only one physical dimension. Now we want to consider three physical dimensions. We need to do that in order to discuss rotations and solve the hydrogen atom.

- In three physics dimensions, the position operator has three components $\hat{x}$, $\hat{y}$ and $\hat{z}$ and the momentum operator has three components $\hat{p}_x$, $\hat{p}_y$ and $\hat{p}_z$.

- There are three independent spatial translations generated by the momentum operators.

$$\hat{U}_x(\epsilon) \;=\; \hat{I} - \frac{i\epsilon}{\hbar}\,\hat{p}_x \qquad \hat{U}_y(\epsilon) \;=\; \hat{I} - \frac{i\epsilon}{\hbar}\,\hat{p}_y \qquad \hat{U}_z(\epsilon) \;=\; \hat{I} - \frac{i\epsilon}{\hbar}\,\hat{p}_z$$

Similarly, there are three independent momentum translations generated by the position operators.

$$\hat{U}_{p_x}(\epsilon) \;=\; \hat{I} + \frac{i\epsilon}{\hbar}\,\hat{x} \qquad \hat{U}_{p_y}(\epsilon) \;=\; \hat{I} + \frac{i\epsilon}{\hbar}\,\hat{y} \qquad \hat{U}_{p_z}(\epsilon) \;=\; \hat{I} + \frac{i\epsilon}{\hbar}\,\hat{z}$$

- The properties of the position and momentum operators are completely specified by their commutation relations.

- Let $x_1 = x$, $x_2 = y$ and $x_3 = z$ and $p_1 = p_x$, $p_2 = p_y$ and $p_3 = p_z$. The we have:

$$[x_i, x_j] \;=\; 0 \qquad [p_i, p_j] \;=\; 0 \qquad [x_i, p_j] \;=\; i\hbar\delta_{ij}$$

These are called the **canonical commutation** relations. All of the operators commute with each other except that x doesn't commute with p_x, y doesn't commute with p_y and z doesn't commute with p_z. You should memorize these.

- **Finite Transformations**
  - As noted above, a finite continuous transformation can be built up out of an infinite number of infinitesimal transformations.

$$\hat{U}_x(x_0) \;=\; \lim_{n\to\infty}\left[\hat{U}_x(x_0/n)\right]^n \;=\; \lim_{n\to\infty}\left[\hat{I} - \frac{i(x_0/n)}{\hbar}\,\hat{p}_x\right]^n$$

  - Using the mathematical identity: $\lim_{n\to\infty}\left(1 - \frac{a}{n}\right)^n = e^{-a}$, we can express this as:

$$\hat{U}_x(x_0) \;=\; e^{-ix_0\hat{p}_x/\hbar}$$

Similarly:

$$\hat{U}_{p_x}(p_0) \;=\; e^{i\hat{x}p_x/\hbar}$$

  - How are we to interpret an operator exponent? It is just an exponential function of the operator. It means nothing more or less that the power series expansion of the function with the operator as the argument.

$$e^{\hat{A}} \;=\; 1 + \hat{A} + \frac{\hat{A}^2}{2!} + \frac{\hat{A}^3}{3!} + \cdots$$

- **Translations of a wave packet**
  - As an example of finite translations, let's look at translations of a Gaussian wave packet. You did this back in Homework Assignment 2 so this should be a review.
  - In HW 2, you found that the Fourier transform of a momentum Gaussian wave packet $\tilde{\psi}(p) = e^{-p^2/4\sigma_p^2}$ is a position Gaussian wave packet.

$$\psi(x) \;=\; \frac{1}{2\pi\hbar}\int e^{ixp'/\hbar}\,\tilde{\psi}(p')\,dp' \;=\; \frac{1}{2\pi\hbar}\int e^{ixp'/\hbar}\,e^{-p'^2/4\sigma_p^2}\,dp' \;=\; e^{-x^2/4\sigma_x^2}$$

    Note that I'm ignoring the uninteresting normalization factors here.
  - Now let's translate by an amount x_0 in x. This is given by the finite translation operator $e^{-ix_0\hat{p}/\hbar}$. In the momentum representation this is just $e^{-ix_0p/\hbar}$. So we can easily do the translation in x by working in the momentum representation.

$$\tilde{\psi}'(p) \;=\; e^{-ix_0p/\hbar}\,\tilde{\psi}(p)$$

    Then, $\psi'(x)$ is given by:

$$\psi'(x) \;=\; \frac{1}{2\pi\hbar}\int e^{ixp'/\hbar}\,\tilde{\psi}'(p')\,dp' \;=\; \frac{1}{2\pi\hbar}\int e^{ixp'/\hbar}\,e^{-ix_0p/\hbar}\,e^{-p'^2/4\sigma_p^2}\,dp'$$

$$=\; \frac{1}{2\pi\hbar}\int e^{i(x-x_0)p'/\hbar}\,e^{-p'^2/4\sigma_p^2}\,dp' \;=\; e^{-(x-x_0)^2/4\sigma_x^2}$$

  - Similarly, we can translate by an amount p_0 in p. This is given by the finite translation operator $e^{i\hat{x}p_0/\hbar}$. In the position representation this is just $e^{ixp_0/\hbar}$. So we can easily do the translation in p by working in the position representation.

$$\psi'(x) \;=\; e^{ixp_0/\hbar}\,\psi(p)$$

    Then, $\tilde{\psi}'(p)$ is given by:

$$\tilde{\psi}'(p) \;=\; \frac{1}{2\pi\hbar}\int e^{-ix'p/\hbar}\,\psi'(x')\,dx' \;=\; \frac{1}{2\pi\hbar}\int e^{-ix'p/\hbar}\,e^{ix'p_0/\hbar}\,e^{-x'^2/4\sigma_x^2}\,dp'$$

$$=\; \frac{1}{2\pi\hbar}\int e^{ix'(p-p_0)/\hbar}\,e^{-x'^2/4\sigma_x^2}\,dp' \;=\; e^{-(p-p_0)^2/4\sigma_p^2}$$