Exam 1 Outline

Bra–Ket Notation

- A *ket* $|\psi\rangle$ represents the state of a system. (ψ is just a label, and is not a wavefunction.)
- Kets have the properties of a Hilbert space (a vector space with an inner product). So $a|\psi\rangle + b|\phi\rangle$ is also a ket, for instance.
- States can also be represented by a *bra* $\langle\psi|$.
- $\langle\psi||\phi\rangle$ or $\langle\psi|\phi\rangle$ is the *inner product* (or dot product) of $|\psi\rangle$ and $|\phi\rangle$, and is equal to a complex number.
- $\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^*$
- The inner product of a state and itself is always a nonnegative real number: $\langle\psi|\psi\rangle \geq 0$.
- A state $|\psi\rangle$ is *normalized* if $\langle\psi|\psi\rangle = 1$.
- Usually we need to normalize kets before we can work with them: $|\psi\rangle \to \frac{|\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}}$
- Two states $|\phi\rangle$ and $|\psi\rangle$ are *orthogonal* if $\langle\phi|\psi\rangle = 0$.
- In a D–dimensional space, any D orthonormal vectors $|v_1\rangle, |v_2\rangle, \ldots, |v_D\rangle$ ($\langle v_i|v_j\rangle = \delta_{ij}$) will span the space: that is, *any* state $|\psi\rangle$ can be written

$$|\psi\rangle = c_1|v_1\rangle + c_2|v_2\rangle + \cdots + c_D|v_D\rangle$$

  where the complex numbers $c_i = \langle v_i|\psi\rangle$. Given these values, you can also write

$$\langle\psi| = c_1^*\langle v_1| + c_2^*\langle v_2| + \cdots + c_D^*\langle v_D|$$

  We'll call a set of D orthonormal vectors a *basis*.

Operators

- An *operator* takes a ket into another ket: e.g. $A|\psi\rangle = |\phi\rangle$.
- If $|\phi\rangle = A|\psi\rangle$, then $\langle\phi| = \langle\psi|A^\dagger$ where $A^\dagger$ is a different operator called the *Hermitian adjoint* of A.
- If $A = A^\dagger$, then we say that A is *Hermitian*.
- Each *physical observable* in the real-world are represented by a *Hermitian operator*. We can also think of the operator as a *measurement*.

- If a certain ket $|a\rangle$ obeys the relationship

$$A|a\rangle = \lambda|a\rangle,$$

  then $|a\rangle$ is an *eigenvector* of A with corresponding *eigenvalue* λ.

- If we apply a measurement A to a system in state $|\psi\rangle$,
  - the only possible results are the eigenvalues λ_i of A.
  - after the measurement, the system will be in the eigenvector $|a_i\rangle$ corresponding to the eigenvalue returned
  - The result λ_i will occur with probability

$$\mathcal{P}_i = |\langle a_i|\psi\rangle|^2$$

    (but only if $\langle a_i|$ and $|\psi\rangle$ are normalized!)

- The *projection operator* of $|a_1\rangle$ is

$$P_{a_1} = |a_1\rangle\langle a_1|$$

  If $|a_1\rangle$ is part of a basis $|a_i\rangle$, and $|\psi\rangle = c_1|a_1\rangle + c_2|a_2\rangle + \ldots$, then $P_{a_1}|\psi\rangle = c_1|\psi\rangle$.

- The *commutator* of two operators is $[A, B] \equiv AB - BA$.
- $[A, B] = -[B, A]$
- $[AB, C] = A[B, C] + [A, C]B$

Spin–1/2 Particles

- The spin of an electron is a 2–dimensional Hilbert space.
- The spin operators along the three axes, and their eigenequations, are

Operator	$\lambda = +\hbar/2$	$\lambda = -\hbar/2$
S_z	$S_z\|\uparrow\rangle = +\frac{\hbar}{2}\|\uparrow\rangle$	$S_z\|\downarrow\rangle = -\frac{\hbar}{2}\|\downarrow\rangle$
S_x	$S_x\|\odot\rangle = +\frac{\hbar}{2}\|\odot\rangle$	$S_x\|\otimes\rangle = -\frac{\hbar}{2}\|\otimes\rangle$
S_y	$S_y\|\rightarrow\rangle = +\frac{\hbar}{2}\|\rightarrow\rangle$	$S_y\|\leftarrow\rangle = -\frac{\hbar}{2}\|\leftarrow\rangle$

(McIntyre writes $|\uparrow\rangle = |+\rangle$, $|\downarrow\rangle = |-\rangle$, $|\odot\rangle = |+_x\rangle$, $|\otimes\rangle = |-_x\rangle$, $|\rightarrow\rangle = |+_y\rangle$, $|\leftarrow\rangle = |-_y\rangle$)

- In the S_z basis,

$$|\odot\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\rangle + |\downarrow\rangle\Big) \qquad |\otimes\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\rangle - |\downarrow\rangle\Big)$$

$$|\rightarrow\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\rangle + i|\downarrow\rangle\Big) \qquad |\leftarrow\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\rangle - i|\downarrow\rangle\Big)$$

- If $|a\rangle$ is one of the eigenvectors $\{|\uparrow\rangle, |\downarrow\rangle, |\rightarrow\rangle, |\leftarrow\rangle, |\odot\rangle, |\otimes\rangle\}$, and $|b\rangle$ is another one of the eigenvectors from a different eigenvector, then

$$|\langle a|b\rangle|^2 = \frac{1}{2}$$

- The spin operator along the axis

$$\hat{n} = \hat{x}\sin\theta\cos\phi + \hat{y}\sin\theta\sin\phi + \hat{z}\cos\theta$$

(where θ is measured from the $\hat{z}$ axis and ϕ is is measured from the $\hat{x}$ axis) is

$$S_{\hat{n}} = \sin\theta\cos\phi\, S_x + \sin\theta\sin\phi\, S_y + \cos\theta\, S_z$$

which has eigenvalues

$$|+_{\hat{n}}\rangle = \cos\frac{\theta}{2}|\uparrow\rangle + \sin\frac{\theta}{2}e^{i\phi}|\downarrow\rangle$$

$$|-_{\hat{n}}\rangle = \sin\frac{\theta}{2}|\uparrow\rangle - \cos\frac{\theta}{2}e^{i\phi}|\downarrow\rangle$$

- $[S_x, S_y] = i\hbar S_z$, $[S_y, S_z] = i\hbar S_x$, $[S_z, S_x] = i\hbar S_y$

- The operator $S^2 = S_x^2 + S_y^2 + S_z^2$ is the magnitude squared of the spin vector. It has the property $S^2|\psi\rangle = \frac{3\hbar^2}{4}|\psi\rangle$ for all $|\psi\rangle$. (That is, it is proportional to the identity operator.) It commutes with all spin operators (e.g. $[S^2, S_x] = 0$).

Matrix Representations

- A matrix representation requires us to choose a *basis*. We can choose whatever basis we like, but some choices may be more convenient than others. In the following section, we'll use the S_z basis (or the $|\uparrow\rangle$–$|\downarrow\rangle$ basis:

$$|\uparrow\rangle \doteq \begin{pmatrix}1\\0\end{pmatrix} \quad \text{and} \quad |\downarrow\rangle \doteq \begin{pmatrix}0\\1\end{pmatrix}$$

- Kets can be represented as column vectors, and bras as row vectors.

$$\text{If } |\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle, \text{ then } |\psi\rangle \doteq \begin{pmatrix}a\\b\end{pmatrix} \quad \text{and} \quad \langle\psi| \doteq (a^*\ b^*)$$

- In the basis $|v_1\rangle$, $|v_2\rangle$, ..., $|v_n\rangle$, we can write

$$|\psi\rangle \doteq \begin{pmatrix} \langle v_1|\psi\rangle \\ \langle v_2|\psi\rangle \\ \vdots \\ \langle v_n|\psi\rangle \end{pmatrix}$$

- An operator A in the same basis can be written

$$A \doteq \begin{pmatrix} \langle v_1|A|v_1\rangle & \langle v_1|A|v_2\rangle & \cdots & \langle v_1|A|v_n\rangle \\ \langle v_2|A|v_1\rangle & \langle v_2|A|v_2\rangle & \cdots & \langle v_2|A|v_n\rangle \\ \vdots & & \ddots & \vdots \\ \langle v_n|A|v_1\rangle & \langle v_n|A|v_2\rangle & \cdots & \langle v_n|A|v_n\rangle \end{pmatrix}$$

  The general form $\langle\phi|A|\psi\rangle$ is called a *matrix element* of A.

- The Hermitian adjoint is the complex transpose of a matrix.

- The eigenvalues λ of a matrix are the solutions to

$$\det(A - I\lambda) = 0$$

  You can then find the corresponding eigenvector by writing the vector as $\vec{v} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}$ and solving the equation $A\vec{v} = \lambda\vec{v}$ for v_i. (Or do it any way you like.)

- In the S_z basis, we can write the spin operators as

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad |\rightarrow\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \quad |\leftarrow\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad |\odot\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad |\otimes\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

- $$S^2 = \frac{3\hbar^2}{4}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \text{ (in any basis)}$$

Measurement

- When a large number of systems in state $|\psi\rangle$ is measured by operator A, the average value returned by A is
$$\langle A\rangle = \langle\psi|A|\psi\rangle$$
- The standard deviation in the measurement is $\Delta A = \sqrt{\langle A^2\rangle - \langle A\rangle^2}$. (This is the standard statistical definition.)
- Operators A and B are *compatible* if $[A, B] = 0$: they have the same set of eigenvectors
- The uncertainty principle:
$$\Delta A\,\Delta B \geq \frac{1}{2i}\langle[A, B]\rangle$$

Schrodinger's Equation

- Schrodinger's Equation:
$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle$$
- $H(t)$ is the energy operator or *Hamiltonian operator*
- H is an observable with eigenvectors
$$H|E_n\rangle = E_n|E_n\rangle$$

Time-Independent Hamiltonian

- If H is independent of time, and
$$|\Psi(0)\rangle = \sum_n c_n|E_n\rangle$$
then
$$|\Psi(t)\rangle = \sum_n c_n e^{-iE_nt/\hbar}|E_n\rangle$$
- In our class we've dubbed $e^{-iE_nt/\hbar}$ the *Schrodinger factor*, though this is not standard in the literature

- An energy eigenstate does not change with time: $|E_n(t)\rangle = e^{-iE_n t/\hbar}|E_n(0)\rangle$ which only varies by an overall phase, which is irrelevant. Energy eigenstates are called *stationary states*.

- In practice,

  1. Find the energy eigenstates, which form the energy basis.
  2. Write the initial state $|\Psi(0)\rangle$ in the energy basis.
  3. Multiply each term by the appropriate Schrodinger factor.

- If $[A, H] = 0$, then A's eigenstates also do not change with time (they are the same as the energy eigenstates)

- Note that all of this section goes out the window if the Hamiltonian has a time dependence. In that case, you need to solve the full Hamiltonian.

Spin Precession

- An electron placed in a magnetic field $B_0\hat{z}$ sees a Hamiltonian

$$H = \omega_0 S_z = \frac{\hbar\omega_0}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

  in the spin-1/2 basis, where $\omega_0 = \frac{eB}{m_e}$.

- The spin of the electron will precess around the z axis with frequency ω_0, the *Larmor frequency*. Be familiar with the calculations we did around this problem.

- If you add an additional magnetic field $B_1\hat{x}$ to the above (and $\omega_1 = eB_1/m_e$), the Hamiltonian is then

$$H = \omega_0 S_z + \omega_1 S_x = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_1 \\ \omega_1 & -\omega_0 \end{pmatrix}$$

  I'd like to calculate The probability $\mathcal{P}_{\Uparrow\to\Downarrow}$ that the electron will flip from $\uparrow$ to $\downarrow$ —that is, if the system starts in the state $|\Psi(0)\rangle = |\uparrow\rangle$, what is the probability that applying the measurement S_z to $|\Psi(t)\rangle$ yields a result of $|\downarrow\rangle$. This probability is given by *Rabi's formula*:

$$\mathcal{P}_{\Uparrow\to\Downarrow} = \frac{\omega_1^2}{\omega_0^2 + \omega_1^2}\sin^2\Big(\frac{\sqrt{\omega_0^2 + \omega_1^2}}{2}t\Big)$$

  This probability only approaches 1 as $\omega_1 \gg \omega_0$.

- Magnetic Resonance. Apply a time-dependent "cross field" to B_0 instead:

$$\vec{B} = B_0\hat{z} + B_1(\hat{x}\cos\omega t + \hat{y}\sin\omega t)$$

The Hamiltonian is now

$$H = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0 \end{pmatrix}$$

and the probability of a spin flip is

$$\mathcal{P}_{\Uparrow\to\Downarrow} = \frac{\omega_1^2}{(\Delta\omega)^2 + \omega_1^2}\sin^2\Big(\frac{\sqrt{(\Delta\omega)^2+\omega_1^2}}{2}t\Big)$$

where $\Delta\omega = \omega - \omega_0$ is the difference between the Larmor frequency of the main magnetic field B_0 and the frequency of rotation of the cross field B_1. By tuning this second frequency to the first, we can get a probability which reaches 100% (periodically).

Function Spaces

- A *state* is represented by a square-integrable function

$$|\psi\rangle \doteq \psi(x), \qquad \int |\psi|^2\,dx < \infty$$

- This is an infinite-dimensional vector space... infinite matrices!
- If $|x\rangle$ is the position eigenstate corresponding to a particle being at position x, then $\psi(x) = \langle x|\psi\rangle$.
- The inner product of two functions is defined as

$$\langle f|g\rangle = \int f(x)^* g(x)\,dx$$

- A set of functions f_n form a basis if $\langle f_n|f_m\rangle = \delta_{mn}$
- If f_n form a basis, any other function can be written as

$$f(x) = \sum_n c_n f_n(x), \qquad c_n = \langle f_n(x)|f(x)\rangle$$

- An operator takes functions into functions.
- The position operator $\hat{x}$ multiples a function by x.
- The momentum operator

$$\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$$

- The standard Hamiltonian is

$$H = \frac{p^2}{2m} + V = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

- A matrix element of A is written

$$\langle \phi | A | \psi \rangle = \int \phi(x)^* A \psi(x) \, dx$$

- Operators have eigenfunctions

$$Af(x) = \lambda f(x)$$