PHYSICS 215B: QUANTUM MECHANICS II

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Lecture 1.

Monday, January 6, 2020

Overview In this course, we'll stay closer to Shankar than in the last class (215A), covering roughly chapters 10-18. The first quarter established the mathematical structure of our theory; the second quarter will be focused on developing the methodologies and applications of quantum mechanics, including its generalization to multi-particle systems. The course is basically divided into two halves:

(a) Symmetries: rotational symmetries, angular momentum, spin, addition of angular momenta, and central force problems
(b) Approximation methods: WKB, variational principle, perturbation theory

Review In QM, the state of a particle is described by a wavefunction, usually expressed in some basis: $\psi(x), \phi(p), \{c_n\}$. The most flexible way to describe a state is in Dirac's bra-ket notation as a state vector, a ray in Hilbert space denoted by $|\psi\rangle$. There are (ket) vectors $|\psi\rangle$ and (bra) dual vectors $\langle\psi|$, which are usually defined by a complex inner product with the property

$$\langle\psi|\phi\rangle \in \mathbb{C}, \quad \langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*. \tag{1.1}$$

This inner product defines a norm,

$$0 \leq \langle\psi|\psi\rangle < \infty, \tag{1.2}$$

such that

$$\langle\psi|\psi\rangle = 0 \iff |\psi\rangle = 0. \tag{1.3}$$

Only the zero vector has zero norm. We often require of our coordinate basis vectors $|x\rangle$ tha thtey are delta function-normalized,

$$\langle x'|x\rangle = \delta(x - x'), \tag{1.4}$$

such that

$$\langle x|\psi\rangle = \psi(x). \tag{1.5}$$

Measurable quantities in QM are linear Hermitian operators (observables):

$$\mathcal{O}^\dagger = \mathcal{O}. \tag{1.6}$$

This guarantees that we get real eigenvalues, and moreover we are guaranteed a complete set of eigenvectors (they admit a spectral decomposition). That is,

$$\mathcal{O}|\lambda_i\rangle = \lambda_i|\lambda_i\rangle, \lambda_i \in \mathbb{R}, \tag{1.7}$$

where

$$\langle\lambda_i|\lambda_j\rangle = \delta_{ij} \tag{1.8}$$

and

$$\sum_i |\lambda_i\rangle\langle\lambda_i| = \mathbb{I}. \tag{1.9}$$

Hence we can decompose a general state as

$$|\psi\rangle = \mathbb{I}|\psi\rangle = \sum_i |\lambda_i\rangle\langle\lambda_i| = \sum_i c_i|\lambda_i\rangle, \quad c_i \equiv \langle\lambda_i|\psi\rangle. \tag{1.10}$$

Measurements of an operator $\mathcal{O}$ give one of the eigenvalues λ_i with probability

$$|\langle\lambda_i|\psi\rangle|^2 = \langle\psi|P_{\lambda_i}|\psi\rangle \tag{1.11}$$

where P_{λ_i} is the projection operator

$$P_{\lambda_i} = |\lambda_i\rangle\langle\lambda_i|. \tag{1.12}$$

Projection operators have the property that

$$P^2 = P, \quad P = P^\dagger. \tag{1.13}$$

In the case of a degenerate subspace (multiple eigenvectors with the same eigenvalue), we instead project onto that subspace and take the expectation value.

One of the most important operators in QM is the Hamiltonian operator $\hat{H}$. It describes the time evolution of states by the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle. \tag{1.14}$$

In the case where $\hat{H}$ is time-independent,[1] we can write a formal solution by

$$|\psi(t)\rangle = U_T(t,t')|\psi(t')\rangle, \tag{1.15}$$

with

$$U_T(t,t') = e^{-\frac{i\hat{H}}{\hbar}(t-t')}. \tag{1.16}$$

Finally, we review changes of (orthonormal) basis. For a basis $\{|i\rangle\}$ satisfying

$$\langle i|j\rangle = \delta_{ij}, \quad \sum_i |i\rangle\langle i| = \mathbb{I} \tag{1.17}$$

and another basis $\{|e_i\rangle\}$ satisfying the same, we can write changes of basis as

$$|e_i\rangle = \sum_j U_{ij}|j\rangle, \tag{1.18}$$

where U is a unitary matrix satisfying

$$U^\dagger U = UU^\dagger = \mathbb{I}. \tag{1.19}$$

[1] The time-dependent form is given by Dyson's formula, which involves time-ordered exponentials.

Multiple degrees of freedom (Shankar Ch. 10) Classically, we can add degrees of freedom to a system by allowing particles to move in more than 1 dimension, or by adding particles to the system. The coordinates and canonical momenta obey Poisson brackets,

$$\{x_i, p_j\} = \delta_{ij}. \tag{1.20}$$

In quantum mechanics, we can describe states in terms of a coordinate basis $|x_1, x_2, \ldots, x_n\rangle$ where the coordinates and momenta are promoted to operators,

$$\hat{X}_1, \hat{X}_2, \ldots, \hat{X}_n, \hat{P}_1, \hat{P}_2, \ldots, \hat{P}_N. \tag{1.21}$$

The only nontrivial commutator is

$$[\hat{X}_i, \hat{P}_j] = i\hbar\delta_{ij}. \tag{1.22}$$

In two dimensions we would have $\hat{X}, \hat{Y}, \hat{P}_x, \hat{P}_y$. For instance, to describe a charged particle in a magnetic field (as we did on the homework last quarter), it's useful to work in a simultaneous eigenbasis of $\hat{X}$ and $\hat{P}_y$.

New states can be defined to obey the inner product

$$\langle x', y'|x, y\rangle = \delta(x - x')\delta(y - y'). \tag{1.23}$$

In particular it's useful to build new states by taking direct (tensor) products,

$$|x, y\rangle = |x\rangle \otimes |y\rangle, \tag{1.24}$$

and if $|x\rangle, |y\rangle \in \mathbb{V}$, then such states live in the tensor product space

$$\mathbb{V} \otimes \mathbb{V} = \mathbb{V}^2. \tag{1.25}$$

The simplest case we might deal with is a particle in 2 dimensions in a separable potential, i.e. $V(x, y) = V_1(\hat{x}) + V_2(\hat{y})$, such that the Hamiltonian is

$$\hat{H}(\hat{x}, \hat{y}, \hat{p}_x, \hat{p}_y) = \frac{\hat{p}_x^2}{2m_1} + \frac{\hat{p}_y^2}{2m_2} + V_1(\hat{x}) + V_2(\hat{y}) = \hat{H}_1(\hat{x}, \hat{p}_x) + H_2(\hat{y}, \hat{p}_y). \tag{1.26}$$

It's a little weird to write two different masses m_1, m_2, since this is really the same particle (though particles may have different effective masses as they move in different directions), but this touches on a key point—is there a difference between one particle moving in 2 dimensions versus 2 particles moving in one dimension? The answer is no when the particles are *distinguishable*, but yes when they are *identical*. We'll see more of this soon.

If we can solve each of the individual Hamiltonians as

$$\hat{H}_1|u_i\rangle = \epsilon_{1i}|u_i\rangle \tag{1.27}$$

$$\hat{H}_2|v_i\rangle = \epsilon_{2i}|v_i\rangle, \tag{1.28}$$

then we can build a complete set of basis states for the 2D problem as

$$|u_i\rangle \otimes |v_j\rangle, \tag{1.29}$$

with energies $\epsilon_{1i} + \epsilon_{2j}$. In such product spaces, we can also construct operators on the full space out of operators that only act on part by taking tensor products. That is,

$$\hat{O}_1 \equiv \hat{O}^{(1)} \otimes \mathbb{I}^{(2)} \tag{1.30}$$

is an operator on the full Hilbert space $\mathbb{V} \otimes \mathbb{V}$ such that

$$\hat{O}^{(1)} \otimes \mathbb{I}^{(2)}|u_i\rangle \otimes |v_j\rangle = \hat{O}^{(1)}|u_i\rangle \otimes I^{(2)}|v_j\rangle. \tag{1.31}$$

Similarly if we define

$$\hat{O}_2 \equiv \mathbb{I}^{(1)} \otimes \hat{O}^{(2)}, \tag{1.32}$$

then

$$\hat{O}_1 \cdot \hat{O}_2 = \hat{O}^{(1)} \otimes \hat{O}^{(2)}, \tag{1.33}$$

where the dot indicates composition of operators (do one, then do the other).

Let us consider two systems. The first has Hamiltonian

$$\hat{H}(\hat{x}, \hat{p}_x, \hat{y}, \hat{p}_y) = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 + \frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\omega^2\hat{y}^2, \tag{1.34}$$

a single particle in a 2D harmonic oscillator potential. The second has Hamiltonian

$$\hat{H}(\hat{x}_1, \hat{p}_1, \hat{x}_2, \hat{p}_2) = \frac{\hat{p}_1^2}{2m} + \frac{1}{2}m\omega^2\hat{x}_1^2 + \frac{\hat{p}_2^2}{2m} + \frac{1}{2}m\omega^2\hat{x}_2^2. \tag{1.35}$$

This is *two particles*, each moving in one dimension in the same harmonic oscillator potential. We claim that if the particles are distinguishable (e.g. they have different charges, masses, something that we can measure to distinguish them), then indeed these are the same problem. But if the particles are truly indistinguishable, then some new physics creeps in.

In quantum mechanics, identical particles are indistinguishable. That is, their intrinsic properties (charge, mass, spin, etc.) are the same.[2] This is different from classical mechanics, where particles with identical properties can generically be distinguished by labels and their trajectories.

Suppose we construct a state

$$|w_i\rangle \otimes |w_j\rangle. \tag{1.36}$$

Then it has a wavefunction

$$(\langle x_1| \otimes \langle x_2|)(|w_i\rangle \otimes |w_j\rangle) = \psi_{w_i}(x_1)\psi_{w_j}(x_2). \tag{1.37}$$

For identical particles, such states are not allowed.[3] Let us define the exchange operator $\hat{P}_{12}$ by

$$\hat{P}_{12}(|w_i\rangle_{(1)} \otimes |w_j\rangle_{(2)}) = |w_j\rangle_{(1)} \otimes |w_i\rangle_{(2)}. \tag{1.38}$$

Notice that

$$(\hat{P}_{12})^2 = \mathbb{I}. \tag{1.39}$$

We can also see that

$$({}_{(2)}\langle w_k| \otimes {}_{(1)}\langle w_l|)(\hat{P}|w_i\rangle_{(1)} \otimes |w_j\rangle_{(}2)) = ({}_{(2)}\langle w_k| \otimes {}_{(1)}\langle w_l|)(|w_j\rangle_{(1)} \otimes |w_i\rangle_{(}2)) = \delta_{jl}\delta_{ik}. \tag{1.40}$$

If we take the dagger, we have instead

$$({}_{(2)}\langle w_k| \otimes {}_{(1)}\langle w_l|P^\dagger)(|w_i\rangle_{(1)} \otimes |w_j\rangle_{(}2)) = ({}_{(2)}\langle w_l| \otimes {}_{(1)}\langle w_k|)(|w_i\rangle_{(1)} \otimes |w_j\rangle_{(}2)) = \delta_{jl}\delta_{ik}. \tag{1.41}$$

We can see that

$$P^\dagger = P, \quad P = P^{-1}, \tag{1.42}$$

so P is both hermitian and unitary. The exchange operator acts on other operators by conjugation, as

$$UOU^\dagger. \tag{1.43}$$

This takes

$$PO_1P^\dagger = O_2, \quad PO_2P^\dagger = O_1, \tag{1.44}$$

since it swaps the particles, acts, and then swaps them back.

For identical particles, we have the property that

$$\hat{P}\hat{H}\hat{P}^\dagger = H \implies [\hat{P}, \hat{H}] = 0. \tag{1.45}$$

We also observe that since $\hat{P}^2 = 1$, it follows that if $\hat{P}|\lambda\rangle = \lambda|\lambda\rangle$, then

$$\lambda^2 = 1 \implies \lambda = \pm 1. \tag{1.46}$$

We can now construct two projection operators, suggestively named S and A:

$$\hat{S} = \frac{1}{2}(\mathbb{I} + \hat{P}) \tag{1.47}$$

$$\hat{A} = \frac{1}{2}(\mathbb{I} - \hat{P}). \tag{1.48}$$

[2] Why are all particles of the same type the same, anyway? One answer comes from quantum field theory—particles are all the same because they're made of the same stuff in a quantized way. That stuff is the field itself.

[3] The states must be symmetric or antisymmetric under exchange of x_1 and x_2. There are also states which pick up a general complex phase, called anyons. See F. Wilczek, "Quantum Mechanics of Fractional-Spin Particles," Phys. Rev. Lett. 49 (1982) 957, or a write-up by the man himself at Quanta Magazine: https://www.quantamagazine.org/how-anyon-particles-emerge-from-quantum-knots-20170228/

These are indeed projections, since $S^2 = S, S^\dagger = S$, and A is similar. We show this explicitly:

$$\begin{aligned} S^2 &= \frac{1}{4}(\mathbb{I} + \hat{P})(\mathbb{I} + \hat{P}) \\ &= \frac{1}{4}(\mathbb{I} + P + P + P^2) \\ &= \frac{1}{2}(\mathbb{I} + \hat{P}) = S. \end{aligned}$$

For two-particle states, we then have

$$S|w_i\rangle \otimes |w_j\rangle = \frac{1}{2}(|w_i\rangle \otimes |w_j\rangle + |w_j\rangle \otimes |w_i\rangle), \tag{1.49}$$

with the antisymmetric projector similar:

$$A|w_i\rangle \otimes |w_j\rangle = \frac{1}{2}(|w_i\rangle \otimes |w_j\rangle - |w_j\rangle \otimes |w_i\rangle). \tag{1.50}$$

In fact, notice that since $S + A = \mathbb{I}$, we have

$$|\psi\rangle = (S + A)|\psi\rangle = S|\psi\rangle + A|\psi\rangle. \tag{1.51}$$

Since these operators commute with the Hamiltonian,[4] particles which are originally in symmetric combinations will stay symmetrized for all time, and the same is true for antisymmetric combinations. There is therefore an additional postulate of quantum mechanics, that identical particles come in two types.

(a) Bosons, which live in the symmetrized subspace of the Hilbert space, and
(b) Fermions, which live in the *anti*-symmetrized subspace of the Hilbert space.

Thus the wavefunction for bosons takes on a symmetric form in x_1, x_2:

$$\psi(x_1, x_2)_S = \psi_{w_i}(x_1)\psi_{w_j}(x_2) + \psi_{w_j}(x_1)\psi_{w_i}(x_2), \tag{1.52}$$

and the wavefunction for fermions is antisymmetric:

$$\psi(x_1, x_2)_A = \psi_{w_i}(x_1)\psi_{w_j}(x_2) - \psi_{w_j}(x_1)\psi_{w_i}(x_2). \tag{1.53}$$

Notice that if we set $w_i = w_j$ then the fermionic wavefunction vanishes, and it also vanishes if $x_1 = x_2$.[5] This is the Pauli exclusion principle. Conversely bosons feel a statistical attraction to each other; we'll revisit this later.

Lecture 2.

Wednesday, January 8, 2020

To recap, if we have a Hamiltonian $\hat{H}(\hat{x}_i, \hat{p}_i)$, we are interested in constructing the spectrum

$$\hat{H}(\hat{x}_i, \hat{p}_i)|w_i\rangle = \epsilon_i|w_i\rangle. \tag{2.1}$$

General states $|\psi\rangle \in V$ can be expressed in the basis $|w_i\rangle$. THe wavefunction is

$$\langle x|\psi\rangle = \psi(x), \tag{2.2}$$

such that $|\psi(x)|^2 = p(x)$, $\int dx|\psi(x)|^2 = 1$.

For a two-particle system, each in the same potential, if the Hamiltonian separates (there are no interactions) then

$$H(\hat{x}_1, \hat{p}_1, \hat{x}_2, \hat{p}_2) = H_1(\hat{x}_1, \hat{p}_1) + H_1(\hat{x}_2, \hat{p}_2). \tag{2.3}$$

The eigenstates of the two-particle system are tensor products of the individual one-particle eigenstates,

$$|w_i\rangle_{(1)} \otimes |w_j\rangle_{(2)} \equiv |w_i, w_j\rangle. \tag{2.4}$$

Generic vectors can be expressed in this basis,

$$|\psi\rangle = \sum_{ij} C_{ij}|w_i, w_j\rangle \in V \otimes V. \tag{2.5}$$

[4] The operators $\mathbb{I}$ and P commute with H, which means that S and A do too.

[5] Slight technicality– by the spin-statistics theorem, fermions have half-integer spin, so in general there's an extra spin degree of freedom which lets us fit e.g. two electrons in the same spot (one spin up, one spin down).

The two-particle wavefunction is simply

$$\langle x_1, x_2|\psi\rangle = \psi(x_1, x_2), \tag{2.6}$$

satisfying the Born rule,

$$P(x_1; x_2) = |\psi(x_1, x_2)|^2, \tag{2.7}$$

the probability of finding the first particle at x_1 and the second at x_2. The normalization[6] is then given by

$$\int |\psi(x_1, x_2)|^2 dx_1 dx_2 = 1. \tag{2.8}$$

If w_1, w_2 are each already normalized with respect to integration over x and orthogonal then the normalization factor is $1/\sqrt{2}$, i.e.[7]

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}}(w_1(x_1)w_2(x_2) \pm w_2(x_1)w_1(x_2)). \tag{2.9}$$

If w_1 and w_2 are the same state the state reduces to

$$w_1(x_1)w_1(x_2). \tag{2.10}$$

In the case of identical particles, we argued that there are extra constraints on our states. We can do this by defining the exchange operator P_{12}, an operator on $V \otimes V$ which acts as

$$P_{12}|w_i, w_j\rangle = |w_j, w_i\rangle. \tag{2.11}$$

It has the properties that

$$P_{12}^\dagger = P_{12}, P_{12}^2 = 1, P_{12} = P_{12}^{-1} \implies P_{12}^\dagger = P_{12}^{-1}. \tag{2.12}$$

Hence P_{12} is in fact unitary.

If we suppose that P commutes with the Hamiltonian (it is a symmetry of our system), i.e.

$$[P_{12}, H] = 0, \tag{2.13}$$

then we can prepare eigenstates of both P and the Hamiltonian. At the non-relativistic level, particles are either bosons or fermions; there are no mixed states. Hence wavefunctions are either symmetric or antisymmetric.

In the coordinate basis, any two-particle wavefunction can be written as

$$w_1(x_1)w_2(x_2) \to \frac{1}{2}(w_1(x_1)w_2(x_2) \pm w_2(x_1)w_1(x_2)). \tag{2.14}$$

Sometimes we write the Hilbert space as a direct sum

$$V \otimes V = |V_{\text{sym}}\rangle \oplus |V_{\text{anti}}\rangle. \tag{2.15}$$

Notice that for distinguishable particles, we talk about the probability density $P(x_1, x_2)$, of finding the first particle at x_1 and the second at x_2. When the particles are identical, our normalization has to change. That is, we can only identify the probability density of finding *one* particle at x_1 and another at x_2; we can't say which is which. Hence the normalizaiton changes to a spatially-ordered integral

$$\int_{-\infty}^{\infty} dx_1 \int_{x_1}^{\infty} dx_2\, P(x_1, x_2) = 1. \tag{2.16}$$

That is, $x_1 < x_2$. Morally speaking, we found one particle at x_1 and then we normalized the probability of finding another particle somewhere later at $x_2 > x_1$.

The probability density for identical particles is related to the wavefunction by

$$P(x_1, x_2) = |\psi(x_1, x_2)|^2 + |\psi(x_2, x_1)|^2. \tag{2.17}$$

This is the only thing that makes sense; it is a symmetrized version of the original distinguishable particle probability density.

For three identical particles, we have a Hilbert space $V \otimes V \otimes V$ and states

$$\langle x_1, x_2, x_3|w_i, w_j, w_k\rangle = w_i(x_1)w_2(x_2)w_k(x_3). \tag{2.18}$$

[6] This was mentioned a little later in the lecture but I think it makes more sense here.

[7] Exercise.

These obey the commutation relations

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}, \tag{2.19}$$

as usual. To study identical particles, we need the exchange operators for this system. They come from the permutation (symmetric) group S_3, if you like.[8] As before we have

$$P_{12}|w_i, w_j, w_k\rangle = |w_j, w_i, w_k\rangle. \tag{2.20}$$

We could similarly define exchange operators P_{13} and P_{23}. Notice that $P_{12}P_{13} \neq P_{13}P_{12}$. Suppose we have elements (a, b, c). Then

$$P_{12}P_{13}(a, b, c) = P_{12}(c, b, a) = (b, c, a), \tag{2.21}$$

whereas

$$P_{13}P_{12}(a, b, c) = P_{13}(b, a, c) = (c, a, b) \neq (b, c, a). \tag{2.22}$$

So this group is not abelian (its elements do not all commute).

The symmetric group S_n is the group of all permutations of n objects. It has $n!$ elements (i.e. choose one element of n to be first, one of $n-1$ to be second, and so on until you run out of elements).

Let's change our notation a bit and write $P_{123} = \mathbb{I}$ to denote the identity operator. That is, $P_{123}(a, b, c) = (a, b, c)$ and other permutations are given by e.g. $P_{132}(a, b, c) = (a, c, b)$. That is, each label in P says which element goes in which slot. For three elements, there are six options:

$$\underbrace{P_{123}, P_{231}, P_{312}}_{\text{even}} \quad \underbrace{P_{213}, P_{321}, P_{132}}_{\text{odd}}. \tag{2.23}$$

The labels even and odd refer to how many pairwise swaps we need to get to that permutation from the identity.

Let us define now two projection operators in analogy to the two-particle case from earlier. The first is

$$S = \frac{1}{N!}\sum_{\alpha} P_\alpha, \tag{2.24}$$

which we call the *symmetric projector*, and

$$A = \frac{1}{N!}\sum_{\alpha} \epsilon_\alpha P_\alpha, \tag{2.25}$$

the *antisymmetric projector*, where $\epsilon_\alpha = +1$ when α is an even permutation and -1 when it is an odd permutation. Note that P_α commutes with S for any permutation α. Since all the permutations are already represented in the sum over α in S, all acting with P_α does is mix up the elements. But we already have all the elements and no two original elements can be mapped to the same one (i.e. $P_\alpha P_i \neq P_\alpha P_j$ unless $i = j$). Hence

$$P_\alpha S = S = S P_\alpha \implies [P_\alpha, S] = 0. \tag{2.26}$$

Similarly, for A we sometimes pick up a minus sign. The swap operator P_{12}, which is odd, gives

$$P_{12}A = \frac{1}{N!}\sum_{\alpha} \epsilon_\alpha P_{12}P_\alpha = \frac{1}{N!}\sum_{\alpha} \epsilon_\alpha P_{\alpha'} = -\frac{1}{N!}\sum_{\alpha'} \epsilon_{\alpha'} P_{\alpha'}. \tag{2.27}$$

That is,

$$P_{12}A = -A, \tag{2.28}$$

and in general

$$P_\alpha A = \epsilon_\alpha A. \tag{2.29}$$

Even permutations mix even and odd permutations amongst themselves, while odd permutations exchange the two sets, taking even to odd and vice versa. We see that

$$P_\alpha A = \epsilon_\alpha A = A P_\alpha, \tag{2.30}$$

so

$$[P_\alpha, A] = 0. \tag{2.31}$$

[8] https://en.wikipedia.org/wiki/Symmetric_group

Let us now check that $S^2 = S$:

$$S^2 = \left(\frac{1}{N!}\sum_\alpha P_\alpha\right) S = \frac{1}{N!}\sum_\alpha S = S, \tag{2.32}$$

while $A^2 = A$ since

$$A^2 = \frac{1}{N!}\sum_\alpha \epsilon_\alpha P_\alpha A = \frac{1}{N!}\sum_\alpha \epsilon_\alpha \epsilon_\alpha A = A, \tag{2.33}$$

since $(\epsilon_\alpha)^2 = 1$ for all α. We conclude that S and A are honest projection operators.

We can project onto the corresponding subspaces, i.e. $S|\psi\rangle$ gives a totally symmetric vector such that

$$\psi_S(x_1, x_i, \dots, x_j, \dots) = +\psi(x_1, x_j, \dots, x_i, \dots), \tag{2.34}$$

while $A|\psi\rangle$ gives a totally antisymmetric vector.[9] The Hilbert space can be decomposed into

$$V^N = V_{\text{sym}} \oplus V_{\text{anti}} \oplus V_{\text{rest}}, \tag{2.35}$$

where the first two subspaces correspond to bosons and fermions respectively, and the rest of the states in the Hilbert space are not allowed.

Note that acting on a general state with S and A give unique states, the maximally (anti)symmetric combinations. In a coordinate basis, our symmetric state is

$$\psi(x_1, \dots, x_N) = \frac{1}{N!}\sum_\alpha w_1(x_{\alpha_1}) w_2(x_{\alpha_2}) w_3(x_{\alpha_3}) \tag{2.36}$$

and the antisymmetric state is

$$\psi(x_1, \dots, x_N) = \frac{1}{N!}\sum_\alpha \epsilon_\alpha w_1(x_{\alpha_1}) w_2(x_{\alpha_2}) w_3(x_{\alpha_3}). \tag{2.37}$$

Note that for the three-particle state, our antisymmetric state (up to a constant factor) is

$$\begin{aligned} &w_1(x_1)w_2(x_2)w_3(x_3) + w_1(x_2)w_2(x_3)w_3(x_1) + w_1(x_3)w_2(x_1)w_3(x_2) \\ &\quad - w_1(x_2)w_2(x_1)w_3(x_3) - w_1(x_3)w_2(x_2)w_3(x_1) - w_1(x_1)w_2(x_3)w_3(x_2). \end{aligned} \tag{2.38}$$

This is precisely the determinant of a matrix:

$$\begin{vmatrix} w_1(x_1) & w_2(x_1) & w_3(x_1) \\ w_1(x_2) & w_2(x_2) & w_3(x_2) \\ w_1(x_3) & w_2(x_3) & w_3(x_3) \end{vmatrix}. \tag{2.39}$$

Question: when can we treat two systems (perhaps very separated in space) as independent? For example, one particle is on the earth and the other is on the moon. Can we write

$$\psi(x_1, x_2) \approx G_E(x_1) G_M(x_2)? \tag{2.40}$$

Sure, if they never overlap:

$$G_E(x_1) G_M(x_1) = 0 \text{ for all } x_1, \tag{2.41}$$

i.e. their supports are disjoint. In the case of identical particles we would write the symmetrized wavefunction

$$\psi_S(x_1, x_2) = \frac{1}{\sqrt{2}}(G_E(x_1)G_M(x_2) + G_M(x_1)G_E(x_2)). \tag{2.42}$$

Then our condition would imply that

$$\psi_S(x_{1M}, x_{2M}) = 0 = \psi_S(x_{1E}, x_{2E}). \tag{2.43}$$

[9] In the three-particle case, we have $S(a,b,c) = \frac{1}{3!}\big((a,b,c) + (b,a,c) + (a,c,b) + (b,c,a) + (c,a,b) + (c,b,a)\big)$, and $A(a,b,c) = \frac{1}{3!}\big((a,b,c) + (b,c,a) + (c,a,b) - (a,c,b) - (b,a,c) - (c,b,a)\big)$. That is, S just adds up all the combinations, while A adds a sign for parity.

Lecture 3.

Monday, January 13, 2020

Symmetries are critical in quantum mechanics, but their study predates quantum mechanics. For instance, if we consider an equilateral triangle, it has some symmetries (namely, the dihedral group D_6). We can leave it alone (identity, I), rotate clockwise by 120 degrees (R_{120}, rotate clockwise by 240 degrees (R_{240}), reflect over the z axis (σ_a), or reflect over one of the two other symmetry axes running through the vertices (σ_b, σ_c).

Note that there are no further symmetries of this object. We can see this by enumerating the possible configurations of the vertices, i.e. we can pick one vertex to be on top (1,2, or 3) and then pick an order for the vertices at the base (e.g. if 1 is on top then either 2 or 3 can be on the bottom). Thus we have 3×2 choices which means there are six elements in the group total.

We also notice that rotations form a *subgroup*, i.e. a group within a group. Specifically, they form the cyclic group $\mathbb{Z}_3$, which is the set of symmetries of the integers modulo 3 under addition.

In quantum mechanics, we have states $|\psi\rangle$ which live in a vector space, and group elements correspond to unitary operators which act on the vector space. The assignment of operators to group elements in a way that respects the group multiplication is called a *representation*., i.e.

$$g_i \mapsto U_{g_i} \text{ such that } U_{g_i}^\dagger = U_{g_i}^{-1}, \quad U_{g_i} U_{g_j} = U_{g_i g_j} \tag{3.1}$$

defines a unitary representation.

Two representations are *equivalent* if they are related by a unitary transformation. That is, they are the same up to a change of basis. A representation is *reducible* if by a unitary transformation it can be put into block diagonal form (all operators $\{U_i\}$ can be block diagonalized). That is,

$$U_i = \begin{bmatrix} U_{1i} & 0 \\ 0 & U_{2i} \end{bmatrix} \tag{3.2}$$

such that the vector space decomposes into a direct sum

$$V = V_1 \oplus V_2. \tag{3.3}$$

The operator acts separately on each of the subspaces V_1, V_2.

In QM, we are interested in irreducible representations. A representation is *irreducible* if it is not reducible. Consider the ammonia molecule. There are three hydrogen atoms at three of the corners of a trigonal pyramid with a nitrogen atom at the last corner. There are the same symmetry operations on this pyramid, i.e. the hydrogen atoms have the same symmetries as the equilateral triangle, so there are therefore six symmetries of this molecule which correspond to its degrees of freedom.[10]

We can also define the character of an element as the trace

$$\chi_i = \operatorname{Tr} U_i, \tag{3.4}$$

and the conjugacy class of an element g_a, which is defined as the set

$$\{g_i g_a g_i^{-1}\}, g_i \in G. \tag{3.5}$$

Note that the identity forms a conjugacy class in itself. One can see that R_{120}, R_{240} forms a conjugacy class and $\sigma_a, \sigma_b, \sigma_c$ form another.

There exist orthogonality theorems which state that if one constructs a vector of the characters of a group in two different representations Γ, Γ', i.e.

$$\sum_{g \in G} \chi^\Gamma(g^{-1}) \chi^{\Gamma'}(g) = N_G \delta_{\Gamma\Gamma'}, \tag{3.6}$$

where N_G is the number of elements in the group. That is, their inner product constructed in this way is zero unless the the representations are identical.

[10] There is a group theory course with notes at http://courses.physics.ucsd.edu/2016/Spring/physics220/.

The number of irreps of a group is equal to its number of conjugacy classes. We can always construct the trivial representation, for instance, assigning the operator 1 to every element, or we could construct an alternating representation assigning operators to ± 1. That is,

	I	R_{120}	R_{240}	σ_a	σ_b	σ_c
A_1	1	1	1	1	1	1
A_2	1	1	1	-1	-1	-1
B	2	a	a	b	b	b

(3.7)

The trace (character) assigned to any element in a conjugacy class must be the same as all other elements in the conjugacy class, since $g_b = g_i g_a g_i^{-1} \implies \mathrm{Tr}\, R(g_b) = \mathrm{Tr}\, R(g_i g_a g_i^{-1}) = \mathrm{Tr}\, R(g_i) R(g_a) R(g_i^{-1}) = \mathrm{Tr}\, R(g_a)$.

One can solve for a and b with a bit of linear algebra using the orthogonality relation. One could also work out the matrix representation in 2 dimensions and find out what the traces are.

There is a "great orthogonality theorem" which states that for 2 irreps $U^\Gamma, U^{\Gamma'}$, we can consider their matrix elements and

$$\sum_{g \in G} U^\Gamma_{ki}(g^{-1}) U^{\Gamma'}_{i'k'}(g) = \frac{N_G}{d_\Gamma} \delta_{\Gamma\Gamma'} \delta_{ii'} \delta_{kk'}. \tag{3.8}$$

Continuous symmetries Continuous symmetries are symmetries where the group elements can be expressed as continuous differentiable functions of some parameters. These are also called *Lie groups.*

One of the simplest examples is translational symmetry. In one dimension, we have a unitary operator T_a such that

$$T_a |x\rangle = |x + a\rangle. \tag{3.9}$$

Consider a general wavefunction $\psi(x)$, which we write as

$$|\psi\rangle = \int dx \psi(x) |x\rangle. \tag{3.10}$$

What happens if we apply T_a to $|\psi\rangle$? We get

$$T_a |\psi\rangle = \int dx \psi(x) |x + a\rangle \tag{3.11}$$

$$= \int dx' \psi(x' - a) |x'\rangle, \tag{3.12}$$

so

$$\psi(x) \to \psi'(x) = \psi(x - a). \tag{3.13}$$

For infinitesimal transformations T_ϵ, we then have

$$\psi_\epsilon(x) = \psi(x - \epsilon) = \psi(x) - \epsilon \frac{\partial \psi}{\partial x} + O(\epsilon^2), \tag{3.14}$$

so that if we assume T has a Taylor expansion in ϵ, then we can expand about $\epsilon = 0$ (the identity) to get

$$T_\epsilon = \mathbb{I} + \epsilon \left(\frac{\partial T}{\partial \epsilon} \right)_{\epsilon = 0} + O(\epsilon^2). \tag{3.15}$$

We can also rewrite this as

$$T_\epsilon = \mathbb{I} - \frac{i\epsilon}{\hbar} \hat{p}, \tag{3.16}$$

where this i accounts for the fact that if T is to be unitary, the generator (the first-order expansion term) must be anti-Hermitian. Notice that if

$$T_\epsilon = 1 + \epsilon A, \quad T_\epsilon^\dagger = 1 + \epsilon A^\dagger, \tag{3.17}$$

then since T is unitary,

$$1 = T_\epsilon T_\epsilon^\dagger = (1 + \epsilon A)(1 + \epsilon A^\dagger) = 1 + \epsilon (A + A^\dagger) + O(\epsilon^2). \tag{3.18}$$

It follows that $A = -A^\dagger$, i.e. A is anti-hermitian.

Comparing orders we find that

$$\langle x | (1 - \frac{i\epsilon}{\hbar} \hat{p}) | \psi \rangle = \psi(x) + \frac{i}{\hbar} \epsilon \hat{p} \psi(x), \tag{3.19}$$

and by construction this is equal to

$$\psi(x) + \epsilon \frac{\partial \psi}{\partial x}. \tag{3.20}$$

Comparing orders we find that

$$\hat{p}_x \psi(x) = -i\hbar \frac{\partial}{\partial x} \psi(x). \tag{3.21}$$

We can construct finite transformations from infinitesimal ones by the exponential map. Equvialently we write

$$T_a = T_\epsilon T_\epsilon \dots T_\epsilon = (T_\epsilon)^N = \left(1 - \frac{ia}{\hbar N}\hat{p}\right)^N = e^{-\frac{ia}{\hbar}\hat{p}}, \tag{3.22}$$

where $\epsilon = a/N$. The last equality results from taking the $N \to \infty$ limit.

Consider the hydrogen atom, which has a 2-particle hamiltonian

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(|\mathbf{r}_1 - \mathbf{r}_2|). \tag{3.23}$$

Notice that with the regular commutation relations, we can define

$$\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}_{\text{cm}} \tag{3.24}$$

so that

$$[\mathbf{p}_{\text{cm}}, \mathbf{r}_1 - \mathbf{r}_2] = 0. \tag{3.25}$$

Lecture 4.

Wednesday, January 15, 2020

Last time, we discussed the generator of translations, which was the momentum operator. That is, the operator

$$\hat{T}_{\mathbf{a}} = e^{-\frac{i\mathbf{a}\cdot\mathbf{p}}{\hbar}}. \tag{4.1}$$

In the coordinate basis, the operator has the form

$$e^{-\frac{ia}{\hbar bar}\left(-i\hbar\frac{\partial}{\partial x}\right)} = e^{-a\frac{\partial}{\partial x}}, \tag{4.2}$$

such that

$$e^{-a\frac{\partial}{\partial x}}\psi(x) = \psi(x-a). \tag{4.3}$$

The translation group is abelian, i.e. its elements all commute with one another. All irreducible representations of the translation group are one-dimensional.

Our orthogonality relations moreover tell us that

$$\int d^3 r e^{-i\frac{\mathbf{v}\cdot\mathbf{p}'}{\hbar}} e^{+i\frac{\mathbf{v}\cdot\mathbf{p}}{\hbar}} = V\delta^{(3)}(\mathbf{p} - \mathbf{p}'), \tag{4.4}$$

where V indicates that this inner product is in a sense the volume of the space we're integrating over.

Rotations in 3D Rotations in 3D are a linear map $\mathbb{R}^3 \to \mathbb{R}^3$, such that $R(\mathbf{0}) = \mathbf{0}$, while $R(\mathbf{a} + \mathbf{b}) = R\mathbf{a} + R\mathbf{b}$. That is, we can add vectors and rotate their sum, or we can rotate each one first and then sum them.

If we write a coordinate system $\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}} : \hat{e}_1, \hat{e}_2, \hat{e}_3$ and some new vectors $\hat{e}_1, \hat{e}_2, \hat{e}_3$.[11]

Let us posit that we can describe rotations by a matrix R_{ij}, so that $b_i' = R_{ij} b_j$. We would like the inner product to be preserved under rotations, such that

$$a_i b_i = a_i' b_i'. \tag{4.5}$$

Let us write this out explicitly.

$$a_i b_i = a_i' b_i' = R_{ij} a_j R_{ik} b_k. \tag{4.6}$$

But

$$a_i b_i = a_j b_j = a_j \delta_{jk} b_k, \tag{4.7}$$

[11] I've redone the exposition here.

so in fact

$$R_{ij}R_{ik} = \delta_{jk} \implies R^T R = \mathbb{I}. \tag{4.8}$$

These are *orthogonal matrices*. Notice that if $R^T R = \mathbb{I}$, then $\det(R^T R) = 1 \implies \det R = \pm 1$.

If we moreover require that $\det(R) = +1$ then we have the group of proper rotations, whereas $\det R = -1$ form the set of improper rotations. The proper rotations define a group $SO(3)$, which is the subgroup of $O(3)$ connected to the identity.

A rotation can be described by Euler angles, which we leave as an exercise. We can also do it by specifying an axis to rotate about $\hat{\mathbf{n}}$ and an angle θ. If we decompose a vector $\mathbf{u}$ into its components parallel $\mathbf{u}_\parallel$ and perpendicular $\mathbf{u}_\perp$ to $\hat{\mathbf{n}}$, then

$$\mathbf{u}_\parallel = \hat{\mathbf{n}}\mathbf{u}\cdot\hat{\mathbf{n}}, \tag{4.9}$$

$$\mathbf{u}_\perp = \mathbf{u} - \mathbf{u}_\parallel = (\hat{\mathbf{n}}\times\mathbf{u})\times\hat{\mathbf{n}}. \tag{4.10}$$

It follows that

$$\mathbf{u}' = \mathbf{u}_\parallel + \cos\theta(\hat{\mathbf{n}}\times\mathbf{u})\times\hat{\mathbf{n}} + \sin\theta(\hat{u}\times\mathbf{u}) \tag{4.11}$$

$$= \hat{\mathbf{n}}(\mathbf{u}\cdot\hat{\mathbf{n}}) + \cos\theta[\mathbf{u} - \hat{\mathbf{n}}(\mathbf{u}\cdot\hat{\mathbf{n}})] + \sin\theta(\hat{\mathbf{n}}\times\mathbf{u}) \tag{4.12}$$

$$= \cos\theta\mathbf{u} + \hat{\mathbf{n}}(\mathbf{u}\cdot\hat{\mathbf{n}})(1-\cos\theta) + \sin\theta(\hat{\mathbf{n}}\times\mathbf{u}). \tag{4.13}$$

One can check that the rotation matrix about the $\hat{\mathbf{z}}$ axis has a simple form,

$$R(\hat{\mathbf{z}},\theta) = \left(R(\hat{\mathbf{z}},\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}. \right) \tag{4.14}$$

For infinitesimal θ we keep terms only to order θ, so

$$\mathbf{u}' = \mathbf{u} + \theta\hat{\mathbf{n}}\times\mathbf{u}. \tag{4.15}$$

From the matrix point of view, let us write

$$R_\epsilon = \mathbb{I} + \epsilon A. \tag{4.16}$$

If R is to be orthogonal, then

$$\mathbb{I} = R_\epsilon^T R = (1+\epsilon A^T)(1+\epsilon A) = \mathbb{I} + \epsilon(A^T + A) + O(\epsilon^2) \implies A^T + A = 0. \tag{4.17}$$

Hence the generator A is antisymmetric. The most general 3×3 antisymmetric matrix takes the form

$$A = \begin{pmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{pmatrix} = a_i \mathscr{J}_i, \tag{4.18}$$

with

$$\mathscr{J}_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \mathscr{J}_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \mathscr{J}_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{4.19}$$

For infinitesimal $\theta = \epsilon$, we have

$$R(\hat{\mathbf{n}},\epsilon) = I + \epsilon\hat{\mathbf{n}}\cdot\mathscr{J}. \tag{4.20}$$

Under matrix multiplication, these generators obey an anticommutator (a Lie bracket, actually):

$$[\mathscr{J}_i, \mathscr{J}] = \epsilon_{ijk}\mathscr{J}_k. \tag{4.21}$$

Note that the matrices actually have the elements $(\mathscr{J}_k)_{ij} = \epsilon_{kij}$, so

$$[(\mathbf{a}\cdot\mathscr{J})\mathbf{u}]_i = (\mathbf{a}\cdot\mathscr{J})_{ij}u_j \tag{4.22}$$

$$= a_k(\mathscr{J}_k)_{ij}u_j \tag{4.23}$$

$$= \epsilon_{kij}a_k u_j = \mathbf{a}\times\mathbf{u}. \tag{4.24}$$

The anticommutator tells us that this group is non-abelian— it has nontrivial commutators.

We can find a general rotation by noticing that

$$\frac{dR(\hat{\mathbf{n}},\theta)}{d\theta} = \lim_{\epsilon\to 0}\frac{R(\hat{\mathbf{n}},\theta+\epsilon) - R(\hat{\mathbf{n}},\theta)}{\epsilon} = \lim_{\epsilon\to 0}\left(\frac{R(\hat{\mathbf{n}},\epsilon)-1}{\epsilon}\right)R(\hat{\mathbf{n}},\theta) = (\hat{\mathbf{n}}\cdot\mathscr{J})R(\hat{\mathbf{n}},\theta). \tag{4.25}$$

We conclude that

$$R(\hat{\mathbf{n}}, \theta) = e^{\theta \hat{\mathbf{n}} \cdot \mathscr{J}}. \tag{4.26}$$

As it turns out,

$$R(\mathbf{a} \times \mathbf{u}) = \det R(R\mathbf{a}) \times (R\mathbf{u}). \tag{4.27}$$

Lecture 5.

Postscript

These notes have been discontinued, since I have received a waiver for this course.