1. Fundamentals

The postulates of quantum mechanics

1) State as a vector in Hilbert space $|\Psi\rangle$.
2) Observables $\leftrightarrow$ Hermitian operators, $|\Psi\rangle = \sum_a c_a |a\rangle$.
3) Measurement: $|\Psi\rangle \to |a\rangle$, $\text{Prob}(a) = |\langle \psi | a\rangle|^2$.
4) Time-evolution

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

Hilbert space. Hilbert space as a vector space. Dual space. Inner product. Adjoint operator and Hermitian operators. Proof that Hermitian operators have real eigenvalues and orthogonal eigenvectors. Unitary operators. Change of basis operator.

Matrix representation of operators. How to find the matrix elements given a basis. You should know how to find the eigenvalues and eigenvectors of an operator (how to diagonalize it).

Degeneracy. The idea of a subspace. How to deal with degeneracy. Linear combination of degenerate eigenstates is also an eigenstate.

Identity operator. $\sum_n |n\rangle \langle n|$, $\int dx\, |x\rangle \langle x|$

Observables. Compatible and incompatible observables. The commutator $[\hat{A}, \hat{B}]$. If two operators commute, the basis vectors for one are also eigenvectors of the other. What happens when a sequence of measurements are made on a system, either involving compatible or incompatible observables (what happens to the state of the system after each measurement). The generalized uncertainty relation

$$\langle (\Delta A)^2\rangle \langle (\Delta B)^2\rangle \gtrsim \frac{1}{4} |\langle [A, B]\rangle|^2 \,.$$

Useful commutators.

$$[x, p] = i\hbar, \qquad [x_i, f(\boldsymbol{p})] = i\hbar \frac{\partial f}{\partial p_i}, \qquad [p_i, g(\boldsymbol{x})] = -i\hbar \frac{\partial g}{\partial x_i}$$

Unitary operators. $U^\dagger U = 1$. Preserves the inner product. Change of basis operator $U = \sum_n |b_n\rangle \langle a_n|$. Unitary equivalent observables A and $U^\dagger A U$ have the same eigenvalue spectrum.

Composite systems. General state (two component system) $\Psi = \sum c_{ab} |a\rangle |b\rangle$ where $|a\rangle$ is a basis in Hilbert space 1 and $|b\rangle$ is a basis in Hilbert space 2. Dimensions of the combined Hilbert space is $n \times m$.

Entanglement and correlated observables. Observables in 1 and 2 are uncorrelated if the state is a product state $|\Psi\rangle = |\Psi_1\rangle |\Psi_2\rangle$; otherwise the state is entangled and observables are correlated. The EPR state $\Psi = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$. The EPR paradox and how Bell's inequalities rule out hidden variable theories.

Quantum computing. The qubit. The general state of the qubit and the Bloch sphere. The basic idea of quantum computing, its advantages, and the challenges in implementing it. Examples of quantum gates (NOT, Hadamard operator, CNOT). The idea of a control register and why it is useful.

The density operator $\rho = \sum_n p_n |n\rangle \langle n|$ and its properties $\mathrm{Tr}(\rho) = 1$, $\langle \bar{A} \rangle = \mathrm{Tr}(\rho A)$. Pure states vs. mixed states. $\mathrm{Tr}(\rho^2) \leq 1$. The reduced density operator. Entanglement with the environment: decoherence and measurement.

2. Time-dependent systems

Time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\ket{\psi} = \hat{H}\ket{\psi}$$

and the idea of time-evolution by expanding in stationary states ($\hat{H}\ket{E} = E\ket{E}$)

$$\ket{\psi} = \sum a_E\ket{E}$$

with

$$a_E(t) = a_E(0)e^{-iEt/\hbar}.$$

Time-energy uncertainty relation. The idea that time-evolution depends on superpositions of stationary states, with observables evolving at a rate that depends on the energy differences. The uncertainty relation $\Delta E \Delta t \gtrsim \hbar$.

Time-evolution operator

$$\ket{\psi(t)} = \hat{U}(t)\ket{\psi(0)}$$

obeys

$$i\hbar\frac{\partial}{\partial t}\hat{U} = \hat{H}\hat{U}.$$

For a time-independent Hamiltonian,

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar} = \sum_E \ket{E}\bra{E}e^{-iEt/\hbar}.$$

Time-dependent Hamiltonian

$$\hat{U}(t) = \exp\left[-\frac{i}{\hbar}\int_0^t \hat{H}(t')dt'\right]$$

where you have to be careful about time-ordering in the integral.

Heisenberg picture. Make sure you understand the differences between Schrödinger and Heisenberg pictures. In the Heisenberg picture, the operators evolve according to $\hat{A}(t) = \hat{U}^\dagger\hat{A}(0)\hat{U}$, states are time-independent, basis vectors $\ket{n(t)} = \hat{U}^\dagger(t)\ket{n(0)}$.

The equation of motion

$$\frac{d\hat{A}}{dt} = \frac{[\hat{A},\hat{H}]}{i\hbar} + \hat{U}^\dagger\frac{\partial\hat{A}}{\partial t}\hat{U}.$$

Mixed states. Density operator evolves in time in Schrödinger according to

$$\frac{d\hat{\rho}}{dt} = \frac{[\hat{H}, \hat{\rho}]}{i\hbar}$$

The interaction picture. $H = H_0 + V(t)$. Use Heisenberg for H_0 and Schrödinger for $V(t)$:

$$i\hbar\frac{\partial}{\partial t}\left|\psi\right\rangle_I = V_I(t)\left|\psi\right\rangle_I,$$

where $V_I(t) = e^{iH_0 t/\hbar}V(t)e^{-iH_0 t/\hbar}$. With $\left|\psi\right\rangle_I$ expanded in stationary states

$$\left|\psi\right\rangle_I = \sum_n c_n(t)\left|n\right\rangle$$

the coefficients obey

$$i\hbar\dot{c}_n = e^{i\omega_{nm}t}V_{nm}c_m$$

$$V_{nm} = \langle n|V(t)|m\rangle, \qquad \hbar\omega_{nm} = E_n - E_m$$

The two state system with $V \propto e^{i\omega t}$ as an example.

Fermi's golden rule. The transition rate from a state $\left|n\right\rangle$ with energy E_n to a state $\left|f\right\rangle$ with energy E_f is

$$\Gamma = \frac{2\pi}{\hbar}\ g(E_f)\ |\langle f|V_0|n\rangle|^2,$$

where $g(E)$ is the density of states in energy (number of states between E and $E + dE$ is $g(E)dE$), $V = V_0 e^{i\omega t}$ is the perturbing potential and $E_f = E_n + \hbar\omega$.

Time-dependent perturbation theory. $c_n(t) = c_n^{(0)}(t) + c_n^{(0)}(t) + c_n^{(0)}(t)...$ For $c_n^{(0)} = \delta_{nm}$ (initially in stationary state m),

$$c_n^{(1)}(t) = -\frac{i}{\hbar}\int_0^t e^{i\omega_{nm}t'}V_{nm}(t')dt'$$

$$c_n^{(2)}(t) = \left(-\frac{i}{\hbar}\right)^2\sum_\ell\int_0^t dt'\int_0^{t'}dt'' e^{i\omega_{n\ell}t'}V_{n\ell}(t')e^{i\omega_{\ell m}t''}V_{\ell m}(t'')$$

Position and momentum eigenstates. The position operator $\hat{x}$ and its eigenstates $\left|x\right\rangle$. Wavefunction $\Psi(x) = \langle x\,|\,\Psi\rangle$. Probability density $|\langle x\,|\,\Psi\rangle|^2$. Orthonormality $\langle x\,|\,x'\rangle = \delta\,(x - x')$. The momentum operator $\hat{p} = -i\hbar\partial/\partial x$ and its eigenstates $\langle x\,|\,p\rangle = (2\pi\hbar)^{-1/2}e^{ipx/\hbar}$.

Adiabatic and sudden transitions. A sudden change in the Hamiltonian leaves the state unchanged. A slow change in the Hamiltonian leads to adiabatic evolution of the state $H(t)\,|n(t)\rangle = E_n(t)\,|n(t)\rangle$. The Berry phase

$$\gamma = i \int_0^t dt' \, \langle n|\frac{\partial}{\partial t} n\rangle$$

and its expression in terms of integrals in parameter space

$$\gamma = \oint d\boldsymbol{R} \cdot \boldsymbol{A}; \qquad \boldsymbol{A} = i \, \langle n|\nabla_R|n\rangle \, .$$

Propagator and path integrals. $K(x,t;x',t') = \langle x,t|x',t'\rangle = \langle x|e^{-iH(t-t')/\hbar}|x'\rangle$. Equal to $\delta(x-x')$ for $t = t'$. Integral solution of Schrödinger's equation

$$\psi(x,t) = \int dx' K(x,t;x',t')\psi(x',t').$$

Free particle propagator

$$K = \sqrt{\frac{m}{2\pi i\hbar(t-t')}} \exp\left(\frac{i(x-x')^2 m}{2\hbar(t-t')}\right)$$

The path integral

$$\langle x,t|x',t'\rangle = \int D[x(t)] \, e^{iS[x(t)]/\hbar}$$

where $S = \int dt \, L(t)$ is the action associated with a particular path.

Harmonic oscillator

$$\hat{H} = \hbar\omega(\hat{a}^\dagger \hat{a} + 1/2)$$

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right), \qquad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - i\frac{\hat{p}}{m\omega}\right)$$

$$a\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle, \qquad a^\dagger\left|n\right\rangle = \sqrt{n+1}\left|n+1\right\rangle, \qquad [\hat{a}, \hat{a}^\dagger] = 1$$

Time-independent perturbation theory

$$\Delta E_n^{(1)} = \langle n^0 | \lambda \hat{H}_1 | n^0 \rangle, \qquad \Delta E_n^{(2)} = \sum_{m \neq n} \frac{\left|\langle m^0 | \lambda \hat{H}_1 | n^0 \rangle\right|^2}{E_n^{(0)} - E_m^{(0)}}$$

$$|n\rangle = |n^0\rangle + \sum_{m \neq n} \frac{\langle m^0 | \lambda \hat{H}_1 | n^0 \rangle}{E_n^{(0)} - E_m^{(0)}} |m^0\rangle$$

Motion in electromagnetic fields

Hamiltonian

$$H = \frac{(\boldsymbol{p} - q\boldsymbol{A})^2}{2m} + q\phi$$

Mechanical momentum

$$\boldsymbol{\pi} = \boldsymbol{p} - q\boldsymbol{A}, \qquad [\hat{\pi}_i, \hat{\pi}_j] = i\hbar q \epsilon_{ijk} B_k$$

Gauge transformation

$$\boldsymbol{A} \to \boldsymbol{A}' = \boldsymbol{A} + \boldsymbol{\nabla}\lambda(\boldsymbol{r}) \qquad \phi \to \phi' = \phi - \frac{\partial\lambda}{\partial t}$$

$$|\psi\rangle \to |\psi'\rangle = e^{iq\lambda(\boldsymbol{r})/\hbar}|\psi\rangle$$

leaves $\langle x \rangle$ and $\langle \pi \rangle$ gauge invariant.

Landau levels. Charged particle in uniform B-field. Energy levels are

$$E_n = \hbar\omega_c\left(n + \frac{1}{2}\right) + \frac{p_z^2}{2m}$$

with cyclotron frequency $\omega_c = qB/m$.

Stationary states in the x-y plane

$$\Psi(x, y) = e^{iky} f_{nk}\left(x - \frac{\hbar}{qB}\right)$$

where $f_{nk}(x)$ is the nth stationary state of the harmonic oscillator with origin shifted to $x = (\hbar/qB)k$. Energy depends only on n, not k.

You should know how to write down the density of states for a free particle

$$dn = \frac{d^3\boldsymbol{k}d^3\boldsymbol{x}}{(2\pi)^3} = \frac{d^3\boldsymbol{p}d^3\boldsymbol{x}}{h^3}$$

Each Landau level has

$$\frac{qB}{2\pi\hbar} = \frac{B}{\Phi_0}$$

states per unit area. (This is just the number of states in energy range $\hbar\omega_c$ for an unmagnetized system "collapsed" into the Landau level.) $\Phi_0 = 2\pi\hbar/q = 4 \times 10^{-15}$ T m^2 is the "flux quantum".

Magnetized Fermi gas: at $T = 0$ a gas of fermions fills the levels up to the Fermi energy. The quantization into Landau levels introduces oscillations in quantities such as the total energy of the gas.

Atomic transitions. Application of Fermi's Golden Rule to atomic transitions. How to write down the vector potential for an electromagnetic wave. The electric dipole approximation. How to write down the density of states for a transition to a bound state or a continuum state. The concept of selection rules and how they arise from the matrix element $\langle f|x|i \rangle$.

3. Multi-particle systems

Non-interacting particles and exchange symmetry If the Hamiltonian can be written as a sum of single-particle Hamiltonians then we can write down the stationary states as a product of single particle stationary states $\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \psi_1(\boldsymbol{r}_1)\psi_2(\boldsymbol{r}_2)$.

Fermions and bosons The stationary states must be either symmetric or antisymmetric under exchange of any two particle labels. Bosons (integer spin) are symmetric; fermions (half-integer spin) are antisymmetric. Consequences:

Pauli-exclusion principle Fermions cannot occupy the same quantum state. E.g. atomic levels, Fermi gas

Bose-Einstein condensation Bosons can occupy the same state. At $T = 0$, can form a condensate, with a macroscopic number of particles in the ground state. Paired fermions can act as bosons, e.g. in superfluids and superconductors.

The helium atom. Use the hydrogen-like atom wavefunctions as single particle states. Solution by perturbation theory or variational principle. Singlet and triplet states can have different energies even without spin terms in the Hamiltonian, because they imply different symmetries for the spatial wavefunction.

Second quantization. Occupation number representation of the state of a multi-particle system $|n_1, n_2, ...n_N\rangle$. Creation and annhiliation operators and their (anti)commutation relations.

$$[a_i^\dagger, a_j^\dagger] = 0, \quad [a_i, a_j] = 0, \quad [a_i, a_j^\dagger] = \delta_{ij} \qquad \text{bosons}$$

$$\{a_i^\dagger, a_j^\dagger\} = 0, \quad \{a_i, a_j\} = 0, \quad \{a_i, a_j^\dagger\} = \delta_{ij} \qquad \text{fermions}$$

An additive single particle operator can be written

$$\mathcal{K} = \sum_i k_i a_i^\dagger a_i$$

in a diagonal basis (where the creation and annhiliation operators add or remove particles from the eigenstates of the operator), or

$$\mathcal{M} = \sum_{i,j} a_i^\dagger a_j \, \langle k_i|M|k_j\rangle$$

for a non-diagonal basis. Pairwise interaction:

$$\mathcal{V} = \frac{1}{2} \sum_{ij} V_{ij} a_i^\dagger a_j^\dagger a_j a_i$$

or

$$\mathcal{V} = \frac{1}{2} \sum_{ij\ell n} \langle ij|V|\ell n\rangle \, a_i^\dagger a_j^\dagger a_n a_\ell,$$

where

$$\langle ij|V|\ell n\rangle = \sum_{\alpha\beta} V_{\alpha\beta} \, \langle k_i|m_\alpha\rangle \, \langle m_\alpha|k_\ell\rangle \, \langle k_j|m_\beta\rangle \, \langle m_\beta|k_n\rangle \, .$$

For a two body potential in the momentum representation

$$\mathcal{V} = \frac{1}{2} \int d^3\boldsymbol{p}_i d^3\boldsymbol{p}_j d^3\boldsymbol{q} \; \tilde{V}(\boldsymbol{q}) \; a_{\mathbf{p}_i+\mathbf{q}}^\dagger a_{\mathbf{p}_j-\mathbf{q}}^\dagger a_{\mathbf{p}_j} a_{\mathbf{p}_i}$$

where $\boldsymbol{q}$ is the momentum transfer and

$$\tilde{V}(\boldsymbol{q}) = \int d^3\boldsymbol{x} \; e^{i\mathbf{x}\cdot\mathbf{q}} \, V(\boldsymbol{x}).$$

Pairing. Cooper instability: an arbitrarily weak attractive potential near the Fermi surface leads to bound states of two electrons. Phonon scattering at low frequency as the origin of the attractive potential between two electrons.

The BCS Hamiltonian

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k n_k + \sum_{k,k'} V_{kk'} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-k'\downarrow} c_{k'\uparrow}$$

and ground state

$$|\psi_G\rangle = \prod_k \left(u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger \right) |0\rangle \, .$$

The broadening of the Fermi surface that allows electrons to interact, lowering the total energy. The condensation energy $-(1/2)g(E_F)\Delta^2$. Size of a Cooper pair $\gg$ electron separation. Excitations: $E_k = (\xi_k^2 + \Delta^2)^{1/2}$.

4. Relativistic quantum mechanics

Klein-Gordon Equation

$$\left[\partial^\mu \partial_\mu - \left(\frac{mc}{\hbar}\right)^2\right]\Psi = \left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 - \left(\frac{mc}{\hbar}\right)^2\right]\Psi = 0$$

Represents spin zero particles (no spin components). Gives the correct energy-momentum relation for free particles $E^2 = (pc)^2 + (mc^2)^2$. Can incorporate EM fields by using $D_\mu \equiv \partial_\mu + iqA_\mu/\hbar c$ (equivalently replace $p_\mu \to p_\mu - qA_\mu/c$), where $A^\mu = (\phi, \boldsymbol{A})$, $p^\mu = (E/c, \boldsymbol{p})$. (Using cgs units for EM here)

Compton wavelength. $\lambda_C = h/mc$. The scale on which particle energies become comparable to their rest mass. The idea that this can lead to particle production, which ultimately leads to the breakdown of the single particle wave equation approach and instead to second quantization / quantum field theory.

Particles and antiparticles. The Klein Gordon equation has positive and negative energy solutions. Interpret them as representing particles or antiparticles. If Ψ solves the KG equation for charge q, Ψ^* solves the KG equation for $-q$. Because the KG equation is second order, we need to specify both $\psi(x)$ and $\partial\psi/\partial t$ at $t = 0$ which we can think of as specifying both the particle and antiparticle components.

Dirac equation.

$$\left(i\gamma^\mu \partial_\mu - \frac{mc}{\hbar}\right)\Psi = 0$$

where Ψ is a four-component spinor that tracks up and down spin and particle/antiparticle. Written as 2x2 matrices of 2x2 matrices, the gamma matrices are

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix},$$

where σ^i are the Pauli spin matrices ($i = x, y, z$). The gamma matrices satisfy $(\gamma^0)^2 = 1$, $(\gamma^i)^2 = -1$,

$$\frac{1}{2}\{\gamma^\mu, \gamma^\nu\} = \eta^{\mu\nu}.$$

Dirac Hamiltonian.

$$H = \boldsymbol{\alpha} \cdot \boldsymbol{p}c + \beta mc^2$$

where $\alpha^i = \gamma^0 \gamma^i$ and $\beta = \gamma^0$. Can use this to derive a probability conservation law

$$\partial_\mu j^\mu = \frac{\partial \rho}{\partial t} + \nabla \cdot \boldsymbol{j} = 0$$

where

$$j^\mu = \bar{\Psi} \gamma^\mu \Psi$$

and $\bar{\Psi} = \Psi^\dagger \gamma^0$. The probability density is $\rho = \Psi^\dagger \Psi = (E/mc^2) \bar{\Psi} \Psi$ and current is $\boldsymbol{j} = \Psi^\dagger \boldsymbol{\alpha} \Psi = \boldsymbol{p} \bar{\Psi} \Psi / mc$. Introducing a magnetic field and taking the non-relativistic limit, we end up with the usual spin Hamiltonian $\pi^2/2m - \boldsymbol{\mu} \cdot \boldsymbol{B}$ where $\mu = g(q/2m)S$ and $S = (\hbar/2)\sigma$.

Free particle solutions:

$$E = +E_p, \quad +\text{helicity} \qquad \psi = (1, 0, pc/(E_p + mc^2), 0)$$

$$E = -E_p, \quad +\text{helicity} \qquad \psi = (-pc/(E_p + mc^2), 0, 1, 0)$$

$$E = +E_p, \quad -\text{helicity} \qquad \psi = (0, 1, 0, -pc/(E_p + mc^2), 0)$$

$$E = -E_p, \quad -\text{helicity} \qquad \psi = (0, pc/(E_p + mc^2), 0, 1)$$

(with normalization factor $2E_p/(mc^2 + E_p)$ omitted and also $\psi \propto \exp(-ip^\mu x_\mu/\hbar)$.)

Helicity $\Sigma \cdot \boldsymbol{p}$ – projection of spin onto the momentum direction. The Dirac Hamiltonian commutes with the helicity operator, so helicity is conserved in a given frame. Lorentz transformation mixes left and right handed helicities.

Charge conjugation: if Ψ is the wavefunction (spinor) for a particle with charge q, then $i\gamma^2 \Psi^\star$ is the wavefunction for the corresponding antiparticle with charge $-q$. [Here the matrix γ^2 is γ^i with $i = 2$.]

We start by reviewing the mathematical
language that we use to describe quantum
systems.

1) <u>Hilbert space</u>   generalized vector space

A quantum state corresponds to a
vector in Hilbert space

$|\psi\rangle$
↖ "ket"

or more correctly a "ray" since it's the
direction that counts. We can multiply a
state by a scalar to normalize it for example
— ie. change the length of the vector —
but it is still the same state

Dimension of the space = how many numbers
we need to describe the state
        (ie. number of possible values of an
            observable)

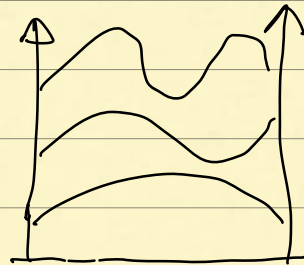eg. spin $\frac{1}{2}$ particle $|\uparrow\rangle, |\downarrow\rangle$ N = 2

eigenstates that we can use as a __basis__ to span the space

general state $|\psi\rangle = a|\uparrow\rangle + b|\downarrow\rangle$

↑

complex coefficients

eg. partide in a box

N = ∞

basis vectors can be the stationary states

$$|\psi\rangle = \sum c_n |n\rangle$$

or position eigenstates

$$|\psi\rangle = \int dx \, \psi(x) |x\rangle$$

Eigenstates of an operator

$$\hat{A} \, |n\rangle = a_n \, |n\rangle \qquad \text{(complex)} \text{ eigenvalue}$$

Same state

Q: Which operators were we using in the examples above?

2) Dual space

one-to-one Correspondence

$$|\psi\rangle \quad \longleftrightarrow \quad \langle\psi|$$

ket   bra

Hilbert space   dual space

$$a\,|\psi\rangle \quad \longleftrightarrow \quad \langle\psi|\, a^{*}$$

Inner product $\langle\phi|\psi\rangle$ Complex number

$$\langle\phi|\psi\rangle^{*} = \langle\psi|\phi\rangle \qquad \text{Complex conjugates}$$
$$(\Rightarrow \langle\phi|\phi\rangle \text{ is real})$$

3) <u>Adjoint operator</u>

$\langle \psi | \hat{A}^\dagger$ is the dual of $\hat{A} | \psi \rangle$

in general $\langle \psi | \hat{A} \neq \langle \psi | \hat{A}^\dagger$

but this <u>is</u> true for <u>Hermitian operators</u>

$$\underline{\hat{A} = \hat{A}^\dagger}$$

Note that $\left(\langle \phi | \hat{A}^\dagger | \psi \rangle \right)^*$

$= \langle \psi | \hat{A} | \phi \rangle$

First, discuss the reading questions from this week

1) $\left(\langle\psi|\hat{A}|\phi\rangle\right)^* = ?$

We know that $\left(\langle\phi|\psi\rangle\right)^* = \langle\psi|\phi\rangle$
so the key thing is to treat
$$\hat{A}|\phi\rangle \quad \text{as another ket}$$

with corresponding bra $\langle\phi|\hat{A}^\dagger$

$\Rightarrow \quad \left(\langle\psi|\hat{A}|\phi\rangle\right)^* = \langle\phi|\hat{A}^\dagger|\psi\rangle.$

2)   Proof that Hermitian operators have real eigenvalues and orthogonal eigenstates.

Consider a Hermitian operator $\hat{A}$, and write

$$\hat{A}|n\rangle = a_n|n\rangle \qquad \text{①}$$

$$\langle m|\hat{A}^\dagger = a_m^*\langle m| \qquad \text{②}$$

$$\text{①} \Rightarrow \qquad \langle m|\hat{A}|n\rangle = a_n\langle m|n\rangle$$

$$\text{②} \Rightarrow \qquad \langle m|\hat{A}^\dagger|n\rangle = a_m^*\langle m|n\rangle$$

$$\Rightarrow \qquad \boxed{0 = (a_n - a_m^*)\langle m|n\rangle}$$

$$\left(\text{where we used the fact that } \hat{A}^\dagger = \hat{A}\right)$$

Either $|m\rangle = |n\rangle$ (same eigenstate)
   then

$$a_n = a_n^* \qquad \underline{\text{real eigenvalues}}$$

or $\qquad |m\rangle \neq |n\rangle$

then since $a_n \neq a_m^*$ in general

$$\langle m|n\rangle = 0 \qquad \underline{\text{eigenstates are}}$$
$$\underline{\text{orthogonal}}$$

The eigenstates of $\hat{A}$ form an orthonormal basis that spans the Hilbert space

$$|\psi\rangle = \sum_n c_n |n\rangle$$

where $c_n = \langle n | \psi \rangle$

Postulates of QM

1. The state of a system is a vector in Hilbert space
$$|\psi\rangle$$
This contains all the information that we have about a system

2. Observables $\longleftrightarrow$ Hermitian operators

$$|\psi\rangle = \sum_a c_a |a\rangle$$

3. Measurement $\qquad |\psi\rangle \xrightarrow{\text{collapses}} |a\rangle$

$$\text{Prob}(\text{measuring } a) = |\langle \psi | a \rangle|^2$$

$$= |c_a|^2$$

(We can also add a 4th postulate that tells us how to time-evolve the state, ie. Schrödinger's equation

$$-i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle$$

but we'll discuss this more in Part 2
when we talk about dynamics).

A couple of more points about the formalism:

1) <u>Identity and projection operators</u>

$$|\psi\rangle = \sum_n c_n |n\rangle$$

$$\Rightarrow \quad \langle m|\psi\rangle = \sum c_n \langle m|n\rangle$$

$$= \sum c_n \, \delta_{mn}$$

$$= c_m$$

So the expansion coefficients are $c_n = \langle n|\psi\rangle$

(similar idea to Fourier expansion etc...)

Therefore we can write

$$|\psi\rangle = \sum_n \langle n|\psi\rangle |n\rangle$$
$$= \sum_n |n\rangle\langle n|\psi\rangle$$
$$= \left(\sum_n |n\rangle\langle n| \right) |\psi\rangle$$

<u>identity operator</u>

$|n\rangle\langle n|$ is the __projection operator__

eg. $\left(|n\rangle\langle n|\right) |\psi\rangle = \langle n|\psi\rangle |n\rangle$

is the component of $|\psi\rangle$ in the direction $|n\rangle$.

When we sum the projection operator over a complete basis, we get the identity operator.

The product $|\psi\rangle\langle\phi|$ is referred to as the __outer product__

$\left(\text{as opposed to inner product } \langle\psi|\phi\rangle\right)$.

2) __Matrix representation of operators__

With the expansion $|\psi\rangle = \sum c_n |n\rangle$

the set of coefficients $\{c_n\}$ specify the state.

Now consider $\hat{A}|\psi\rangle$ for some operator $\hat{A}$.

$$\hat{A}|\psi\rangle = \sum c_n \hat{A}|n\rangle$$

$$\Rightarrow \hat{A}|\psi\rangle = \sum_n c_n \sum_m |m\rangle\langle m|\hat{A}|n\rangle$$

(insert identity operator)

$$= \sum_m \left(\underbrace{\sum_n c_n \langle m|\hat{A}|n\rangle} \right) |m\rangle$$

these are the coefficients that represent the ket $\hat{A}|\psi\rangle$

$$\text{ie. } \hat{A}|\psi\rangle = \sum b_m |m\rangle$$

$$\text{with} \quad b_m = \sum_n A_{mn} c_n$$

$$\text{and} \quad A_{mn} = \langle m|\hat{A}|n\rangle$$

We see that we can write
$$|\phi\rangle = \hat{A}|\psi\rangle$$

as a matrix multiplication $\underline{b} = \underline{\underline{A}} \cdot \underline{c}$

The quantities $A_{mn} = \langle m| \hat{A} |n\rangle$

are the "matrix elements"
of $\hat{A}$ in the basis $\{|n\rangle\}$

Notes
- Hermitian operator has $A_{mn} = A_{nm}^{*}$
  (Hermitian matrix)

- if $\{|n\rangle\}$ are the eigenvectors of $\hat{A}$
  then A_{mn} is diagonal

$$\langle n| \hat{A} |m\rangle = a_m \langle n|m\rangle$$
$$= a_m \delta_{nm}$$

- we can think of bra's as row vectors and kets as column vectors

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} \qquad \langle\psi| = \begin{pmatrix} c_1^* & c_2^* & \cdots & c_N^* \end{pmatrix}$$

then $\langle\psi|\psi\rangle$ is a scalar (dot product);

$|\psi\rangle\langle\psi|$ is a matrix (outer product)

End with a bit of discussion about
measurement

Consider measuring two observables $\hat{A}$ and $\hat{B}$.

Important quantity is the commutator

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

If $[\hat{A}, \hat{B}] = 0$ then $\hat{A}$ and $\hat{B}$ have a
complete set of simultaneous eigenstates.
We refer to them as <u>compatible observables</u>.

To see this, use the eigenstates of $\hat{A}$ as
a basis
$$\hat{A}|n\rangle = a_n|n\rangle$$

and then ask is $\langle n|\hat{B}|m\rangle$ diagonal
in this basis?

If we assume $[\hat{A}, \hat{B}] = 0$
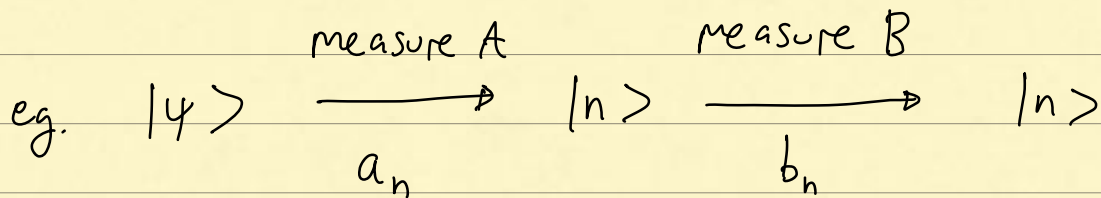
then $\langle n|[\hat{A}, \hat{B}]|m\rangle = 0$

$$\Rightarrow \quad \langle n| \hat{A}\hat{B} |m\rangle - \langle n| \hat{B}\hat{A} |m\rangle = 0$$

$$a_n \langle n| \hat{B} |m\rangle - a_m \langle n| \hat{B} |m\rangle = 0$$

$$(a_n - a_m) \langle n| \hat{B} |m\rangle = 0$$

$$\Rightarrow \quad \langle n| \hat{B} |m\rangle \; \propto \; \delta_{nm}$$

ie. $\hat{B}$ is diagonal in this
basis if $[\hat{A}, \hat{B}] = 0$ ✓

eg. $|\psi\rangle \xrightarrow[a_n]{\text{measure A}} |n\rangle \xrightarrow[b_n]{\text{measure B}} |n\rangle$

Last time, we began to discuss measurement.
Main ideas:

Observables $\longleftrightarrow$ Hermitian operators

- real eigenvalues
- orthogonal eigenstates

Measurement postulate

$$|\psi\rangle \xrightarrow[a_n]{\hat{A}} |n\rangle$$

Probability of measuring a_n is $|\langle n|\psi\rangle|^2$.

Compatible observables commute

$$[\hat{A}, \hat{B}] = 0$$

$\Rightarrow$ $\hat{A}$ and $\hat{B}$ have a common eigenbasis

$$|\psi\rangle \xrightarrow[a_n]{\hat{A}} |n\rangle \xrightarrow[b_n]{\hat{B}} |n\rangle$$

Discussion of reading question 2

What happens if there is degeneracy?

eg.
$$\hat{A} |n\rangle = a |n\rangle$$

$$\hat{A} |m\rangle = a |m\rangle$$

Important points:

— any linear combination of $|m\rangle$ and $|n\rangle$ is also an eigenstate with the same eigenvalue

$$\hat{A} \left[\alpha |n\rangle + \beta |m\rangle \right] = \alpha \hat{A} |n\rangle + \beta \hat{A} |m\rangle$$

$$= a \left[\alpha |n\rangle + \beta |m\rangle \right]$$

— we say that there is a degenerate subspace of the Hilbert space

dimension = # degenerate states

— We can construct an orthogonal basis for the subspace using linear combinations of $|m\rangle$ and $|n\rangle$.

Example (problem 1.23 from Sakurai)

Operator $\hat{A}$ has representation

$$\begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix}$$

with basis vectors $|1\rangle$, $|2\rangle$, $|3\rangle$

$|2\rangle$ and $|3\rangle$ have the same eigenvalue $(-a)$
— there is a 2D subspace

Any orthogonal linear combinations of $|2\rangle$ and $|3\rangle$ would give the same matrix for $\hat{A}$.

Now consider a second operator $\hat{B}$. With the same basis vectors,

1.23 Consider a three-dimensional ket space. If a certain set of orthonormal kets—say, $|1\rangle$, $|2\rangle$, and $|3\rangle$—are used as the base kets, the operators A and B are represented by

$$A \doteq \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix}, \quad B \doteq \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix}$$

with a and b both real.

(a) Obviously A exhibits a degenerate spectrum. Does B also exhibit a degenerate spectrum?

(b) Show that A and B commute.

(c) Find a new set of orthonormal kets that are simultaneous eigenkets of both A and B. Specify the eigenvalues of A and B for each of the three eigenkets. Does your specification of eigenvalues completely characterize each eigenket?

$$\hat{B} = \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix}. \qquad \left(\begin{array}{c} \text{Can show} \\ \text{that } [\hat{A}, \hat{B}] = 0 \end{array} \right)$$

We see that $|1\rangle$ is an eigenvector of $\hat{B}$ but $|2\rangle$ and $|3\rangle$ are not.

The eigenvectors and eigenvalues of

$$\begin{pmatrix} 0 & -ib \\ ib & 0 \end{pmatrix} \quad \text{are} \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} \quad b$$

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \quad -b$$

Note that both of these are eigenvectors of $\hat{A}$ with eigenvalue $-a$.

So in this problem where we are interested in $\hat{A}$ and $\hat{B}$, a natural basis to use is

$$|a\ b\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |-a\ b\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ i \end{pmatrix}$$

$$|-a\ -b\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -i \end{pmatrix}.$$

Now imagine measuring $\hat{A}$ then $\hat{B}$:

If the measurement of $\hat{A}$ returns $+a$, this is straight forward :

$$|\psi> \xrightarrow[a]{\hat{A}} \quad |a \; b> \xrightarrow[b]{\hat{B}} |a \; b>$$

If $\hat{A}$ returns $(-a)$ then the state of the system must be a linear combination of $|-a \; b>$ and $|-a \; -b>$ after the measurement.

Which linear combination depends on the initial state $|\psi>$
— after the measurement, the state will be the projection of $|\psi>$ into the subspace

eg. $|\psi> = c_0 |a \; b> + c_1 |-a \; b>$

$$+ \; c_2 |-a \; -b>$$

$$|\psi\rangle \xrightarrow[(-a)]{\hat{A}} \frac{c_1 |-a \; b\rangle + c_2 |-a \; -b\rangle}{\sqrt{|c_1|^2 + |c_2|^2}}$$

For a similar example, see Shankar p132.

measurement, though the eigenvalue will not, as the following example will show. Consider two operators Λ and Ω on $\mathbb{V}^3(R)$. Let $|\omega_3\lambda_3\rangle$ be one common eigenvector. Let $\lambda_1 = \lambda_2 = \lambda$. Let $\omega_1 \neq \omega_2$ be the eigenvalues of Ω in this degenerate space. Let us use as a basis $|\omega_1\lambda\rangle$, $|\omega_2\lambda\rangle$, and $|\omega_3\lambda_3\rangle$. Consider a normalized state

$$|\psi\rangle = \alpha|\omega_3\lambda_3\rangle + \beta|\omega_1\lambda\rangle + \gamma|\omega_2\lambda\rangle \tag{4.2.16}$$

Let us say we measure Ω first and get ω_3. The state becomes $|\omega_3\lambda_3\rangle$ and the subsequent measurement of Λ is assured to give a value λ_3 and to leave the state alone. Thus $P(\omega_3, \lambda_3) = |\langle\omega_3\lambda_3|\psi\rangle|^2 = \alpha^2$. Evidently $P(\omega_3, \lambda_3) = P(\lambda_3, \omega_3)$.

Suppose that the measurement of Ω gave a value ω_1. The resulting state is $|\omega_1\lambda\rangle$ and the probability for this outcome is $|\langle\omega_1\lambda|\psi\rangle|^2$. The subsequent measurement of Λ will leave the state alone and yield the result λ with unit probability. Thus $P(\omega_1, \lambda)$ is the product of the probabilities:

$$P(\omega_1, \lambda) = |\langle\omega_1\lambda|\psi\rangle|^2 \cdot 1 = |\langle\omega_1\lambda|\psi\rangle|^2 = \beta^2 \tag{4.2.17}$$

Let us now imagine the measurements carried out in reverse order. Let the result of the measurement be λ. The state $|\psi'\rangle$ after measurement is the projection of $|\psi\rangle$ in the degenerate λ eigenspace:

$$|\psi'\rangle = \frac{\mathbb{P}_\lambda|\psi\rangle}{|\langle\mathbb{P}_\lambda\psi|\mathbb{P}_\lambda\psi\rangle|^{1/2}} = \frac{\beta|\omega_1\lambda\rangle + \gamma|\omega_2\lambda\rangle}{(\beta^2 + \gamma^2)^{1/2}} \tag{4.2.18}$$

where, in the expression above, the projected state has been normalized. The probability for this outcome is $P(\lambda) = \beta^2 + \gamma^2$, the square of the projection of $|\psi\rangle$ in the eigenspace. If Ω is measured now, both results ω_1 and ω_2 are possible. The probability for obtaining ω_1 is $|\langle\omega_1\lambda|\psi'\rangle|^2 = \beta^2/(\beta^2 + \gamma^2)$. Thus, the probability for the result $\Lambda = \lambda$, $\Omega = \omega_1$, is the product of the probabilities:

$$P(\lambda, \omega_1) = (\beta^2 + \gamma^2) \cdot \frac{\beta^2}{\beta^2 + \gamma^2} = \beta^2 = P(\omega_1, \lambda) \tag{4.2.19}$$

Thus $P(\omega_1, \lambda) = P(\lambda, \omega_1)$ independent of the degeneracy. *But this time the state suffered a change due to the second measurement* (unless by accident $|\psi'\rangle$ has no component along $|\omega_2\lambda\rangle$). Thus compatibility generally implies the invariance under the second measurement of the *eigenvalue* measured in the first. Therefore, the state can only be said to remain in the same eigenspace after the second measurement. If the first eigenvalue is non-degenerate, the eigenspace is one dimensional and the state vector itself remains invariant.

In our earlier discussion on how to produce well-defined states $|\psi\rangle$ for testing quantum theory, it was observed that the measurement process could itself be used as a preparation mechanism: if the measurement of Ω on an arbitrary, unknown initial state given a result ω, we are sure we have the state $|\psi\rangle = |\omega\rangle$. But this presumes ω is not a degenerate eigenvalue. If it is degenerate, we cannot nail down the state, except to within an eigenspace. It was therefore suggested that we stick to variables with a nondegenerate spectrum. We can now lift that restriction. Let us

An example with incompatible observables

See Sakurai p 32, Fig 1·8 (I added it on the next page).

Equations (1.4.46) and (1.4.47) give the probability of measuring $|c'\rangle$ given the input $|a'\rangle$, ie. $|\langle c'|a'\rangle|^2$
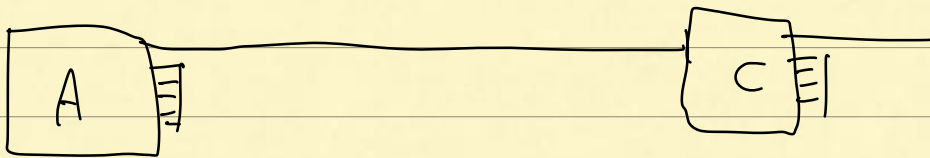
In this case, where B is measured as well,

A ⊏ B ⊏ C
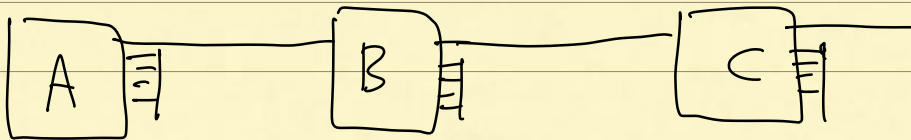
it is (summed over all possible B measurements)

$$\sum_b |\langle c'|b'\rangle|^2 \, |\langle b'|a'\rangle|^2 \qquad\qquad ─\text{①}$$

whereas for

A ⊏ C

it is
$$\left| \sum_b \langle c' | b' \rangle \langle b' | a' \rangle \right|^2 \quad - ②$$

These are not the same! Even though we average over all b' values, the act of measuring B changes the state and removes the cross-terms that are present in ②.

(This has echoes of the double slit experiment — in ② the different b' choices interfere (cross-terms) whereas in ① they do not because we measure b' in each case.)
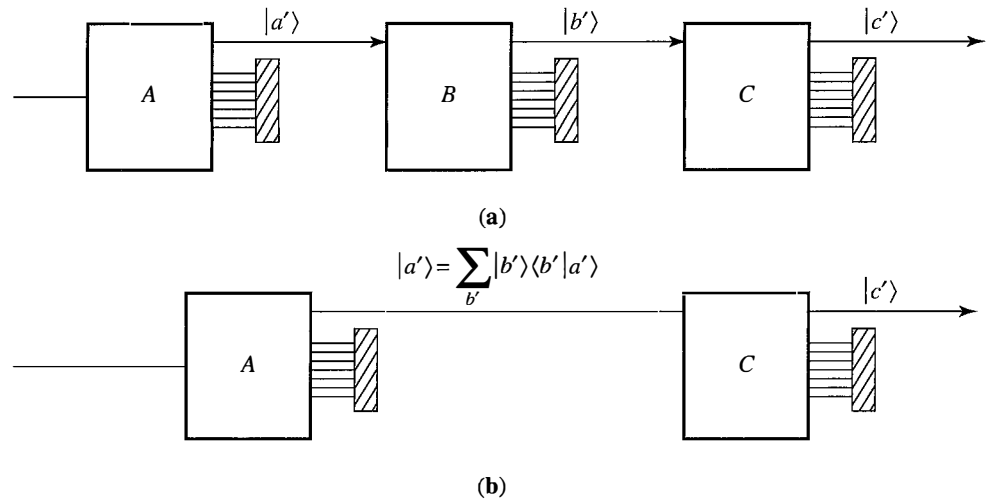
FIGURE 1.8   Sequential selective measurements.

Likewise,

$$BA|a',b'\rangle = Ba'|a',b'\rangle = a'b'|a',b'\rangle; \qquad (1.4.43)$$

hence,

$$AB|a',b'\rangle = BA|a',b'\rangle, \qquad (1.4.44)$$

and thus $[A,B] = 0$ in contradiction to the assumption. So, in general, $|a',b'\rangle$ does not make sense for incompatible observables. There is, however, an interesting exception; it may happen that there exists a subspace of the ket space such that (1.4.44) holds for all elements of this subspace, even though A and B are incompatible. An example from the theory of orbital angular momentum may be helpful here. Suppose we consider an $l = 0$ state (s-state). Even though L_x and L_z do *not* commute, this state *is* a simultaneous eigenstate of L_x and L_z (with eigenvalue zero for both operators). The subspace in this case is one-dimensional.

We already encountered some of the peculiarities associated with incompatible observables when we discussed sequential Stern-Gerlach experiments in Section 1.1. We now give a more general discussion of experiments of that type. Consider the sequence of selective measurements shown in Figure 1.8a. The first (A) filter selects some particular $|a'\rangle$ and rejects all others, the second (B) filter selects some particular $|b'\rangle$ and rejects all others, and the third (C) filter selects some particular $|c'\rangle$ and rejects all others. We are interested in the probability of obtaining $|c'\rangle$ when the beam coming out of the first filter is normalized to unity. Because the probabilities are multiplicative, we obviously have

$$|\langle c'|b'\rangle|^2|\langle b'|a'\rangle|^2. \qquad (1.4.45)$$

Now let us sum over b' to consider the total probability for going through all possible b' routes. Operationally this means that we first record the probability of

obtaining c' with all but the first b' route blocked; then we repeat the procedure with all but the second b' blocked, and so on; then we sum the probabilities at the end and obtain

$$\sum_{b'} |\langle c'|b'\rangle|^2 |\langle b'|a'\rangle|^2 = \sum_{b'} \langle c'|b'\rangle\langle b'|a'\rangle\langle a'|b'\rangle\langle b'|c'\rangle. \qquad (1.4.46)$$

We now compare this with a different arrangement, where the B filter is absent (or not operative); see Figure 1.8b. Clearly, the probability is just $|\langle c'|a'\rangle|^2$, which can also be written as follows:

$$|\langle c'|a'\rangle|^2 = \left|\sum_{b'} \langle c'|b'\rangle\langle b'|a'\rangle\right|^2 = \sum_{b'}\sum_{b''} \langle c'|b'\rangle\langle b'|a'\rangle\langle a'|b''\rangle\langle b''|c'\rangle. \quad (1.4.47)$$

Notice that expressions (1.4.46) and (1.4.47) are different! This is remarkable because in both cases the pure $|a'\rangle$ beam coming out of the first (A) filter can be regarded as being made up of the B eigenkets

$$|a'\rangle = \sum_{b'} |b'\rangle\langle b'|a'\rangle, \qquad (1.4.48)$$

where the sum is over all possible values of b'. The crucial point to be noted is that the result coming out of the C filter depends on whether or not B measurements have actually been carried out. In the first case, we experimentally ascertain which of the B eigenvalues are actually realized; in the second case, we merely imagine $|a'\rangle$ to be built up of the various $|b'\rangle$'s in the sense of (1.4.48). Put in another way, actually recording the probabilities of going through the various b' routes makes all the difference even though we sum over b' afterwards. Here lies the heart of quantum mechanics.

Under what conditions do the two expressions become equal? It is left as an exercise for the reader to show that for this to happen, in the absence of degeneracy, it is sufficient that

$$[A, B] = 0 \quad \text{or} \quad [B, C] = 0. \qquad (1.4.49)$$

In other words, the peculiarity we have illustrated is characteristic of incompatible observables.

The Uncertainty Relation

The last topic to be discussed in this section is the uncertainty relation. Given an observable A, we define an **operator**

$$\Delta A \equiv A - \langle A\rangle, \qquad (1.4.50)$$

where the expectation value is to be taken for a certain physical state under consideration. The expectation value of $(\Delta A)^2$ is known as the **dispersion** of A. Because we have

$$\langle(\Delta A)^2\rangle = \langle(A^2 - 2A\langle A\rangle + \langle A\rangle^2)\rangle = \langle A^2\rangle - \langle A\rangle^2, \qquad (1.4.51)$$

Last time:
- Compatible and incompatible observables
- how measurement works when there is degeneracy

The fact that compatible observables share eigenstates means that we can know the values of both observables at the same time — measurement of one doesn't affect measurement of the other.

This is generally written in the form of the

uncertainty relation

$$\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq \frac{1}{4} \left| \langle [\hat{A}, \hat{B}] \rangle \right|^2$$

where $\Delta \hat{A} = \hat{A} - \langle A \rangle$

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle$$

$$= \sum |\langle a_n | \psi \rangle|^2 \, a_n$$

is the expectation value of $\hat{A}$ given the state $|\psi\rangle$.

$$\langle (\Delta A)^2 \rangle = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$$

$$= \langle \psi | \hat{A}^2 | \psi \rangle - \langle \psi | \hat{A} | \psi \rangle^2$$

(variance)

You can find the proof of the uncertainty relation in

      Sakurai $\S 1.4.5$ p33

or

      Shankar $\S 9.2$ p237

Examples $[\hat{x}, \hat{p}_x] = i\hbar$

$$\Rightarrow \quad \Delta x \, \Delta p_x \geq \hbar/2$$

$[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z$ $[\hat{x}, \hat{p}_z] = 0$

$[\hat{L}^2, \hat{L}_z] = 0$ $[\hat{x}, \hat{y}] = 0$

Composite states and Entanglement

See Binney & Skinner Chapter 6 for a
good discussion of this topic.

eg. <u>electron in H atom</u>

$$|\psi\rangle = |n\ \ell\ m\rangle \otimes |s\rangle$$

infinite Hilbert
Space

2D Hilbert space

$$a|\uparrow\rangle + b|\downarrow\rangle$$

$$\psi(\vec{x}) = \langle \vec{x} | n\ \ell\ m\rangle$$

The $\otimes$ indicates that we are taking the
"direct product" of two vectors from different
Hilbert spaces. We usually don't need to
write it because it will be obvious from the
context what we mean.

eg. when we write $\hat{J} = \hat{L} + \hat{S}$

what we really mean is $\hat{L} \otimes \hat{1} + \underline{\hat{1}} \otimes \hat{S}$

Often we would just use the shorthand

$$| n \; \ell \; m \; s \rangle$$ to represent the state,

but it's important to realize that when we do so we are implicitly talking about two seperate Hilbert spaces.

Another example is a multiple particle system

eg. two spin-$\frac{1}{2}$ particles

$$|\psi\rangle = a |\uparrow\rangle |\uparrow\rangle + b |\uparrow\rangle |\downarrow\rangle$$

$$+ c |\downarrow\rangle |\uparrow\rangle + d |\downarrow\rangle |\downarrow\rangle$$

particle 1   particle 2

Note that

$$\text{dimension of product space} = \text{product of dimensions of constituent spaces}$$

$$|\psi\rangle = \sum_{n,m} c_{nm} |n\rangle |m\rangle$$

basis for Hilbert space 1

basis for Hilbert space 2

product space has dimensions $N \times M$

ie. we need $N \times M$ coefficients c_{nm} to specify the state.

This can get very large very quickly as we add more components / particles to a system !

A product state $|\psi\rangle = |A\rangle|B\rangle$

$$= \left(\sum_n a_n |n\rangle \right) \left(\sum_m b_m |m\rangle \right)$$

$$= \sum_{n,m} a_n b_m |n\rangle|m\rangle$$

is a special case where we only need
to specify N + M coefficients

$$\left(N \text{ for the } \{a_n\} \text{ and } M \text{ for } \{b_m\} \right)$$

States of the form $|A\rangle|B\rangle$ have the
property that measurements of $\hat{A}$ and $\hat{B}$
are uncorrelated.

If $|\psi\rangle$ can not be written as a product
we say that the state is "entangled"

Measurements of $\hat{A}$ and $\hat{B}$ are then
correlated.

eg. $|\psi\rangle = \alpha |\uparrow\rangle|\uparrow\rangle$

$$+ |\downarrow\rangle (\beta |\uparrow\rangle + \gamma |\downarrow\rangle)$$

(this is from Binney & Skinner § 6.1.1)

Measure the spin of particle 1:

1) the result is $\uparrow$

$$\Rightarrow |\psi\rangle \longrightarrow |\uparrow\rangle|\uparrow\rangle$$

if we then measure the spin of particle 2,
we are guaranteed to get $\uparrow$.

2) the result is $\downarrow$

$$\Rightarrow |\psi\rangle \longrightarrow \frac{\beta |\downarrow\rangle|\uparrow\rangle + \gamma |\downarrow\rangle|\downarrow\rangle}{\sqrt{\beta^2 + \gamma^2}}$$

measure particle 2:

$$\text{Prob} (\uparrow) = \frac{\beta^2}{\beta^2 + \gamma^2} \quad , \quad \text{Prob} (\downarrow) = \frac{\gamma^2}{\gamma^2 + \beta^2}$$

Summarize in a table:

A measurement	B measurement	P(B|A)
$\uparrow$	$\uparrow$	100%
$\uparrow$	$\downarrow$	0%
$\downarrow$	$\uparrow$	$\dfrac{\beta^2}{\beta^2 + \gamma^2}$
$\downarrow$	$\downarrow$	$\dfrac{\gamma^2}{\beta^2 + \gamma^2}$

The outcome of the $\hat{B}$ measurement depends on what we measured for $\hat{A}$.

The two particles in this case are <u>entangled</u>.

Exercise: make the table for the case where we measure B and then A.

EPR state

Classic example

e^+

• nucleus with spin
zero decays

e^-
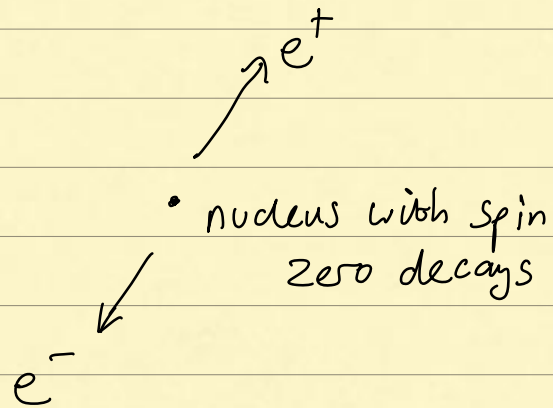
$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle \right)$$

$$= \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$

(spin singlet)

One observer measures the spin of the electron.
The result is either

$$|\psi\rangle \rightarrow |\uparrow\downarrow\rangle$$
$$\text{or } |\psi\rangle \rightarrow |\downarrow\uparrow\rangle.$$

Take the first one — the electron is measured
to have $S_z(e^-) = \uparrow$.

If a second observer then measures the positron
spin in the same direction, they are guaranteed

to get $S_z(e^+) = \downarrow$.

But they might choose a different axis, e.g. if they measure S_x instead they will get

$$S_x = +1 \qquad 50\% \text{ probability}$$

or

$$S_x = -1 \qquad 50\% \text{ probability.}$$

So depending on the relative choice of axes that the two observers make, their measurements can be anywhere between fully - correlated or not correlated at all.

"<u>Non-locality</u>" Observation of one of the particles collapses the wavefunction of the whole system — no matter how far away the 2nd particle is.

EPR "Paradox" Einstein, Podolsky, Rosen
(1935)

EPR made a similar argument involving position & momentum measurements and argued that QM must be incomplete.

Last time —

Composite systems

$$|\psi\rangle = \sum c_{ij} |a_i\rangle |b_j\rangle$$

If $|\psi\rangle$ can <u>not</u> be written as a product

$$|\psi\rangle = \left(\sum \alpha_i |a_i\rangle \right) \left(\sum \beta_j |b_j\rangle \right)$$

then the state is ENTANGLED.

Measurements of observables associated with different components of the system are correlated.

- Discussion of Reading Question 3.

Quantum computing

To simulate a quantum system requires keeping track of a large number of amplitudes.

eg.   N coupled 2-state systems

→   total dimension 2^N

This can quickly get out of hand, eg. $2^{1000} \simeq 10^{300}$ Impossible to simulate on a (classical) computer. But turning this around, can we use a quantum system to perform computations out of reach of classical machines?

Basic building block: $\boxed{\text{qubit}}$

2 state system
linear combination of $|0\rangle$ and $|1\rangle$

eg. 2 qubits $|\psi\rangle = a_{00}|00\rangle + a_{01}|01\rangle$

$+ a_{10}|10\rangle + a_{11}|11\rangle$

3 qubits $\quad |\psi\rangle = a_{000}|000\rangle + a_{001}|001\rangle$

$\quad + a_{010}|010\rangle + a_{011}|011\rangle$

$\quad + a_{100}|100\rangle + a_{101}|101\rangle$

$\quad + a_{110}|110\rangle + a_{111}|111\rangle$

2^N terms

In a classical byte for example, we have 8 bits (8 ones or zeros)
But with 8 qubits we have $2^8 = 256$ possible terms that form the state of the system.
All values $0 \dots 255$ are present at once in the superposition.

Perform computations by evolving the system in time
- Massively parallel computations "for free"
- Challenging to maintain coherence
- How to "read out" the answer?

Bloch sphere

Write $|0\rangle$ and $|1\rangle$ as eigenstates of operator $\hat{Z}$

$$\hat{Z}|0\rangle = |0\rangle$$
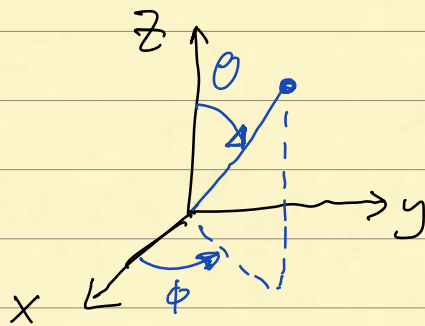$$\hat{Z}|1\rangle = -|1\rangle$$

in this basis, $\hat{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$\left\lceil \text{analogous to} \quad \hat{S}_z|\uparrow\rangle = +\frac{\hbar}{2}|\uparrow\rangle \right.$$
$$\left. \hat{S}_z|\downarrow\rangle = -\hbar/2 \, |\downarrow\rangle \right\rfloor$$

Most general state of a qubit

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2} e^{i\phi}|1\rangle$$

Vector $|\psi\rangle$ lies on the <u>Bloch sphere</u>

- What angles correspond to $|\psi\rangle = |0\rangle$ and $|\psi\rangle = |1\rangle$?

- HW 1 Q2 $\theta = \pi/2$ $|\psi\rangle$ lies in the x-y plane

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle + e^{i\phi} |1\rangle \right).$$

Unitary operators

$$U^\dagger U = 1 = UU^\dagger$$

Preserves the inner product

$$|\phi'\rangle = U|\phi\rangle$$
$$\langle\psi'| = \langle\psi|U^\dagger$$

$$\langle\psi'|\phi'\rangle = \langle\psi|U^\dagger U|\phi\rangle = \langle\psi|\phi\rangle$$

An example is the <u>change of basis operator</u>

$$U = \sum |b_n\rangle\langle a_n|$$

changes basis from $|a_n\rangle$ to $|b_n\rangle$

$$U|a_n\rangle = \sum_m |b_m\rangle\langle a_m|a_n\rangle$$

$$= |b_n\rangle$$

acts on nth basis
vector in $|a_n\rangle$ basis

to give the n-th
basis vector in $|b_n\rangle$ basis

The matrix element of U is

$$\langle a_m | U | a_n \rangle = \langle a_m | b_n \rangle$$

(similar to a rotation matrix in 3D)

Consider a state expanded in the $|a_n\rangle$ basis

$$|\psi\rangle = \sum |a_n\rangle \langle \psi | a_n \rangle$$

The b-coefficients are

$$\langle b_m | \psi \rangle = \sum \langle b_m | a_n \rangle \langle a_n | \psi \rangle$$

$$= \sum \langle a_m | U^\dagger | a_n \rangle \langle a_n | \psi \rangle$$

ie.
$$\begin{pmatrix} b \end{pmatrix} = \begin{pmatrix} U^\dagger \end{pmatrix} \begin{pmatrix} a \end{pmatrix}$$

Similarly, $\quad A' = U^\dagger A U$

matrix representation of A
in the $|b_n\rangle$ basis

matrix representation
of A in the
$|a_n\rangle$ basis

For a general unitary operator U,

A and $U^\dagger A U$ are <u>unitary equivalent</u>

<u>observables</u>

They have the same eigenvalue spectrum

$$\hat{A} \, |a\rangle = a \, |a\rangle$$

$$(U^\dagger A U)(U^\dagger |a\rangle) = a (U^\dagger |a\rangle)$$

eg. $\hat{S}_x$ and $\hat{S}_z$, which are related by a (unitary) rotation operator.

Another important example of a unitary operator is the time-evolution operator

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

eg. time-independent Hamiltonian

$$\hat{U}(t, t_0) = \exp\left[-i\hat{H}(t-t_0)/\hbar\right]$$

We'll say more about this later.

Quantum gates

A quantum gate is a unitary operator that evolves a single qubit or system of qubits. An example is the NOT gate that acts on a single qubit as follows:

$$\hat{X}\left|0\right\rangle = \left|1\right\rangle$$
$$\hat{X}\left|1\right\rangle = \left|0\right\rangle$$

Just a reminder that the states $\left|0\right\rangle$ and $\left|1\right\rangle$ are eigenstates of the $\hat{Z}$ operator. In this *computational basis*, the $\hat{Z}$ operator is

$$\hat{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Questions:

1. Write down the matrix representation of $\hat{X}$

   Computing the matrix elements, e.g. $\langle 1|\hat{X}|0\rangle = \langle 1|1\rangle = 1$ etc. gives

   $$\hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

2. What happens when $\hat{X}$ operates on the general state $\alpha\left|0\right\rangle + \beta\left|1\right\rangle$?

   $$\hat{X}\left(\alpha\left|0\right\rangle + \beta\left|1\right\rangle\right) = \alpha\left|1\right\rangle + \beta\left|0\right\rangle$$

   or if we write the state as a vector,

   $$\hat{X}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \beta \\ \alpha \end{pmatrix}.$$

3. What are the eigenvectors of $\hat{X}$ (let's refer to them as $\left|+\right\rangle$ and $\left|-\right\rangle$) in terms of $\left|0\right\rangle$ and $\left|1\right\rangle$?

   We already know the answer from the Pauli spin matrices,

   $$\left|+\right\rangle = \frac{1}{\sqrt{2}}\left(\left|0\right\rangle + \left|1\right\rangle\right) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

   $$\left|-\right\rangle = \frac{1}{\sqrt{2}}\left(\left|0\right\rangle - \left|1\right\rangle\right) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

4. Write down the operator that changes basis from $|0\rangle$, $|1\rangle$ to $|+\rangle$, $|-\rangle$. This is an important operator known as the **Hadamard operator**. What is the matrix representation of this operator in the $|0\rangle$, $|1\rangle$ basis?

The operator that changes $|0\rangle$ to $|+\rangle$ and $|1\rangle$ to $|-\rangle$ is

$$\hat{U}_H = |+\rangle\langle 0| + |-\rangle\langle 1| = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

5. What does $\hat{Z}$ do to $|+\rangle$ and $|-\rangle$?

$$\hat{Z}|+\rangle = |-\rangle, \qquad \hat{Z}|-\rangle = |+\rangle$$

Note that this means $\hat{Z}$ acts like a NOT operator for the $|+\rangle$ $|-\rangle$ basis.

6. Are $\hat{X}$ and $\hat{Z}$ unitary?

Yes, you can verify that $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = 1$ for both $\hat{X}$ and $\hat{Z}$.

Now consider a two qubit system, with general state $a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$. We can write this as a 4-component vector

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$$

7. Write down the matrix representation of the operator that applies a NOT to qubit 2 but leaves qubit 1 unchanged.

We need an operator that changes

$$|00\rangle \rightarrow |01\rangle$$

$$|01\rangle \rightarrow |00\rangle$$

$$|10\rangle \rightarrow |11\rangle$$

$$|11\rangle \rightarrow |10\rangle$$

The matrix representation is

$$
\begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}.
$$

Finally consider N qubits.

8. If we initialize each one in the state $|0\rangle$ and then apply the Hadamard operator to each one in turn, what is the resulting state?

The Hadamard operator acts on a single qubit and takes $|0\rangle \to |+\rangle$. So if we operate on each qubit with the Hadamard operator, the state becomes

$$
\Psi = |+\rangle \, |+\rangle \, |+\rangle \, ... \, |+\rangle
$$

or multiplying out in terms of $|0\rangle$ and $|1\rangle$

$$
\Psi = \frac{1}{2^{N/2}} \left(|0\rangle \, |0\rangle \, ... \, |0\rangle + |0\rangle \, |0\rangle \, ... \, |1\rangle + ... + |1\rangle \, |1\rangle \, .. \, |1\rangle \right)
$$

which we can write as

$$
\Psi = \frac{1}{2^{N/2}} \left(|0\rangle + |1\rangle + |2\rangle + ... + |2^N - 1\rangle + |2^N - 1\rangle \right).
$$

This state is an equal superposition of all possible states for the N qubits. This is the maximally entangled state.

Quantum computation

By applying the Hadamard operator to each of N qubits that are in the $|0\rangle$ state, we can create a state that is an equal superposition of the 2^N available states:

$$\frac{1}{2^{N/2}} \left(|0\rangle + \cdots + |2^N - 1\rangle \right)$$

One could then imagine a sequence of operations (gates) that evaluate a function f:

$$\hat{U} |n\rangle \longrightarrow |f(n)\rangle$$

$$\left(\begin{array}{l} \text{where } f(n) \text{ is an integer in the range} \\ \quad 0 \ldots 2^N - 1 \end{array} \right)$$

However this doesn't work in general if different values of n give the same value of f:

$$\langle n | \hat{U}^\dagger \hat{U} | m \rangle \longrightarrow \langle f(n) | f(m) \rangle$$
$$= \langle f(n) | f(n) \rangle = \underline{1}$$

but $\quad \langle n | \hat{U}^\dagger \hat{U} | m \rangle = \langle n | m \rangle = 0$
$$\text{for } n \neq m$$

Instead, a common approach is to have a control register as well as a data register

Then $\quad | n \rangle | m \rangle \longrightarrow$

$$\hat{U} | n \rangle | m \rangle = | n \rangle | m + f(n) \rangle$$

The states are orthogonal even for two values of n that have the same value of f.

Another common example is the CNOT
(controlled NOT)

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

takes
$$00 \rightarrow 00$$
$$01 \rightarrow 01$$
$$10 \rightarrow 11$$
$$11 \rightarrow 10$$

Generating the Bell (EPR) state

Simulation results

Perhaps the simplest example of a quantum algorithm is the _Deutsch algorithm._

one-bit function f maps $\{0,1\} \rightarrow \{0,1\}$

either _constant_ or _balanced_

$f(0)$	$f(1)$	
0	0	constant
1	1	constant
0	1	balanced
1	0	balanced

How can we tell if f is constant or balanced?

Use the operator

$$\hat{U}\, |n\rangle\, |m\rangle \longrightarrow |n\rangle\, |m \oplus f(n)\rangle$$

$$(\text{mod } 2 \text{ addition})$$

with $|m\rangle = |-\rangle = \dfrac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle \right)$

if $f(n) = 0 \qquad \hat{U}\,|n\rangle|-\rangle = |n\rangle\,|-\rangle$

$f(n) = 1 \qquad \hat{U}\,|n\rangle\,|-\rangle = \dfrac{1}{\sqrt{2}}\left(|n\rangle|1\rangle \right.$

$$\left. - |n\rangle|0\rangle \right)$$

$$= - |n\rangle|-\rangle$$

$\Rightarrow \qquad \hat{U}\,|n\rangle\,|-\rangle = (-1)^{f(n)}\, |n\rangle\,|-\rangle$

Now compute

$$\hat{U}\,|+\rangle|-\rangle = \frac{1}{\sqrt{2}}\Big(\hat{U}\,|0\rangle|-\rangle$$
$$+ \hat{U}\,|1\rangle|-\rangle\Big)$$

$$= \frac{1}{\sqrt{2}}\Big((-1)^{f(0)}\,|0\rangle|-\rangle$$
$$+ (-1)^{f(1)}\,|1\rangle|-\rangle\Big)$$

$$= \frac{1}{\sqrt{2}}\Big[(-1)^{f(0)}\,|0\rangle + (-1)^{f(1)}\,|1\rangle\Big]\,|-\rangle$$

$f(0)$	$f(1)$	output
0	0	$\quad|+\rangle|-\rangle$
1	1	$-\;|+\rangle|-\rangle$
0	1	$\quad|-\rangle|-\rangle$
1	0	$-\;|-\rangle|-\rangle$

if we read the control register with $\hat{X}$
then we will get $|+\rangle$ for constant
$|-\rangle$ for balanced

We get the answer with one measurement, whereas it would take two computations with a classical computer (ie. evaluate $f(0)$ and $f(1)$ and compare).

This may seem like a trivial example, but it can be generalized to functions of N-bits

$$f(n) = 0 \quad \text{or} \quad 1$$

for n in the range $0 \ldots 2^N - 1$.

Deutsch-Josza algorithm — determine whether $f(n)$ is constant (all 0's or 1's) or balanced (half 0, half 1) in one operation, compared to $\sim 2^{N-1}$ classically.

$\longrightarrow$ An _exponential speed up_!

This time we set the control register to the maximally-entangled state

$$\frac{1}{2^{N/2}} \sum_{n=0}^{2^N-1} |n\rangle = |\psi\rangle$$

using Hadamard operators acting on $|0\rangle$.

Then
$$\hat{U} |\psi\rangle |-\rangle$$

$$= \left(\frac{1}{2^{N/2}} \sum_{n=0}^{2^N-1} (-1)^{f(n)} |n\rangle \right) |-\rangle$$

For a <u>constant</u> function, this is $\pm |\psi\rangle |-\rangle$

So, we operate with Hadamard operators again, and if the control register goes back to $|0\rangle$ then the function was constant.

Q: what does the control register go to if the function is balanced? Can you show that $\text{Prob}(0) = 0$ in this case?

The density operator

Often we don't know which state a system is in. Even if we try to prepare a state with a measurement of an observable, there is experimental error for example.

But we may know the probability of being in state $|n\rangle$ for example, call this p_n.

⌐ Note we are not saying that the state of the system is $|\psi\rangle = \sum \sqrt{p_n} |n\rangle$
That would be a definite quantum state! ⌐

eg.
$$\overline{\langle A\rangle} = \sum_n p_n \langle n| \hat{A} |n\rangle$$
averaged over the ensemble

Inserting $\sum_i |a_i\rangle\langle a_i|$ identity operator

$$\overline{\langle A\rangle} = \sum_i \sum_n p_n \langle n| \hat{A} |a_i\rangle \langle a_i|n\rangle$$

$$a_i |a_i\rangle$$

$$\Rightarrow \quad \overline{\langle A \rangle} = \sum_{n,i} p_n \left| \langle a_i | n \rangle \right|^2 a_i \qquad (*)$$

Prob. of being
in state $|n\rangle$

Prob. of
measuring a_i when in
state $|n\rangle$

The __density operator__ is defined as

$$\rho \equiv \sum_n p_n |n\rangle \langle n| \; .$$

The p_n's represent our (incomplete) state of knowledge about which state $|n\rangle$ the system is in.

Consider

$$\rho A = \sum_n p_n |n\rangle \langle n| \sum_i a_i |a_i\rangle \langle a_i|$$

$$= \sum_{n,i} p_n a_i |n\rangle \langle n| a_i \rangle \langle a_i|$$

$$\langle m | \rho A | m \rangle = \sum_{n,i} p_n a_i \langle m | n \rangle \langle n | a_i \rangle \langle a_i | m \rangle$$

$$\underbrace{}_{\delta_{mn}}$$

$$= \sum_i p_m a_i |\langle m | a_i \rangle|^2$$

If we sum over m, we get

$$\sum_m \langle m | \rho A | m \rangle = \overline{\langle A \rangle} \qquad \left(\begin{array}{c}\text{using}\\ \text{eq. } *\end{array}\right)$$

This is the trace of the operator ρA

$$\rightarrow \boxed{\text{Tr}(\rho A) = \overline{\langle A \rangle}}$$

Properties of ρ

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

- $\rho = \rho^\dagger$ Hermitian

- $Tr(\rho) = \sum p_i = 1$

- $\langle\phi|\rho|\phi\rangle = \sum_i p_i |\langle\phi|\psi_i\rangle|^2$

$$= \text{Prob of finding the system to be in state } |\phi\rangle.$$

This implies the diagonal entries are always non-negative.
(Off-diagonal elements can be <0).

- $Tr(\rho) = 1 \Rightarrow \sum \lambda_k = 1$

  for eigenvalues λ_k.

- $Tr(\rho^2) = \sum \lambda_k^2 \leq 1$

$\boxed{\text{Pure state}}$ then $\rho = |\psi\rangle\langle\psi|$

$$Tr(\rho^2) = 1$$

$\boxed{\text{Mixed state}}$ $\rho = \sum p_i |\psi_i\rangle\langle\psi_i|$

$$Tr(\rho^2) < 1 \qquad \text{``purity''}$$

eg. imagine we have an experiment in which
we try to prepare qubits in the state
$|0\rangle$, but it fails now and again and with
probability p produces a $|1\rangle$.

What is ρ?
What is $Tr(\rho^2)$?

Repeat for the case where the failure mode
is to produce a $|+\rangle$ state.

eg. a qubit is in the state $\alpha|0\rangle + \beta|1\rangle$
what is ρ? $Tr(\rho^2)$?

Density operator

1. Imagine we have an experiment in which we try to prepare qubits in the state $|0\rangle$, but it fails now and again and with probability p produces a $|1\rangle$.

(a) Write down ρ. What is $\text{Tr}(\rho^2)$?

$$\rho = (1-p)\,|0\rangle\langle 0| + p\,|1\rangle\langle 1|$$

To find the matrix representation of ρ, calculate the matrix elements $\langle 0|\rho|0\rangle$, $\langle 0|\rho|1\rangle$ etc. This gives

$$\rho = \begin{pmatrix} 1-p & 0 \\ 0 & p \end{pmatrix}.$$

Multiplying the matrix by itself gives

$$\rho^2 = \begin{pmatrix} (1-p)^2 & 0 \\ 0 & p^2 \end{pmatrix}.$$

Therefore the purity is

$$\text{Tr}(\rho^2) = (1-p)^2 + p^2 = 1 - 2p(1-p).$$

Note that $\text{Tr}(\rho^2) = 1$ for $p = 0$ and $p = 1$, as expected since the system is then in a definite quantum state. The minimum value of $\text{Tr}(\rho^2)$ is $1/2$, when $p = 1/2$, which is the state of maximum uncertainty ($|0\rangle$ or $|1\rangle$ are equally likely).

(b) Repeat for the case where the failure mode is to produce a $|+\rangle$ state.

Now we write
$$\rho = (1-p)\,|0\rangle\langle 0| + p\,|+\rangle\langle +|$$

(this emphasizes the point that the states in the sum do not have to be orthogonal to one another). Using $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$, we find

$$\rho = \begin{pmatrix} 1-p/2 & p/2 \\ p/2 & p/2 \end{pmatrix}.$$

$$\rho^2 = \begin{pmatrix} 1-p+p^2/2 & p/2 \\ p/2 & p^2/2 \end{pmatrix}.$$

$$\mathrm{Tr}(\rho^2) = 1 - p + p^2 = 1 - p(1 - p).$$

This has the correct limits as before. Note that the minimum value is now greater than $1/2$.

2. A qubit is in the state $\alpha \left|0\right\rangle + \beta \left|1\right\rangle$. What is ρ? What is $\mathrm{Tr}(\rho^2)$?

$$\rho = \left|\Psi\right\rangle \left\langle\Psi\right| = |\alpha|^2 \left|0\right\rangle \left\langle0\right| + |\beta|^2 \left|1\right\rangle \left\langle1\right| + \alpha^\star\beta \left|1\right\rangle \left\langle0\right| + \beta^\star\alpha \left|0\right\rangle \left\langle1\right|$$

$$\rho = \begin{pmatrix} |\alpha|^2 & \beta^\star\alpha \\ \alpha^\star\beta & |\beta|^2 \end{pmatrix}.$$

$$\rho^2 = \begin{pmatrix} |\alpha|^2 & \beta^\star\alpha \\ \alpha^\star\beta & |\beta|^2 \end{pmatrix}.$$

$$\mathrm{Tr}(\rho^2) = |\alpha|^2 + |\beta|^2 = 1.$$

As expected since we are in a definite state, so $\rho^2 = \left|\Psi\right\rangle \left\langle\Psi\right| \left|\Psi\right\rangle \left\langle\Psi\right| = \left|\Psi\right\rangle \left\langle\Psi\right| = \rho$ (since $\left\langle\Psi|\Psi\right\rangle = 1$). *

Last time, we discussed the <u>density operator</u>

$$\hat{\rho} = \sum p_i |\psi_i\rangle\langle\psi_i|$$

for a single system, where $|\psi_i\rangle$ are possible states of the system.

Ideas from last time:

- Expectation value $\overline{\langle A\rangle} = \text{Tr}(\rho A)$

- Purity $\text{Tr}(\rho^2) \leq 1$

  Pure state $\text{Tr}(\rho^2) = 1$
  Mixed state $\text{Tr}(\rho^2) < 1$

Now consider composite systems. We'll see that things get interesting!

First, note that we can write the
density operator in terms of its matrix elements
in some basis $|n\rangle$ as

$$\hat{\rho} = \sum_{i,j} \rho_{ij} \ |i\rangle\langle j|$$

since this gives

$$\langle n | \hat{\rho} | m \rangle = \sum_{i,j} \rho_{ij} \ \langle n|i\rangle\langle j|m\rangle$$

$$= \rho_{nm} \quad \checkmark$$

(this is true for any operator).

Now let's do this for a composite
system:

$$\hat{\rho}_{12} = \sum_{i,j,k,\ell} |a_i\rangle |b_j\rangle \, \rho_{ijk\ell} \, \langle a_k| \langle b_\ell| \qquad (*)$$

basis vectors in
Hilbert space 1

basis vectors in
Hilbert space 2

eigenstates of
operator $\hat{A}$

eigenstates of
operator $\hat{B}$.

Consider observable $\hat{Q}$ in Hilbert space 1,
ie. Q acts only on the $|a_i\rangle$ states, not the
$|b_i\rangle$ states.

We know that $\overline{\langle Q \rangle} = \mathrm{Tr}(\rho Q)$

$$= \sum_{m,n} \langle a_n| \langle b_m| \, \rho_{12} Q \, |a_n\rangle |b_m\rangle.$$

Now insert $(*)$

$$= \sum_{mn} \langle a_n b_m | \left(\sum_{ijkl} |a_i b_j \rangle \, \rho_{ijkl} \, \langle a_k b_l | \right)$$

$$Q \, |a_n b_m \rangle$$

We have terms:

$$\langle a_n b_m | a_i b_j \rangle = \delta_{ni} \, \delta_{mj}$$

$$\langle a_k b_l | Q | a_n b_m \rangle = \delta_{lm} \, \langle a_k | Q | a_n \rangle$$

$$\Rightarrow \quad \mathrm{Tr}(\rho Q) = \sum_{mnk} \rho_{nmkm} \, \langle a_k | Q | a_n \rangle$$

$$= \sum_{nk} \langle a_k | Q | a_n \rangle \sum_m \rho_{nmkm}$$

(✲)

a <u>partial trace</u> over the eigenstates of Hilbert space 2

We define the reduced density matrix

$$\hat{\rho}_1 = \sum_n \langle b_n | \hat{\rho}_{12} | b_n \rangle$$

(take the trace over the B eigenstates)

$$= \sum_{nijkl} \langle b_n | b_j \rangle | a_i \rangle \rho_{ijkl} \langle a_k | \langle b_l | b_n \rangle$$

$$= \sum_{nik} | a_i \rangle \rho_{inkn} \langle a_k |$$

with matrix elements

$$\rho_{jl} = \langle a_j | \hat{\rho}_1 | a_l \rangle$$

$$= \sum_n \rho_{jnln} \, .$$

Comparing with (*) we see that

$$\overline{\langle Q \rangle} = \sum_{nk} \langle a_k | Q | a_n \rangle \, \rho_{nk}$$

But $\text{Tr}(\rho_1 Q)$

$$= \sum_m \langle a_m | \left(\sum_{nik} |a_i\rangle \, \rho_{inkn} \langle a_k| \right) Q | a_m\rangle$$

$$= \sum_{mnk} \rho_{mnkn} \, \langle a_k | Q | a_m\rangle$$

$$= \sum_{mk} \rho_{mk} \, \langle a_k | Q | a_m\rangle \, .$$

$$\Rightarrow \boxed{\overline{\langle Q \rangle} = \text{Tr}(\rho_1 Q)}$$

So once we calculate the reduced density matrix, we can just use it as usual as the density matrix for Hilbert space 1.

Reduced density operator

Consider two particles in the EPR state

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \left(|01\rangle - |10\rangle \right).$$

(a) Write down the density matrix using the basis $(|00\rangle, |01\rangle, |10\rangle, |11\rangle)$. Verify that it has the properties you expect for a density matrix of a pure state.

(b) Taking the trace over particle 1, derive the reduced density matrix for particle 2. Write out the matrix using the basis $|0\rangle, |1\rangle$ for particle 2. Does this reduced density matrix correspond to a pure state or a mixed state?

(c) How does the reduced density matrix you found in part (b) compare with the density matrix for a single particle in the pure state $|\Psi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$?

Reduced density operator

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|01\rangle - |10\rangle \right)$$

(a)   This is a pure state

$$\hat{\rho} = \sum p_i |\psi_i\rangle\langle\psi_i|$$

has only one term : $\hat{\rho} = |\psi\rangle\langle\psi|$

$$= \frac{1}{2} \left(|01\rangle\langle 01| \; \longrightarrow \; |10\rangle\langle 01| \; - \; |01\rangle\langle 10| \right.$$
$$\left. + \; |10\rangle\langle 10| \right)$$

Now calculate the matrix elements

use the basis $(|00\rangle, \; |01\rangle, \; |10\rangle, \; |11\rangle)$

We need $\langle 00| \hat{\rho} |00\rangle$
$$\langle 00| \hat{\rho} |01\rangle$$
etc. $\Rightarrow$ 16 terms

$$\hat{\rho} = \frac{1}{2} \begin{array}{cccc} |00\rangle & |01\rangle & |10\rangle & |11\rangle \end{array}$$

$$\hat{\rho} = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{array}{l} \langle 00| \\ \langle 01| \\ \langle 10| \\ \langle 11| \end{array}$$

$\text{Tr}(\rho) = 1 \quad \checkmark$

$$\rho^2 = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$\text{Tr}(\rho^2) = 1 \qquad$ as expected for a

pure state $\checkmark$

(b) We need to take the partial trace over the particle 1 states.

The reduced density operator is

$$\hat{\rho}_2 = \sum_n \langle n | \hat{\rho} | n \rangle$$

$$\underset{\uparrow}{\text{particle 1 eigenstates}}$$

matrix elements in the $\left(|0\rangle_2, |1\rangle_2 \right)$ basis

$$\langle 0 | \hat{\rho}_2 | 0 \rangle = \sum_{i=0,1} \langle i0 | \hat{\rho} | i0 \rangle$$

$$= 0 + \frac{1}{2} = \frac{1}{2}$$

$$\langle 0 | \hat{\rho}_2 | 1 \rangle = \sum_{i=0,1} \langle i0 | \hat{\rho} | i1 \rangle$$

$$= 0 + 0 = 0$$

$$\langle 1 | \hat{\rho}_2 | 0 \rangle = \sum_{i=0,1} \langle i1 | \hat{\rho} | i0 \rangle$$

$$= 0 + 0 = 0$$

$$\langle 1 | \hat{\rho}_2 | 1 \rangle = \sum_{i=0,1} \langle i1 | \hat{\rho} | i1 \rangle$$

$$= \frac{1}{2} + 0 = \frac{1}{2}$$

Therefore $\hat{\rho}_2 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

In Dirac notation, this is

$$\hat{\rho}_2 = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$$

$$\text{———(*)}$$

$\text{Tr}(\rho^2) = \frac{1}{2} \quad \Rightarrow \quad \underline{\text{mixed state}}$

In fact, this is the maximally disordered state (minimum purity).

(c) For the pure state $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$

$$\hat{\rho} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

which has $\text{Tr}(\rho^2) = 1$

In part (b) we ended up with something similar, but with the off-diagonal elements vanishing.

From the point of view of an observer who can only measure particle 2, it is not in a pure state corresponding to a superposition of $|0\rangle$ and $|1\rangle$; instead it is in the mixed state (*).

There is information loss on taking the partial trace.

Last time —

loss of information on taking the partial
trace

eg. $|\psi\rangle = \frac{1}{\sqrt{2}} (|10\rangle - |01\rangle)$

partial trace $\longrightarrow$ $\rho_1 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$

Note the off-diagonal zeros — this is
a mixed state with the same density
matrix as a classical ensemble.

Two applications

1) decoherence

$|\psi\rangle = |computer\rangle |environment\rangle$
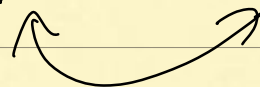
become entangled over
time

2) "measurement problem"

Copenhagen interpretation ~ two pieces

- $i\hbar \dfrac{\partial |\psi\rangle}{\partial t} = \hat{H} |\psi\rangle$

- $|\psi\rangle \longrightarrow |a\rangle$ on measurement
  collapse

Many worlds interpretation

only have $i\hbar \dfrac{\partial |\psi\rangle}{\partial t} = \hat{H} |\psi\rangle$

Everett 1960s
Entanglement decouples parts of the
wavefunction.

eg Bousso (2012) et al.

$(|0\rangle + |1\rangle)_S \; |0\rangle_A$

       $\nearrow$ $\nwarrow$ measuring apparatus
      system

interaction
$\longrightarrow$ $\quad a \, |0\rangle_S \, |0\rangle_A \;+\; b \, |1\rangle_S \, |1\rangle_A$

Now add environment

$$|\psi\rangle \;=\; a \, |0\rangle_S \, |0\rangle_A \, |0\rangle_E \;+\; b \, |1\rangle_S \, |1\rangle_A \, |1\rangle_E$$

We don't keep track of the environmental degrees of freedom

$$\rho_{SA} \;=\; \mathrm{Tr}_E \, |\psi\rangle\langle\psi|$$

$$=\; \begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix}$$

There is a decoupling of the outcomes. Looks like a classical ensemble with probabilities $|a|^2$, $|b|^2$.

Part 2 — Quantum dynamics

Time-dependence in quantum mechanics:

- Schrödinger equation $i\hbar \frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$

- Stationary states $\hat{H}|E\rangle = E|E\rangle$

  have time-dependence $\propto e^{-iEt/\hbar}$

Basic recipe is

- write the initial state as a sum of stationary states
- evolve each one in time with $e^{-iEt/\hbar}$
- sum to get the state at time t

- Dynamics comes from energy differences, since then a relative phase develops between different stationary states.

eg. two-level system

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

$$\Rightarrow \quad |\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle e^{-iE_0 t/\hbar} + |1\rangle e^{-iE_1 t/\hbar}\right)$$

Can show that

$$|\langle\psi(t)|\psi(0)\rangle|^2 = \cos^2\left(\frac{\Delta E\, t}{2\hbar}\right)$$

where $\Delta E = E_1 - E_0$.

Starts dropping below 1 (ie. the state at time t is becoming uncorrelated with the initial state) for times

$$\boxed{t \gtrsim \hbar/\Delta E}$$

Time-energy uncertainty relation.

Time evolution operator

We can write down the recipe above as an operator.

$$|\psi(t)\rangle = \sum_E \langle E|\psi(0)\rangle \, e^{-iEt/\hbar} \, |E\rangle$$

$$\Rightarrow \quad |\psi(t)\rangle = U(t) \, |\psi(0)\rangle$$

where
$$U(t) = \sum_E |E\rangle\langle E| \, e^{-iEt/\hbar}.$$

Notes:
- This is a unitary operator

- We can also write $U(t) = e^{-i\hat{H}t/\hbar}$

$\left(\text{in general} \quad f(\hat{A}) = \sum f(\lambda_i) \, |\lambda_i\rangle\langle\lambda_i| \right.$

where $|\lambda_i\rangle$ is the basis in which $\hat{A}$ is diagonal. This works if $f(\hat{A})$ has a polynomial expansion $f(A) = \sum c_n A^n.$ $\Big)$

- Has the properties

$$U^\dagger(t_2 - t_1) = U(t_1 - t_2)$$
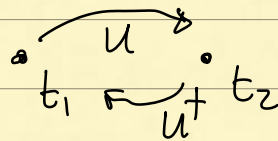
$$U(t_3 - t_1) = U(t_3 - t_2) U(t_2 - t_1)$$
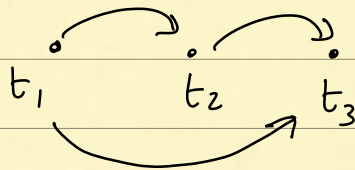
- If $\hat{H}$ is time-dependent, then

$$U(t) = \exp\left[-\frac{i}{\hbar} \int_0^t \hat{H}(t') \, dt'\right].$$

Need to be careful about time-ordering in the integral if $\hat{H}$ at different times do not commute — ie. we need time to increase right to left in the integrand.

Heisenberg & Schrödinger pictures

Consider the matrix element

$$\langle \phi | \hat{A} | \psi \rangle \quad \text{evaluated at time } t$$

$$= \langle \phi(0) | U^\dagger \hat{A} U | \psi(0) \rangle .$$

There are two ways to look at this:

Schrödinger	Heisenberg
$\langle \phi(0) | U^\dagger \hat{A} U | \psi(0) \rangle$	$\langle \phi(0) | U^\dagger \hat{A} U | \psi(0) \rangle$
$= \langle \phi(t) | \hat{A} | \psi(t) \rangle$	$= \langle \phi | \hat{A}(t) | \psi \rangle$
Time-dependence is in the states	Time-dependence is in the operator

There is a geometric interpretation of this which becomes clear when we look at the basis vectors

The basis kets are defined by $\hat{A}|a\rangle = a|a\rangle$.

Schrödinger picture: $\hat{A}$ is constant, so the basis vectors are also constant in time

Heisenberg picture: $\hat{A}$ is time-dependent, so the basis vectors are also time-dependent.

They evolve according to $|a\rangle \longrightarrow U^{\dagger}|a\rangle$

Since then we always satisfy

$$\hat{A}(t)\,|a\rangle(t) = a\,|a\rangle(t)$$

$\lceil$ since the left hand side is

$$U^{\dagger}\hat{A}(0)\,U\,U^{\dagger}\,|a\rangle(0)$$

$$= U^{\dagger}\hat{A}(0)\,|a\rangle(0) = a\,U^{\dagger}|a\rangle(0)$$

$$= a\,|a\rangle(t) \checkmark \rfloor$$

So in the Schrödinger picture, the basis
vectors are fixed, the state $|\psi\rangle$ evolves.
Because the time-evolution operator is unitary,
we can think of it as a rotation in Hilbert
space, $|\psi\rangle \longrightarrow U|\psi\rangle$

In the Heisenberg picture, the state is
fixed, and instead the basis vectors rotate,
but in the opposite direction

$$|a\rangle \longrightarrow U^\dagger |a\rangle.$$

The expansion coefficients $\langle\psi|a\rangle$ are
the same in each case:

Schrödinger $\qquad \langle\psi(t)|a\rangle$

$$= \langle\psi(0)|\, U^\dagger\, |a\rangle$$

Heisenberg $\qquad \langle\psi|\, a(t)\rangle$

$$= \langle\psi|\, U^\dagger\, |a(0)\rangle$$

the
same
✓

Last time – Schrödinger vs. Heisenberg pictures

Schrödinger $\quad |\psi(t)\rangle = U |\psi(0)\rangle$

Heisenberg $\quad |\psi\rangle$ fixed

$$\hat{A}(t) = U^\dagger \hat{A} U$$

$$|a(t)\rangle = U^\dagger |a\rangle$$

Expansion coefficients

$$|\psi\rangle = \sum \langle \psi | a \rangle |a\rangle$$

Schrödinger: $\quad |\psi(t)\rangle = \sum \langle \psi(t) | a \rangle |a\rangle$

$$= \sum \langle \psi(0) | U^\dagger |a\rangle |a\rangle$$

$c_a(t)$ – projection of the
time-dependent state onto
fixed basis vectors

Heisenberg $\quad |\psi\rangle = \sum \langle \psi | a(t) \rangle \, |a(t)\rangle$

$$= \sum \underbrace{\langle \psi | U^{\dagger} | a(0) \rangle}_{C_a(t)} \; U^{\dagger} |a(0)\rangle$$

Notice that the values of $C_a(t)$ are the same in each case — probability of measuring observable a is the same.

An example that uses both pictures:

Two state system with a time-dependent potential

$$H = H_0 + V(t)$$

$$H_0 |n\rangle = E_n |n\rangle$$

We are interested in transitions between the states caused by the potential $V(t)$.

"Interaction picture"   (Sakurai §5.5)
— use Heisenberg for the evolution
according to H_0, and Schrödinger for
the interaction part $V(t)$.

$$|\alpha\rangle_I = e^{iH_0 t/\hbar} |\alpha\rangle_S$$

remove the background H_0
time-dependence from the
Schrödinger state

and add it to the operators:

$$A_I = e^{iH_0 t/\hbar} A_S e^{-iH_0 t/\hbar}$$

— Then we have

$$i\hbar \frac{\partial}{\partial t} |\alpha\rangle_I = i\hbar e^{iH_0 t/\hbar} \frac{\partial}{\partial t} |\alpha\rangle_S$$

$$- H_0 e^{iH_0 t/\hbar} |\alpha\rangle_S$$

$$= e^{iH_0 t/\hbar} (H_0 + V) |\alpha\rangle_S$$

$$- H_0\, e^{iH_0 t/\hbar} |\alpha\rangle_S$$

these commute so the H_0 terms cancel

$$\Rightarrow\ i\hbar \frac{\partial}{\partial t} |\alpha\rangle_I = e^{iH_0 t/\hbar}\, V\, |\alpha\rangle_S$$

$$= e^{iH_0 t/\hbar}\, V\, e^{-iH_0 t/\hbar}\, e^{+iH_0 t/\hbar} |\alpha\rangle_S$$

$$= V_I(t)\, |\alpha\rangle_I$$

$$\boxed{\ i\hbar \frac{\partial}{\partial t} |\alpha\rangle_I = V_I(t)\, |\alpha\rangle_I\ } \quad \neg(*)$$

We just need to solve the Schrödinger equation for the interaction part.
Note that $|\alpha\rangle_I$ doesn't change if $V = 0$.

We can solve this by expanding

$$|\alpha\rangle_I = \sum c_n(t) |n\rangle$$

[Note that this is equivalent to

$$|\alpha\rangle_S = \sum c_n(t) e^{-i H_0 t/\hbar} |n\rangle$$

So we see that the H_0 time-dependence has been taken out]

Now do $\langle n | $ eq. $*\rangle$:

$$i\hbar \, \dot{c}_n = \langle n | V_I | \alpha \rangle_I$$

$$= \sum_m c_m(t) \langle n | V_I | m \rangle$$

$$\langle n | V_I | m \rangle = e^{i(E_n - E_m)t/\hbar} \langle n | V | m \rangle$$

$$= e^{i \omega_{nm} t} V_{nm}$$

$$\Rightarrow \quad i\hbar \, \dot{c}_n = \sum_m e^{i \omega_{nm} t} V_{nm} \, c_m$$

$$
\begin{pmatrix} \\ \\ \end{pmatrix} = \begin{pmatrix} & \\ & \\ & \end{pmatrix} \begin{pmatrix} \\ \\ \end{pmatrix}
$$

An example with analytic solution is an oscillating potential

$$V_{11} = V_{22} = 0$$

$$V_{12} = \gamma e^{i\omega t}, \quad V_{21} = \gamma e^{-i\omega t}$$

initially $\quad C_1 = 1 \quad\quad$ (ground state)
$$C_2 = 0$$

solution is

$$
|c_2|^2 = \frac{\gamma^2/\hbar^2}{\frac{\gamma^2}{\hbar^2} + (\omega - \omega_{21})^2/4}
$$

$$
\times \quad \sin^2\left[\left(\frac{\gamma^2}{\hbar^2} + \frac{(\omega - \omega_{21})^2}{4} \right)^{1/2} t \right]
$$

$|c_2|^2_{max}$

resonance

$$FWHM = \frac{4\gamma}{\hbar}$$

ω_{21}

ω

at resonance,

$|c_2|^2$

1

$\frac{\pi \hbar}{\gamma}$

t
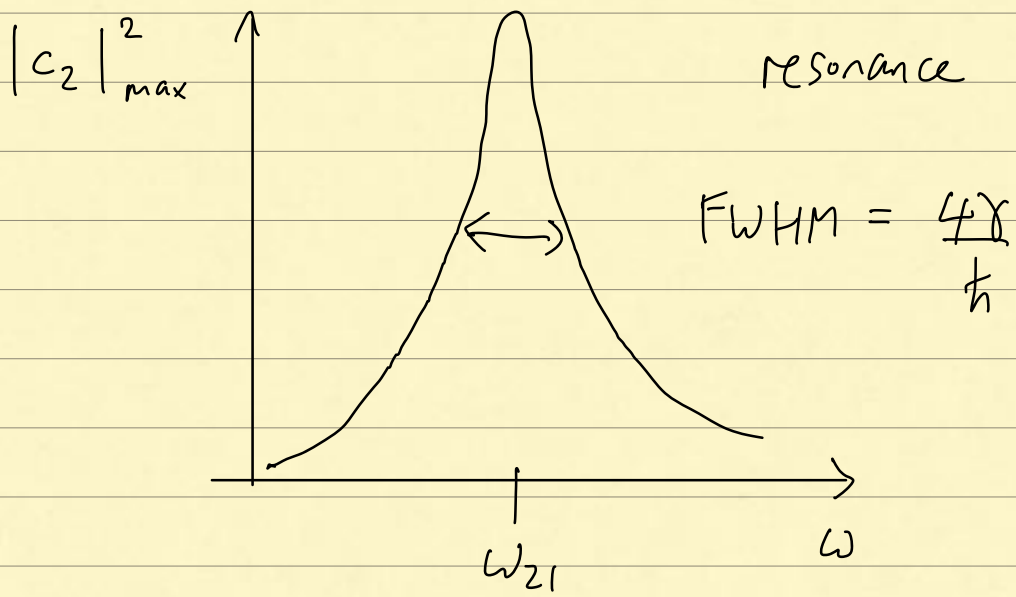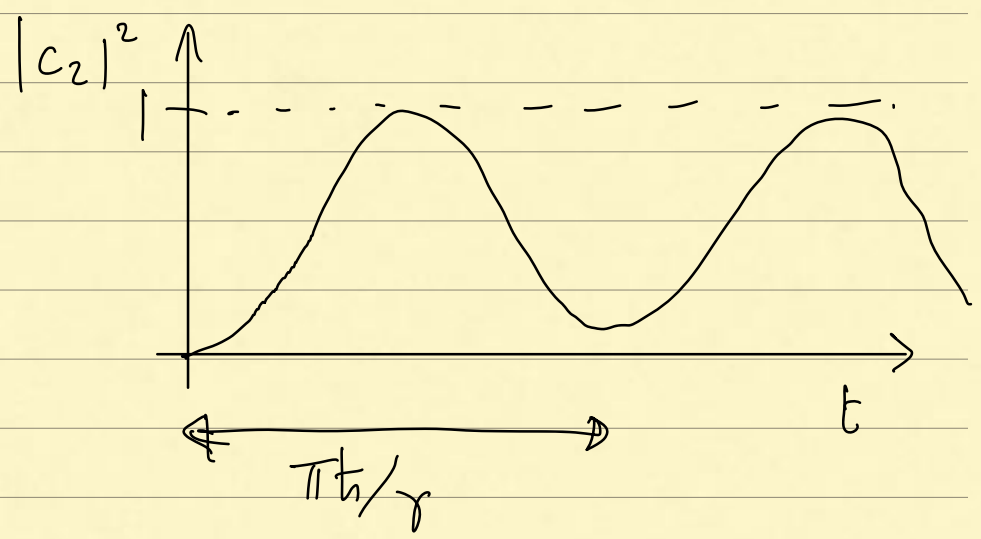
absorption and emission cycle

Heisenberg equation of motion

$$\hat{A}(t) = U^\dagger \hat{A} U$$

$$\Rightarrow \frac{d\hat{A}}{dt} = \frac{dU^\dagger}{dt} \hat{A} U + U^\dagger \frac{d\hat{A}}{dt} U + U^\dagger \hat{A} \frac{dU}{dt}$$

But
$$\frac{dU}{dt} = -\frac{i}{\hbar} \hat{H} U$$

$$\frac{dU^\dagger}{dt} = \frac{i}{\hbar} \hat{H} U^\dagger$$

$$\Rightarrow \frac{d\hat{A}}{dt} = \frac{i}{\hbar} \left[\hat{H} U^\dagger \hat{A} U - U^\dagger \hat{A} \hat{H} U \right]$$

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

$$+ \dot{\hat{A}}(t)$$

$$\Rightarrow \boxed{ \frac{d\hat{A}}{dt} = \frac{[\hat{A}(t), \hat{H}]}{i\hbar} + \dot{\hat{A}}(t) }$$

Check $\dfrac{d}{dt} \langle \psi | \hat{A} | \psi \rangle$

$$= \langle \psi | \dfrac{d\hat{A}}{dt} | \psi \rangle \qquad \begin{pmatrix} \text{use Heisenberg,} \\ \text{so } |\psi\rangle \text{ is time-} \\ \text{independent} \end{pmatrix}$$

$$= \underbrace{\dfrac{\langle [\hat{A}, \hat{H}] \rangle}{i\hbar}} + \langle \dfrac{\partial A}{\partial t} \rangle$$

This is Ehrenfest's theorem which you may have seen before derived from the TDSE.

Particle in a 1D potential

$$\hat{H} = \dfrac{\hat{p}^2}{2m} + V(\hat{x})$$

Let's calculate $\dfrac{d\hat{p}}{dt}$, $\dfrac{d\hat{x}}{dt}$

Use the results $[x_i, f(\vec{p})] = i\hbar \dfrac{\partial f}{\partial p_i}$

$$[p_i, g(\vec{x})] = -i\hbar \dfrac{\partial g}{\partial x_i}$$

1) $[\hat{p}, \hat{H}] = [\hat{p}, V(\hat{x})] = -i\hbar \frac{\partial V}{\partial x}$

$\Rightarrow$ $$\boxed{\frac{d\hat{p}}{dt} = -\frac{\partial V(\hat{x})}{\partial x}}$$

2) $[\hat{x}, \hat{H}] = \frac{[\hat{x}, \hat{p}^2]}{2m}$

$[\hat{x}, \hat{p}\hat{p}] = \hat{x}\hat{p}\hat{p} - \hat{p}\hat{p}\hat{x}$

$= [\hat{x},\hat{p}]\hat{p} + \hat{p}[\hat{x},\hat{p}]$

$= 2i\hbar \hat{p}$

$\Rightarrow$ $$\boxed{\frac{d\hat{x}}{dt} = \frac{\hat{p}}{m}}$$

We see here a connection to classical mechanics

classical $\longrightarrow$ quantum

canonical variables $\longrightarrow$ operators

Poisson brackets $\longrightarrow$ commutator
$\{\,,\,\}$ $\dfrac{[\,,\,]}{i\hbar}$

Hamiltonian formulation of classical mechanics: $H(q, p)$

equations of motion
$$\dot{p} = -\frac{\partial H}{\partial q}$$
$$\dot{q} = \frac{\partial H}{\partial p}$$

A function $f(p, q)$ evolves according to

$$\frac{df}{dt} = \{f, H\}$$

$$= \sum_i \left(\frac{\partial f}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial H}{\partial q_i} \right)$$

Notice that $\{q_i, p_j\} = \delta_{ij}$

More on transitions between states

Interaction picture:

$$\hat{H} = \hat{H}_o + \hat{V}(t)$$

$$|\alpha\rangle_I = \sum c_n(t) |n\rangle$$

with $\qquad i\hbar \dot{c}_n = \sum_m e^{i\omega_{nm}t} V_{nm} c_m$

$$\hbar \omega_{nm} = E_n - E_m \; ; \qquad V_{nm} = \langle n | \hat{V} | m \rangle$$

Now consider the initial condition $(t=0)$

$$c_n = 1 \quad \text{for some } n \quad \text{and}$$
$$c_j = 0 \quad \text{for } j \neq n.$$

then

$$\dot{c}_j \simeq \frac{1}{i\hbar} e^{i\omega_{jn}t} V_{jn} c_n \underset{\nearrow}{\overset{c_n \simeq 1}{}}$$

If $V(t) = V_0 e^{-i\omega t}$

$$V_{jn} = \langle j | V | n \rangle = e^{-i\omega t} \langle j | V_0 | n \rangle$$

$$\Rightarrow \quad \dot{c}_j \simeq \frac{1}{i\hbar} e^{i(\omega_{jn} - \omega)t} \langle j | V_0 | n \rangle$$

Integrate

$$c_j(t) \simeq \frac{e^{i(\omega_{jn} - \omega)t} \Big|_0^t \langle j | V_0 | n \rangle}{-\hbar(\omega_{jn} - \omega)}$$

Transition probability

$$\boxed{|c_j|^2(t) = \frac{4 |\langle j | V_0 | n \rangle|^2}{\hbar^2 (\omega_{jn} - \omega)^2} \sin^2\left(\frac{(\omega_{jn} - \omega)t}{2}\right)}$$

This is the same as our exact result from last time, but with γ (strength of potential) small ($\gamma^2 \ll \hbar^2(\omega - \omega_{21})^2$).

Fermi's Golden Rule

Typically there is a continuum of end states with energy E and

density of states $g(E)$

Such that the total transition probability is

$$P = \int dE_j \, g(E_j) \, |c_j|^2$$

$$= \int dE_j \, g(E_j) \, \frac{4|\langle j|V_0|n\rangle|^2}{\hbar^2 (\omega_{jn}-\omega)^2} \sin^2 \frac{(\omega_{jn}-\omega)t}{2}$$

Change variables $\quad x = (\omega_{jn}-\omega)/2$

$$= (E_j - E_n - \hbar\omega)/2\hbar$$

$$\Rightarrow \quad E_j = 2\hbar x + E_n + \hbar\omega$$

$$\Rightarrow P = \frac{2}{\hbar} \int dx \, g(E_n + \hbar\omega + 2\hbar x) \, \frac{\sin^2 xt}{x^2}$$

$$\times \, |\langle E_n + \hbar\omega + 2\hbar x|V_0|E_n\rangle|^2$$

The function $\dfrac{\sin^2 xt}{x^2}$ looks like

height is t^2

$\left(\dfrac{\sin^2 xt}{x^2} \to t^2 \right.$
$\left. \text{as } x \to 0 \right)$

$-\dfrac{2\pi}{t}$ $-\dfrac{\pi}{t}$ 0 $\dfrac{\pi}{t}$ $\dfrac{2\pi}{t}$ X

width $\propto \dfrac{1}{t}$

area $= \pi t$
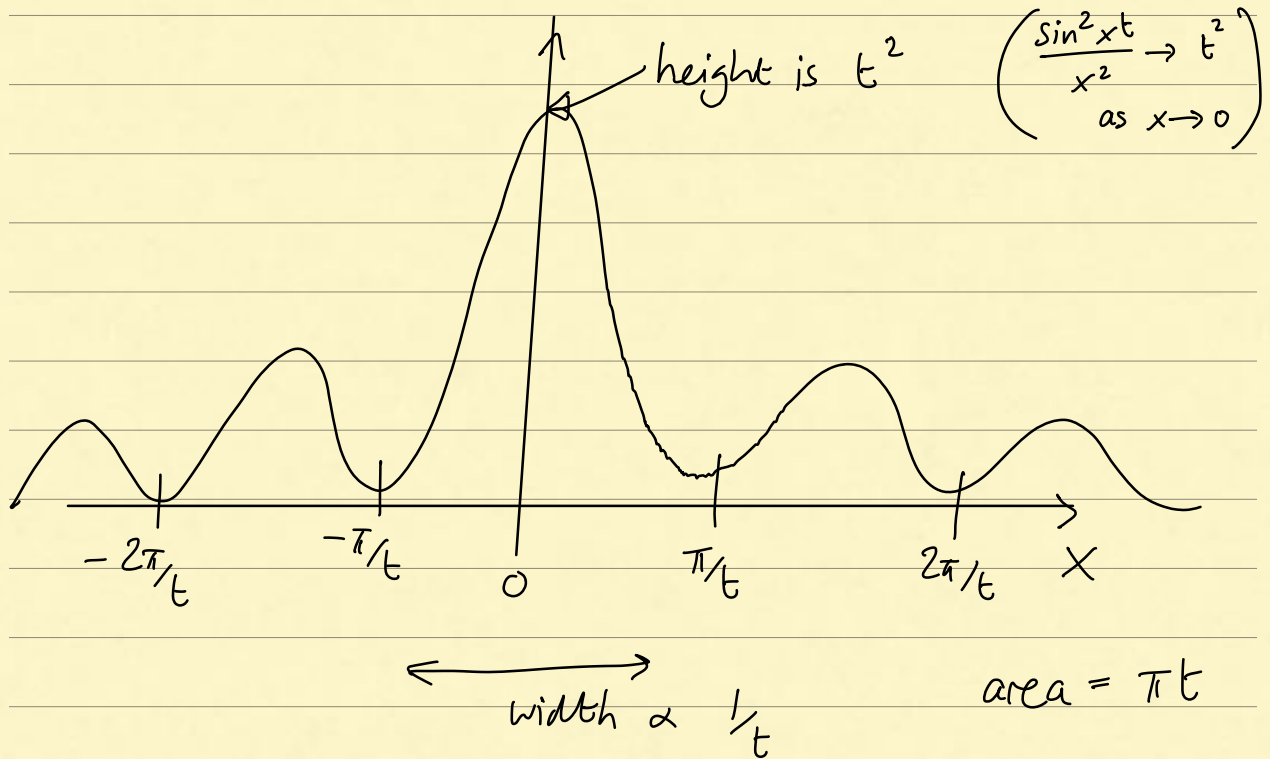
- As t grows, it becomes more peaked and concentrated near $x \simeq 0$, ie. final states with $\omega_{jn} \approx \omega$. $[\Delta E \, \Delta t \gtrsim \hbar]$.

- The area is linear in t. At early times, we can tolerate some uncertainty in energy $\Rightarrow$ more available states (more width).

- As t becomes large $\dfrac{\sin^2 xt}{x^2} \longrightarrow \pi t \, \delta(x)$

With the replacement $\dfrac{\sin^2 xt}{x^2} \longrightarrow \pi t \, \delta(x)$,

we have

$$P = \frac{2\pi}{\hbar} \, t \, g(E_n + \hbar\omega) \, \left| \langle E_n + \hbar\omega | V_0 | E_n \rangle \right|^2$$

The <u>transition rate</u> is

$$\boxed{\Gamma = \frac{2\pi}{\hbar} \, g(E_n + \hbar\omega) \, \left| \langle E_n + \hbar\omega | V_0 | E_n \rangle \right|^2}$$

" Fermi's Golden Rule "

transition rate =

$$\left(\frac{2\pi}{\hbar}\right) \times \left(\begin{array}{c}\text{density of final}\\ \text{states}\end{array}\right) \times \left|\begin{array}{c}\text{matrix}\\ \text{element}\end{array}\right|^2$$

$$\Gamma = \frac{2\pi}{\hbar} \, g(E_f) \, |M_{fi}|^2$$

Time-dependent perturbation theory

We've actually been doing perturbation theory to first order.

See Sakurai § 5.7.

Look for a solution

$$C_n(t) = c_n^{(0)}(t) + c_n^{(1)}(t) + c_n^{(2)}(t) + \ldots$$

$\uparrow$ $\quad\quad\quad$ $\uparrow$ $\quad\quad\quad$ $\uparrow$

$$O(1) \quad\quad O\left(\frac{V}{H_o}\right) \quad\quad O\left(\frac{V}{H_o}\right)^2$$

If $|\alpha\rangle = |n\rangle$ initially, then

$$c_m^{(0)}(t) = \delta_{nm}$$

$$c_m^{(1)}(t) = -\frac{i}{\hbar} \int_0^t e^{i\omega_{mn} t'} V(t') \, dt'$$

$$C_m^{(2)}(t) = \left(\frac{-i}{\hbar}\right)^2 \sum_\ell \int_0^t dt' \int_0^{t'} dt''$$

$$e^{i\omega_{m\ell} t'} V_{m\ell}(t') e^{i\omega_{\ell n} t''} V_{\ell n}(t'')$$

- For $V = V_0 e^{-i\omega t}$ you can check that $C_n^{(1)}(t)$ is what we were using above.

- Note that in the second order expression, we are summing over intermediate states ℓ.

If you include this term in the Fermi's Golden Rule derivation, you'll see that the delta function $\delta(x)$ assures energy conservation between initial and final states, but the in between transitions $n \to \ell, \quad \ell \to m$ are energy non-conserving. "Virtual transitions".

Adiabatic and sudden transitions

We've been discussing a periodic potential $V(t)$. More generally, $V(t)$ might represent a change in the Hamiltonian over time.

Two limits:

1) <u>Sudden</u>   rapid change over time $\ll \omega_{nm}^{-1}$

   eg. atomic β decay $Z \to Z+1$

   The state remains the same. But now will be a mixture of stationary states of the new Hamiltonian.

2) <u>Adiabatic</u>   slow change over time $\gg \omega_{nm}^{-1}$

   If we are in a stationary state initially, stay in the slowly evolving stationary state of $H(t)$.

size of the atom $\simeq \dfrac{a_0}{Z}$

time to eject the electron $\simeq \dfrac{a_0}{cZ} = \tau$

hydrogenic atoms $E = -\dfrac{1}{2} Z^2 \alpha^2 m_e c^2$

$$\left(\alpha = \frac{1}{137} \right)$$

energy difference between states is

$$\Delta E \sim Z^2 \alpha^2 m_e c^2$$

$\Rightarrow \quad \dfrac{\Delta E \, \tau}{\hbar} \simeq \dfrac{Z^2 \alpha^2 m_e c^2}{\hbar} \cdot \dfrac{a_0}{cZ}$

Use $\quad a_0 = \dfrac{\hbar}{\alpha m_e c}$

$\Rightarrow \quad \dfrac{\Delta E \, \tau}{\hbar} \simeq \alpha Z \simeq \dfrac{Z}{137} \cdot$

Berry phase

For a time-independent Hamiltonian, if the system is in stationary state $|n\rangle$ at $t=0$, the state at time t is

$$|\psi\rangle = e^{-iE_n t/\hbar} |n\rangle .$$

What about a slowly varying Hamiltonian $H(t)$? At each time we solve for the stationary states and their energies

$$\hat{H}(t) |n(t)\rangle = E_n(t) |n(t)\rangle .$$

For $|\psi\rangle = |n\rangle$ at $t=0$, we might expect

$$|\psi\rangle(t) = \exp\left(-\frac{i}{\hbar} \int_0^t E_n(t') \, dt'\right) |n(t)\rangle$$

but it turns out that this is not quite right. We need to add an additional phase — the <u>Berry phase</u>.

$$|\psi\rangle = e^{i\gamma(t)} \exp\left(-\frac{i}{\hbar} \int_0^t E_n(t') \, dt'\right) |n(t)\rangle$$

Substitute into $i\hbar \frac{\partial}{\partial t} |\psi\rangle = H(t) |\psi\rangle$

$\Rightarrow$ $i\hbar \frac{\partial}{\partial t} |n(t)\rangle - \hbar \dot{\gamma} \, |n(t)\rangle = 0$

$\Rightarrow$ $i \langle n(t) | \frac{\partial}{\partial t} |n(t)\rangle = \dot{\gamma}$

$\Rightarrow$

$$\gamma = i \int_0^t \langle n(t') | \frac{\partial}{\partial t} |n(t')\rangle \, dt'$$

This phase factor is actually measurable!
There is a topological phase that develops
when the parameter controlling the Hamiltonian
is taken back to its starting value (ie. does a
"loop" in parameter space).

eg parameters $\underline{R}$ $H(\underline{R}(t))$

then $\gamma = i \int_0^t \langle n | \nabla_R | n \rangle \cdot \dot{\underline{R}} \; dt'$

$= i \oint d\underline{R} \cdot \langle n | \nabla_R | n \rangle$

vector field $\underline{A} \equiv i \langle n | \nabla_R | n \rangle$

$\gamma = \oint d\underline{R} \cdot \underline{A}$

$= \int d\underline{a} \cdot (\nabla_R \times \underline{A})$

area of
the loop.

Note that γ is unchanged by multiplying
the basis vector by an arbitrary phase

$$| n \rangle \rightarrow e^{i\delta(\underline{R})} | n \rangle$$

$\Rightarrow \quad \underline{A} \rightarrow \underline{A} - \nabla_R \delta$

leaving $\nabla \times \underline{A}$ unchanged !

What matters is the topology of the path
through the $\underline{R}$ space, not the phase variation
along the path.

eg. Holstein (1989); Sakurai § 5.6.3, § 5.6.4

$$H(t) = -\frac{2\mu}{\hbar} \, \underline{S} \cdot \underline{B}$$

spin-$\frac{1}{2}$ particle in a magnetic field that
is changing direction

$$\longrightarrow \quad \gamma_{\pm} = \mp \frac{1}{2} \int \frac{\hat{\underline{B}} \cdot d\underline{a}}{|\underline{B}|^2} = \mp \frac{1}{2} \Omega$$
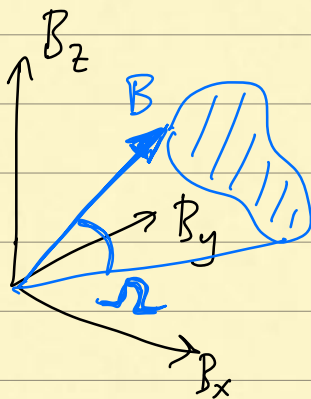
Solid angle
subtended by the
path of the $\underline{B}$ vector

Richardson (1988) — measurements using ultracold
neutrons

[Propagator and Path Integrals]

Position eigenstates $\hat{x}|x\rangle = x|x\rangle$

orthogonality $\langle x'|x\rangle = \delta(x-x')$

$$|\psi\rangle = \int dx \; \psi(x) \, |x\rangle$$

$$\psi(x) = \langle x|\psi\rangle$$

identity operator $\int dx \, |x\rangle\langle x|$

Propagator

The amplitude for going from $|x'\rangle$ at time t' to $|x\rangle$ at time t

$$K(x,t; x',t') = \langle x| \, e^{-iH(t-t')/\hbar} \, |x'\rangle$$

$$= \sum_n \langle x|n\rangle\langle n|x'\rangle \, e^{-iE_n(t-t')/\hbar}$$

We can use it to evolve the wavefunction

$$\int dx' \; K(x,t; x't') \; \Psi(x',t')$$

$$= \int dx' \; \langle x | e^{-iH(t-t')/\hbar} | x' \rangle \langle x' | \Psi(t') \rangle$$

$$\underbrace{\qquad\qquad\qquad\qquad}_{\text{identity}}$$

$$= \langle x | e^{-iH(t-t')/\hbar} | \Psi(t') \rangle$$

$$= \langle x | \Psi(t) \rangle$$

$$= \Psi(x, t) \qquad\qquad \text{(Green's function solution)}$$

Properties of K
- satisfies the TDSE

$$-\frac{\hbar^2}{2m} \nabla^2 K + V K = i\hbar \frac{\partial K}{\partial t}$$

- $K(x, t'; x', t') = \delta(x-x')$

Now consider $\langle x | U(t-t') | x' \rangle$

write $e^{-iH(t-t')/\hbar}$ as $U(t-t')$

break this into two pieces:

$$U(t-t') = U(t-t'') U(t''-t')$$

$\Rightarrow \quad \langle x | U(t-t') | x' \rangle$

$$= \int dx'' \; \langle x | U(t-t'') | x'' \rangle \langle x'' | U(t''-t') | x' \rangle$$

we have to consider all possible intermediate locations.

propagators to and from intermediate location x''

We could break this up into more and more pieces

x', t' $\quad t_1 \quad t_2 \quad t_3 \quad t_4 \quad t_5 \quad$ x, t
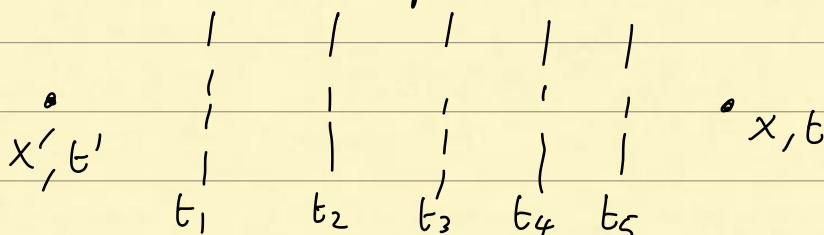
With many integrals over the intermediate
coordinates $\int dx_1 \, dx_2 \, dx_3 \, dx_4 \, dx_5 \ldots$

We soon see that an equivalent way of
writing the propagator is as an integral over
all possible paths
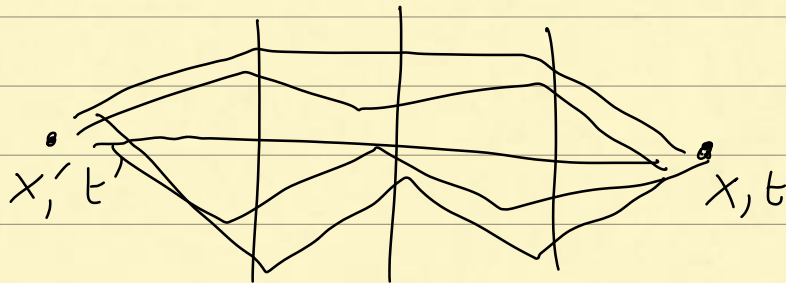
x', t' x, t

Classically, there is a unique path from
(x', t') to (x, t) — the path that minimizes
the action $\quad S = \int_{t'}^{t} L(x, \dot{x}) \, dt$

In QM, we need to consider all paths.
In fact

$$\langle x, t \,|\, x', t' \rangle \sim \sum_{\text{paths}} e^{\, i S[\text{path}]/\hbar}$$

This is Feynman's path integral formulation of QM. We will go into the details next time, but one thing to note now is that it reproduces the classical path in the limit $\hbar \to 0$ (large S) since paths near the classical one have similar S values ($\delta S = 0$) and so constructively add together, whereas further away the variations in S give a rapidly oscillating phase that cancels.

Propagator for a free particle

Since $\hat{H} = \dfrac{\hat{p}^2}{2m}$ the momentum eigenstates

are eigenstates of $\hat{H}$ and so we can write

$$K(x,t;x',t') = \langle x| \int dp \, |p\rangle\langle p| \, e^{-iE(p)\Delta t/\hbar} \, |x'\rangle$$

$$= \int dp \, \langle x|p\rangle\langle p|x'\rangle \, e^{-iE(p)\Delta t/\hbar}$$

with $E(p) = \dfrac{p^2}{2m}$, $\Delta t = t - t'$

Momentum eigenstates $\hat{p}|p\rangle = p|p\rangle$

$$\langle p|p'\rangle = \delta(p-p') \qquad \hat{p} \rightarrow -i\hbar \frac{\partial}{\partial x}$$

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

$$\Rightarrow \quad K = \frac{1}{2\pi\hbar} \int dp \, e^{ipx/\hbar} \, e^{-ipx'/\hbar} \, e^{-ip^2\Delta t/2m\hbar}$$

We can do the integral by completing the square:

$$p(x-x') - \frac{p^2(t-t')}{2m}$$

$$= -\left(\frac{t-t'}{2m}\right)\left[\left(p - \frac{(x-x')m}{(t-t')}\right)^2\right.$$

$$\left. - \frac{m^2(x-x')^2}{(t-t')^2}\right]$$

You can see that there is a factor

$$e^{i(x-x')^2m/2(t-t')\hbar}$$

and the rest is a Gaussian integral.

The result is

$$\boxed{K = \sqrt{\frac{m}{2\pi i\hbar(t-t')}}\; e^{i\frac{(x-x')^2 m}{2\hbar(t-t')}}}$$

The classical action for a free particle is

$$S_c = \int_{t'}^{t}\left[\frac{m\dot{x}^2}{2} - V(x)^{0}\right] dt''$$

along the trajectory with $\dot{x} = $ constant

$$= \frac{x - x'}{t - t'}$$

$$\Rightarrow \quad S_c = \int_{t'}^{t} \frac{m}{2} \frac{(x - x')^2}{(t - t')^2} \, dt''$$

$$= \frac{m}{2} \frac{(x - x')^2}{(t - t')}$$

We see that the free particle propagator is

$$A(t) \, e^{\, i \, S_c / \hbar}$$

with $A(t)$ such that $K \rightarrow \delta(x - x')$

as $t \rightarrow t'$.

$$\left[\lim_{\varepsilon \to 0} \frac{1}{\sqrt{\pi \varepsilon}} \, e^{-x^2 / \varepsilon} = \delta(x) \right]$$

(Note that it is not generally the case
that $K \propto e^{\, i \, S_c / \hbar}$. Holds for $V(x, \dot{x})$ up to
quadratic in x or $\dot{x}$.

Derivation using path integral:

Evaluate $\quad K(x_N, t_N; x_0, t_0)$

$$= \int_{x_0}^{x_N} D[x(t)] \; e^{i S[x(t)]/\hbar}$$

We consider N discrete steps $\quad t_n = t_0 + n\varepsilon$

with time spacing $\quad \varepsilon = (t_N - t_0)/N$

and later take the limit $\varepsilon \to 0$.

$$S = \int_{t_0}^{t_N} L(t) \, dt = \int_{t_0}^{t_N} \frac{1}{2} m \dot{x}^2 \, dt$$

$$\longrightarrow \qquad S = \sum_{i=0}^{N-1} \frac{m}{2} \left(\frac{x_{i+1} - x_i}{\varepsilon} \right)^2 \varepsilon$$

The integral is

$$K = \lim_{\varepsilon \to 0} A \int dx_1 \int dx_2 \ldots \int dx_{N-1} \; e^{iS/\hbar}$$

↗ normalization constant

We have a series of integrals of the form

$$\int_{-\infty}^{\infty} dy_1 \; \exp\left[-\frac{1}{i}\left[(y_2-y_1)^2 + (y_1-y_0)^2 \right] \right]$$

$$= \left(\frac{i\pi}{2} \right)^{1/2} \exp\left(-(y_2-y_0)^2 \Big/ 2i \right)$$

After integrating over all the x_i's, this gives

$$K = A \left(\frac{2\pi \hbar \varepsilon i}{m} \right)^{N/2} \left(\frac{m}{2\pi \hbar i N \varepsilon} \right)^{1/2} \exp\left(\frac{im(x_N-x_0)^2}{2\hbar N \varepsilon} \right)$$

$\underbrace{\phantom{K = A \left(\frac{2\pi \hbar \varepsilon i}{m} \right)^{N/2}}}$ this should be 1

$\underbrace{\phantom{\left(\frac{m}{2\pi \hbar i N \varepsilon} \right)^{1/2} \exp}}$ this is the free particle propagator

$$\Rightarrow A = \left(\frac{m}{2\pi \hbar \varepsilon i} \right)^{N/2}$$

$$\equiv B^{-N}$$

$$\Rightarrow \int D[x(t)] = \lim_{\varepsilon \to 0} \frac{1}{B} \int \frac{dx_1}{B} \int \frac{dx_2}{B} \cdots \int \frac{dx_{N-1}}{B}$$

Formulation of the path integral

Divide the time evolution into N steps

$$e^{-iHt/\hbar} = \left[e^{-iH\Delta t/\hbar} \right]^N$$

Factorize

$$e^{-iH\Delta t/\hbar} \simeq e^{-iT\Delta t/\hbar} e^{-iV\Delta t/\hbar} + O(\Delta t)^2$$

where $H = T + V = \dfrac{p^2}{2m} + V$

Then write

$$\langle x_N | U_H(t) | x_0 \rangle$$

$$= \langle x_N | \left(U_H(\Delta t) \right)^N | x_0 \rangle$$

$$= \langle x_N | U_T(\Delta t) \, U_V(\Delta t) \, U_T(\Delta t) \cdots$$

$$\cdots \cdots U_T(\Delta t) \, U_V(\Delta t) | x_0 \rangle$$

Now insert identity operators as we did previously but now over position and momentum

$$\int dx_i \int dp_i \ |x_i\rangle\langle x_i| \ p_i\rangle\langle p_i|$$

(where i labels the timestep)

$$\longrightarrow \ \langle x_N| \ U_H(t) \ |x_0\rangle$$

$$= \int dx_1 ... dx_{N-1} \ \frac{dp_1 ... dp_N}{(2\pi\hbar)^N} \quad \times$$

$$\exp\left[-\frac{i\Delta t}{\hbar} \sum_{n=0}^{N-1} \left(V(x_n) + T(p_{n+1}) - \frac{p_{n+1}(x_{n+1} - x_n)}{\Delta t} \right)\right]$$

$\underbrace{\hspace{3cm}}$ this is from the time evolution operators

$\underbrace{\hspace{3cm}}$ this is from the $|p\rangle$ eigenstates

$$\left(\langle x|p\rangle = \frac{e^{ipx}}{(2\pi\hbar)^{1/2}} \right)$$

In the continuum limit $(N \to \infty)$ this is

$$\langle x_N | e^{-iHt/\hbar} | x_0 \rangle =$$

$$\int D(x,p) \exp\left[\frac{i}{\hbar} \int_0^t dt' \left(p\dot{x} - H(p,x)\right)\right]$$

where $\quad D[x,p] = dx_1 \ldots dx_{N-1} \dfrac{dp_1 \ldots dp_N}{(2\pi\hbar)^N}$

This is the Hamiltonian formulation of the path integral. The integration is over paths in phase space $(p$ and $x)$.

The integrand is in fact the Lagrangian L since the Legendre transform relating H and L is

$$H(p,x) = p\dot{x} - L(p,x).$$

For a quadratic K.E. $p^2/2m$, the momentum

integral can be carried out (Gaussian integral)
which gives

$$\langle x_N | e^{-iHt/\hbar} | x_0 \rangle =$$

$$\int D[x] \exp\left[\frac{i}{\hbar} \int_0^t dt' L(x, \dot{x}) \right]$$

and $\quad D[x] = \lim_{N \to \infty} \left(\frac{Nm}{i 2\pi \hbar t} \right)^{N/2} dx_1 \dots dx_{N-1}$

This agrees with what we had earlier.

Last time —

- ## Propagator for a free particle

$$K = \left(\frac{m}{2\pi i \hbar (t-t')} \right)^{1/2} \exp \left(\frac{i m (x-x')^2}{2\hbar (t-t')} \right)$$

This might remind you of the Green's function for the diffusion equation.

$$\psi(x,t) = \int dx' \, K(x,t; x',t') \, \psi(x',t')$$

- ## Path integral

$$K = \int_{x'}^{x} D[x(t)] \, e^{i S[x(t)]/\hbar}$$

$$\lim_{\varepsilon \to 0} \left(\frac{m}{2\pi \hbar \varepsilon i} \right)^{N/2} \int dx_1 \, dx_2 \cdots dx_{N-1}$$

- **General recipe:**

1. Divide evolution into N steps

$$e^{-iHt/\hbar} = \left[e^{-iH\Delta t/\hbar} \right]^N$$

2. Factorize

$$e^{-iHt/\hbar} \simeq e^{-i\frac{p^2 t}{2m\hbar}} \, e^{-iVt/\hbar} + O(\Delta t)^2$$

3. Introduce identity operators

$$\int dx_i \, |x_i\rangle\langle x_i| \int dp_i \, |p_i\rangle\langle p_i|$$

$$\longrightarrow \quad \langle x_N | U(t) | x_0 \rangle = \int dx_1 \cdots dx_{N-1} \, \frac{dp_1 \cdots dp_N}{(2\pi\hbar)^N}$$

$$\times \exp\left[-\frac{i\Delta t}{\hbar} \sum_{n=0}^{N-1} \left(V(x_n) + \frac{p_n^2}{2m} - \frac{p_{n+1}(x_{n+1}-x_n)}{\Delta t} \right) \right]$$

4. Take the continuum limit $\qquad N \to \infty \qquad \Delta t \to 0$

$$\langle x_N | e^{-iHt} | x_0 \rangle =$$

$$\int D[x,p] \, \exp\left[\frac{i}{\hbar} \int_0^t dt' \left(p\dot{x} - H(p,x) \right) \right]$$

where

$$D[x,p] = \lim_{N \to \infty} \frac{dx_1 \cdots dx_{N-1} \, dp_1 \cdots dp_N}{(2\pi\hbar)^N}$$

Two further points to make about this:

1. the factor $p\dot{x} - H$ is actually the Lagrangian L

$$L = p\dot{x} - H \qquad \text{(Legendre transform)}$$

2. For K.E. $= \frac{p^2}{2m}$ (quadratic) we can

do the momentum integral (Gaussian integral)
(Complete the square like last time)

$\rightarrow \quad \langle x_N | e^{-iHt/\hbar} | x_0 \rangle =$

$$\int D[x(t)] \; \exp\left[\frac{i}{\hbar} \int_0^t L(x, \dot{x}) \; dt' \right]$$

with $\quad D[x(t)] = \lim_{N \to \infty} \left(\frac{Nm}{2\pi i \hbar t} \right)^{N/2} dx_1 \ldots dx_{N-1}$

this factor that we had last time
comes from the momentum integration

Semiclassical approximation

We saw that for a free particle (or linear or quadratic potentials), $K \propto \exp\left(\frac{iS_c}{\hbar}\right)$

where S_c is the action of the classical path. As we discussed, this is maybe not surprising since the classical path is where $\delta S = 0$.

We can expand around the classical path $x(t) = x_c(t)$:

$$S[x] = S[x_c + \delta x]$$
$$= S[x_c] + \ldots$$

no 1st order term
$(\delta S = 0)$

$$+ \frac{1}{2} \int dt' \; \delta x^2(t) \left.\frac{\delta^2 S}{\delta x^2}\right|_{x=x_c}$$

$$+ \ldots$$

2nd order term

Because the leading term is quadratic, we again get a Gaussian integral!

$$K \sim \left(\frac{i}{2\pi\hbar} \frac{\partial^2 S_c}{\partial x^2} \right)^{1/2} e^{iS_c/\hbar}$$

Expand $S = \int_0^t dt' \left(\frac{m\dot{x}^2}{2} - V(x) \right)$

$$= S[x_c] + \int_0^t dt' \left(\frac{m}{2} \delta\dot{x}^2 - \frac{1}{2} V''(x_c) \delta x^2 \right)$$

$$+ \dots$$

$$= S[x_c] + \int_0^t \frac{dt'}{2} \left(m \frac{\partial^2}{\partial t^2} - V'' \right) \delta x^2$$

$$\rightarrow \quad K = \left(\frac{m}{2\pi i \hbar t} \right)^{1/2} \frac{1}{\sqrt{\det\left(m\frac{\partial^2}{\partial t^2} - V'' \right)}} e^{iS_c/\hbar} .$$

$$\wp$$

$$(\det = \text{product of eigenvalues})$$
$$\text{over the } N \text{ steps}$$

Lagrangian and Hamiltonian with EM fields

The Lagrangian $L = \frac{1}{2} m v^2 - q\phi + \frac{q}{c} \underline{v} \cdot \underline{A}$

gives the correct equation of motion (EOM)

$$\frac{d}{dt} \left(m \underline{v} \right) = q \left(\underline{E} + \frac{\underline{v} \times \underline{B}}{c} \right)$$

$$\underbrace{\qquad\qquad}_{\text{Lorentz force}}$$

Canonical momentum $\quad p_i = \dfrac{\partial L}{\partial \dot{x}_i}$

is

$$\underline{p} = m \underline{v} + \frac{q}{c} \underline{A}.$$

Hamiltonian $\quad H = \underline{p} \cdot \underline{v} - L$

$$= \frac{1}{2} m v^2 + q\phi$$

$$= \frac{\left(\underline{p} - q\underline{A}/c \right)^2}{2m} + q\phi \quad .$$

(which gives the correct $\dot{x}_i = \dfrac{\partial H}{\partial p_i}$, and

$\dot{p}_i = -\dfrac{\partial H}{\partial x_i}$ gives the correct EOM)

Units

cgs / Gaussian	SI
(Shankar,	(Binney & Skinner)
Sakurai & Napolitano)	

$$\vec{p} = m\underline{v} + \frac{q\underline{A}}{c}$$

$$\vec{p} = m\underline{v} + q\underline{A}$$

$$\underline{F} = q\left(\underline{E} + \frac{\underline{v}}{c} \times \underline{B}\right)$$

$$\underline{F} = q\left(\underline{E} + \underline{v} \times \underline{B}\right)$$

$$\underline{E} = -\underline{\nabla}\phi - \frac{1}{c}\frac{\partial \underline{A}}{\partial t}$$

$$\underline{E} = -\underline{\nabla}\phi - \frac{\partial \underline{A}}{\partial t}$$

$$\underline{\nabla} \cdot \underline{E} = 4\pi\rho$$

$$\underline{\nabla} \cdot \underline{E} = \rho/\varepsilon_0$$

$$\underline{\nabla} \times \underline{E} = -\frac{1}{c}\frac{\partial \underline{B}}{\partial t}$$

$$\underline{\nabla} \times \underline{E} = -\frac{\partial \underline{B}}{\partial t}$$

$$\underline{\nabla} \cdot \underline{B} = 0$$

$$\underline{\nabla} \times \underline{B} = \frac{1}{c}\frac{\partial \underline{E}}{\partial t} + \frac{4\pi}{c}\underline{J}$$

$$\underline{\nabla} \times \underline{B} = \frac{1}{c^2}\frac{\partial \underline{E}}{\partial t} + \mu_0 \underline{J}$$

Aharanov - Bohm Effect

The additional term in the Lagrangian $\frac{q}{c} \underline{v} \cdot \underline{A}$ can be observed.

partide paths

$\otimes B$

imperetrable cylinder with uniform magnetic field $\underline{B}$
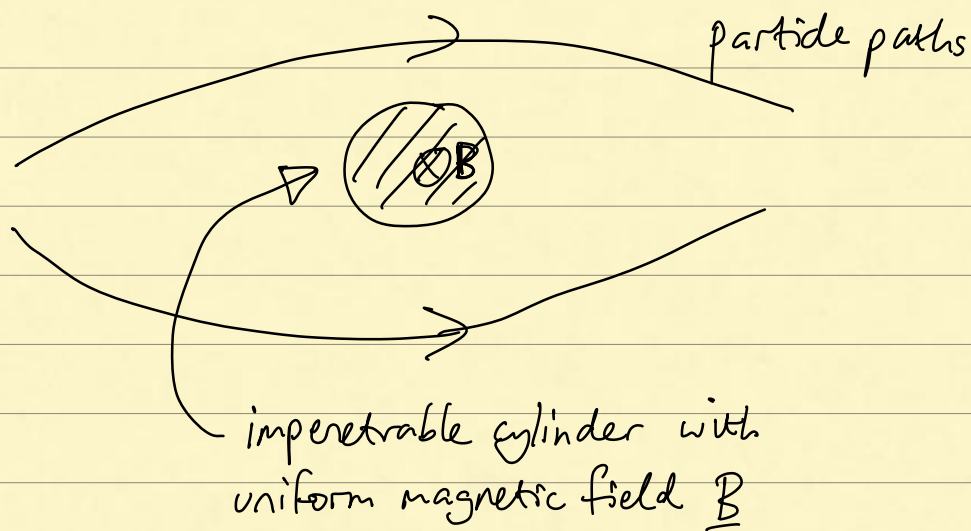
Outside the cylinder $\quad 2\pi r A_\phi = B \times$ area of cylinder
$$= \Phi$$

r
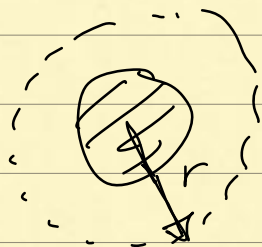
$$\Rightarrow \quad A_\phi = \frac{\Phi}{2\pi r}$$

Even though B vanishes outside the cylinder, A does not!

Contribution to the action is

$$\int_0^t \frac{q}{c} \underline{v} \cdot \underline{A} \, dt' = \int_{path} \frac{q}{c} \underline{A} \cdot d\underline{\ell}$$

Consider pairs of trajectories going above and below the cylinder

net phase is $\quad \frac{1}{\hbar} \oint \frac{q}{c} \underline{A} \cdot d\underline{\ell}$

$$= \frac{q \Phi}{\hbar c}.$$

phase difference 2π is accumulated for

$$\Phi = \frac{2\pi \hbar c}{q} \equiv \Phi_o \qquad \text{"flux quantum"}$$

$$= 4 \times 10^{-15} \, T_M^2.$$

Last time —

- EM Lagrangian $\qquad L = \frac{1}{2}mv^2 - q\phi + q\frac{v \cdot A}{c}$

  Hamiltonian $\qquad H = \frac{1}{2}mv^2 + q\phi$

  $$= \frac{(p - qA/c)^2}{2m} + q\phi$$

Distinguish between canonical momentum $p = \pi - q\frac{A}{c}$
and mechanical momentum $\pi = mv$.

- Aharanov Bohm effect

magnetic flux Φ
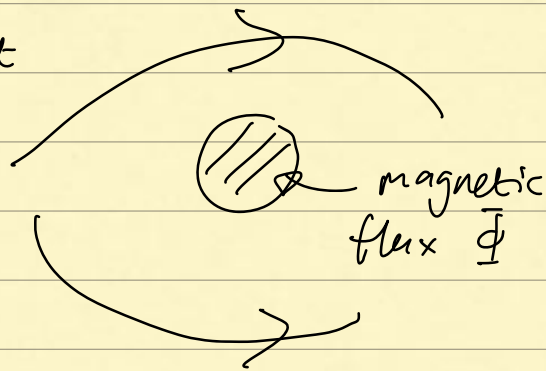
net phase $\qquad \frac{1}{\hbar} \oint \frac{q}{c} A \cdot d\ell$

$$= \frac{1}{\hbar} \frac{q}{c} \Phi = \frac{2\pi \Phi}{\Phi_0}$$

flux quantum $\underline{\Phi}_0 = \dfrac{2\pi\hbar c}{q} = 4.1 \times 10^{-7}\, G\, cm^2$

$$\left[\text{in } SI: \quad \underline{\Phi}_0 = \dfrac{2\pi\hbar}{q} = 4 \times 10^{-15}\, Tm^2. \right]$$

Gauge invariance

We discussed the fact that the Berry phase

$$\gamma = i \oint \langle n | \underline{\nabla}_R | n \rangle \cdot d\underline{R}$$

$$= \oint \underline{A}_B \cdot d\underline{R} \quad = \int d\underline{a} \cdot \underline{\nabla}_R \times \underline{A}_B$$

is unchanged if we change our phase convention
for $|n\rangle$:

$$|n\rangle \;\longrightarrow\; e^{i\delta(R)} |n\rangle$$

since then

$$\underline{A}_B \;\longrightarrow\; \underline{A}_B - \underline{\nabla}_R \delta$$

$$\Rightarrow \quad \underline{\nabla} \times \underline{A}_B \text{ is unchanged.}$$

What about gauge changes in EM? We know
that we are free to choose a gauge

$$\underline{A} \rightarrow \underline{A} + \underline{\nabla} \lambda$$

which leaves the physical field
$$\underline{B} = \underline{\nabla} \times \underline{A} \quad \text{unchanged.}$$
(Since $\underline{\nabla} \cdot \underline{B} = 0$, $\underline{B}$ only has two independent
components, whereas $\underline{A}$ has 3 — this leads to
the gauge freedom represented by the freedom to
choose λ.)

So it might seem strange that the gauge-
dependent quantity $\underline{A}$ is now appearing in
the Hamiltonian!

The Aharanov-Bohm phase depended on Φ,
so it's gauge invariant — because we integrated
around a loop $\Delta \phi \sim \oint \underline{A} \cdot d\underline{\ell} \sim \int \underline{\nabla} \times \underline{A} \cdot d\underline{S}$

But in general, consider the path from
$\underline{r}'$ to $\underline{r}$:

$$S = \int_{t'}^{t} L \, dt''$$

$$= \int_{t'}^{t} dt'' \left(\frac{1}{2} m \dot{x}^2 + q \frac{\underline{v} \cdot \underline{A}}{c} - q\phi \right)$$

Now make a gauge change $\quad \underline{A} \to \underline{A} + \underline{\nabla}\lambda$
$$\phi \to \phi - \frac{1}{c}\dot{\lambda}$$

$$\left(\text{since } \underline{B} = \underline{\nabla} \times \underline{A}, \quad \underline{E} = -\underline{\nabla}\phi - \dot{\underline{A}}/c \right)$$

$$\Rightarrow \quad S \to S + \Delta S$$

$$\Delta S = \int_{t'}^{t} dt'' \left(\frac{q \, \underline{v} \cdot \underline{\nabla}\lambda}{c} + \frac{q}{c}\dot{\lambda} \right)$$

$$= \int_{t'}^{t} dt'' \, \frac{q}{c} \underbrace{\left(\frac{\partial}{\partial t} + \underline{v} \cdot \underline{\nabla} \right) \lambda}$$

this is the total derivative
along the path

$$\Rightarrow \quad \Delta S = \frac{q}{c} \left[\lambda(\underline{r}) - \lambda(\underline{r}') \right]$$

The change in the propagator is

$$K(\underline{r},t; \underline{r}',t') \rightarrow K \times e^{\frac{iq}{\hbar c}\left[\lambda(\underline{r}) - \lambda(\underline{r}')\right]}$$

or

$$\langle \underline{r},t | \underline{r}',t \rangle \rightarrow \langle \underline{r},t | e^{\frac{iq\lambda(\underline{r})}{\hbar c}} e^{\frac{-iq\lambda(\underline{r}')}{\hbar c}} | \underline{r}',t' \rangle$$

we can absorb the gauge change into a redefinition of the phase of the basis vectors

Gauge invariance in QM:

$$\underline{A} \rightarrow \underline{A}' = \underline{A} + \nabla\lambda$$

$$|\psi\rangle \rightarrow |\psi'\rangle = e^{iq\lambda/\hbar c} |\psi\rangle$$

Notes:

1. unitary $\langle \psi' | \psi' \rangle = \langle \psi | \psi \rangle$

   (as it should be since we derived it from $e^{i \Delta S / \hbar}$)

2. $\langle \psi' | \hat{x} | \psi' \rangle = \langle \psi | \hat{x} | \psi \rangle$

   $\Rightarrow \langle x \rangle$ gauge independent

3. What about $\langle \pi \rangle = \langle p - \frac{qA}{c} \rangle$?

$$e^{-iq\lambda/\hbar c} \; \hat{\underline{p}} \; e^{iq\lambda/\hbar c}$$

$$= e^{-iq\lambda/\hbar c} \underbrace{\left[\hat{\underline{p}}, e^{iq\lambda/\hbar c} \right]}_{-i\hbar \underline{\nabla} e^{i\lambda q/\hbar c}} + \hat{\underline{p}}$$

$$= e^{i\lambda q/\hbar c} \underline{\nabla} \lambda \; q/c$$

$$= \frac{q}{c} \underline{\nabla} \lambda + \hat{\underline{p}}$$

So the gauge change gives an extra term in $\langle p \rangle$ that cancels the change in $\langle \frac{qA}{c} \rangle$

$\Rightarrow \langle \pi \rangle$ is gauge invariant.

Landau levels

Spinless particle in a uniform magnetic field

$$\underline{B} = B \hat{z} \qquad \underline{A} = \frac{1}{2} B \left(-y, x, 0 \right)$$

$$\Rightarrow H = \frac{1}{2m} \left[\left(P_x + \frac{1}{2} \frac{qBy}{c} \right)^2 + \left(P_y - \frac{1}{2} \frac{qBx}{c} \right)^2 + p_z^2 \right]$$

$$= \frac{1}{2m} \left(\Pi_x^2 + \Pi_y^2 \right) + \frac{p_z^2}{2m}$$

Define the Larmor frequency $\omega = \frac{qB}{mc}$

then $\qquad \Pi_x = P_x + \frac{1}{2} m \omega y$

$$\Pi_y = P_y - \frac{1}{2} m \omega x$$

Note that whereas p_x and p_y commute, Π_x and Π_y do not!

$$\left[\pi_x, \pi_y\right] = \left[p_x + \tfrac{1}{2}m\omega y, \; p_y - \tfrac{1}{2}m\omega x\right]$$

$$= -\tfrac{1}{2}m\omega \underbrace{\left[p_x, x\right]}_{-i\hbar} + \tfrac{1}{2}m\omega \underbrace{\left[y, p_y\right]}_{i\hbar}$$

$$= i\, m\omega\hbar$$

Now define the ladder operators:

$$\hat{a} = \frac{1}{\sqrt{2m\hbar\omega}}\left(\hat{\pi}_x + i\hat{\pi}_y\right)$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}\left(\hat{\pi}_x - i\hat{\pi}_y\right)$$

$$a^\dagger a = \frac{1}{2m\hbar\omega}\left(\pi_x^2 + \pi_y^2 + i\underbrace{\left[\hat{\pi}_x, \hat{\pi}_y\right]}_{-m\omega\hbar}\right)$$

$$\hbar\omega\, a^\dagger a = \frac{\pi_x^2 + \pi_y^2}{2m} - \tfrac{1}{2}\hbar\omega$$

So we see that

$$H = \hbar\omega \left(a^\dagger a + \tfrac{1}{2} \right) + \frac{p_z^2}{2m}$$

with

$$[a, a^\dagger] = 1$$

The particle moves freely along the magnetic field direction (p_z^2 term) but has quantized motion perpendicular to the field, with energies $(n + \tfrac{1}{2})\hbar\omega$.

Clarification about last time:

Gauge change $\quad \underline{A} \rightarrow \underline{A}' = \underline{A} + \underline{\nabla}\lambda$

Propagator
$$\langle \underline{r} | U(t) | \underline{r}' \rangle \rightarrow$$

$$\langle \underline{r} | e^{\frac{iq\lambda(\underline{r})}{\hbar c}} U(t) e^{-\frac{iq\lambda(\underline{r}')}{\hbar c}} | \underline{r}' \rangle$$

$\Rightarrow$ propagator will remain the same if we apply a phase change to the basis vectors

$$| \underline{r} \rangle \rightarrow e^{-i\lambda(\underline{r})q/\hbar c} | \underline{r} \rangle.$$

The wavefunction then picks up a phase of the <u>opposite</u> sign

$$\psi(\underline{r}) = \langle \underline{r} | \psi \rangle \rightarrow e^{i\lambda(\underline{r})q/\hbar c} \psi(\underline{r})$$

Alternatively, we can apply the phase change to the states directly
$$| \psi \rangle \rightarrow e^{iq\lambda/\hbar c} | \psi \rangle.$$

Landau levels

Particle in a uniform magnetic field $\underline{B} = B\hat{z}$

$$H = \frac{\pi^2}{2m} = \frac{(p - qA/c)^2}{2m}$$

Last time we wrote $\underline{A} = \frac{1}{2} B(-y, x, 0)$

$$\text{Symmetric gauge}$$

$$\Rightarrow \quad H = \left(\frac{1}{2} + a^\dagger a\right) \hbar \omega_B + \frac{p_z^2}{2m}$$

$$\omega_B = \frac{qB}{mc} \quad \text{Larmor frequency}$$

$\Rightarrow$ Quantized motion perpendicular to $\underline{B}$.
Energies $E_n = \hbar \omega_B \left(n + \frac{1}{2}\right) \qquad n = 0, 1 \ldots$

Note that we went from two degrees of freedom (π_x, π_y) to one $(n) \Rightarrow$ there is a large degeneracy in each Landau level. To investigate this, we need the wavefunctions.

Landau level wavefunctions

   Simplest way to derive the wavefunctions is to use the Landau gauge $\underline{A} = B(0, x, 0)$

then
$$H = \frac{p_x^2}{2m} + \frac{(p_y - qBx/c)^2}{2m}$$

(consider horizontal motion only)

Notice that $[H, p_y] = 0$ which suggests

$$\psi(x,y) = f(x)\, e^{iky}$$

$$\Rightarrow H\psi = \left[\frac{p_x^2}{2m} + \frac{(\hbar k - qBx/c)^2}{2m} \right] \psi$$

$$= \left[\frac{p_x^2}{2m} + \frac{1}{2} m\omega_B^2 \left(x - \frac{\hbar c\, k}{qB} \right)^2 \right] \psi$$

This is a harmonic oscillator with a shifted origin at

$$x = \frac{\hbar k}{qB/c}$$

$\Rightarrow$ the stationary states are

$$\Psi_{nk}(x,y) = e^{iky} f_{nk}(x)$$

$$\uparrow$$
harmonic oscillator
shifted to $x = \frac{\hbar k}{qB/c}$

Energies do not depend on k

$$E_n = \hbar \omega_B \left(n + \tfrac{1}{2}\right).$$

Note that if we had instead chosen
$$A = B(-y, 0, 0)$$
we would get wavefunctions $\Psi \sim e^{ikx} f_{nk}(y)$

The form of the wavefunction depends on the gauge chosen. When we choose a gauge, we are choosing one of the symmetries of the problem (symmetric gauge $\rightarrow$ rotationally symmetric

Landau gauge $\rightarrow$ translational symmetry)
and thereby which constant of the motion to use to label the degenerate eigenfunctions.

[See HW 4 and 2020 midterm Q2 for more.]

Density of states

Free particle with $B = 0$
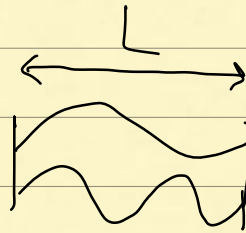
Periodic b.c.'s over length L $\Rightarrow$ $\lambda = \dfrac{L}{n}$

$$\Rightarrow \quad k = \frac{2\pi}{L} n$$

$\Rightarrow$ number of states in interval dk
is $\dfrac{L\,dk}{2\pi}$.

In 3D this becomes $\dfrac{L^3 \, d^3k}{(2\pi)^3}$

$\Rightarrow$ phase space density is $\boxed{\dfrac{1}{(2\pi)^3} \, d^3x \, d^3k}$

You might have seen this before in stat. mech.

In our case, we have a free particle wavefunction in the y-direction but a localized wavefunction in the x-direction.

Consider an area $\quad L_x \times L_y$

L_x

L_y
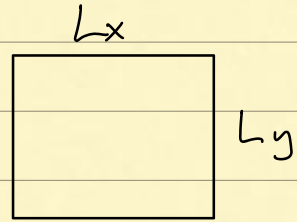
The shift in the localized states is $\dfrac{\hbar c}{qB} k_y$

$\Rightarrow$ we need $k_y < \dfrac{qB L_x}{\hbar c}$

$\Rightarrow$ total number of states $= \dfrac{L_y \Delta k_y}{2\pi}$

$\qquad\qquad\qquad = L_x L_y \dfrac{qB}{2\pi\hbar c}$

$\Rightarrow$ number of states per unit area is

$$\dfrac{qB}{2\pi\hbar c} = \dfrac{B}{\Phi_0} = \dfrac{B}{4\times10^{-15} \, Tm^2}$$

With $B = 0$ the density of states is

$$\frac{dk_x \, dk_y}{(2\pi)^2} = \frac{dp_x \, dp_y}{(2\pi\hbar)^2} = \frac{2\pi p \, dp}{(2\pi\hbar)^2}$$

$$= \frac{\pi \, d(p^2)}{(2\pi\hbar)^2} = \frac{2m\pi}{(2\pi\hbar)^2} \, d\varepsilon \qquad \left(\varepsilon = \frac{p^2}{2m} \right)$$

$\Rightarrow$ in an energy range $\hbar\omega_B$, the number of
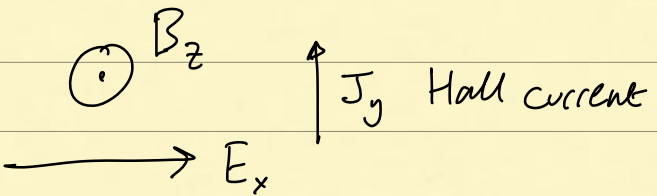
states is $\quad \dfrac{2\pi m \hbar \omega_B}{(2\pi\hbar)^2} = \dfrac{m}{2\pi\hbar} \dfrac{qB}{mc}$

$$= \frac{qB}{2\pi\hbar c}$$

ie. all the $B = 0$ states "collapse" onto the
Landau level

$$B > 0$$

$g(\varepsilon)$

$B = 0, \quad g(\varepsilon) = \dfrac{m}{2\pi\hbar^2}$
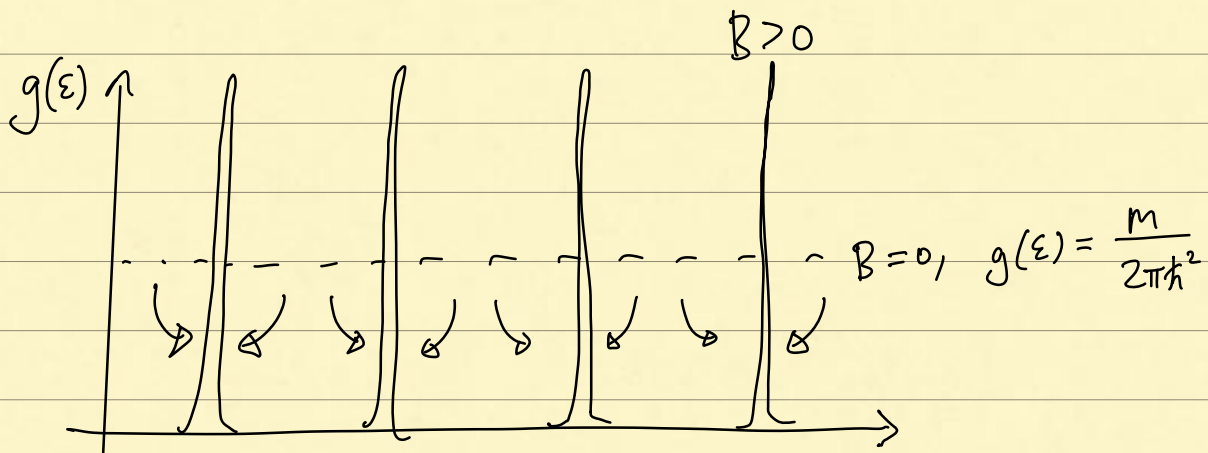
Quantum Hall effect

Hall effect reminder:

$\odot \, {}^{B_z}$

$\longrightarrow E_x$

$\uparrow J_y$ Hall current

number density

current $\qquad J_x = \sigma E_x = nq v$

electrical conductivity

drift velocity

$\Rightarrow \qquad v = \dfrac{\sigma E_x}{nq}$.

charges feel a force in the y-direction

$$q\left(\dfrac{v}{c} \times B\right) = \dfrac{\sigma E_x B_z}{nc}$$

which implies a $\underline{\text{Hall current}}$ $\qquad \sigma\left(\dfrac{v}{c} \times B\right)$

$$\boxed{J_H = \dfrac{\sigma^2}{nqc} \, \underline{E} \times \underline{B}.}$$

(We've assumed that the scattering time τ is short compared to ω_B^{-1} — in the opposite limit J_H is divided by $(\omega_B \tau)^2$.)

Now think about the quantum case. Add
$\underline{E} = E \; \hat{\underline{x}}$ to our Hamiltonian for free electrons.

$$\phi = - E x$$

$$\Rightarrow \quad H = \frac{1}{2m} \left[p_x^2 + \left(p_y - q \frac{Bx}{c} \right)^2 \right] - q E x$$

To simplify, we can complete the square. Compared to previously, there is an additional shift in x:

$$x \rightarrow x - \frac{\hbar k}{q B / c} - \frac{m c^2 E}{q B^2}$$

The energies are now

$$E_{n,k} = \hbar \omega_B \left(n + \tfrac{1}{2} \right) - q E \overbrace{\left(\frac{\hbar k}{q B / c} + \frac{q E}{m c \omega_B^2} \right)}^{\Delta x}$$

$$+ \frac{m c^2}{2} \frac{E^2}{B^2} \quad .$$

harmonic oscillator as
before

kinetic energy

electrostatic
energy

Note that E_{nk} now depends on k!
(Because there is an energy cost to changing position
in the electric potential).

New look at the current:

x-direction $\langle \Psi_{nk} | \pi_x | \Psi_{nk} \rangle = 0$

(no net momentum in the H.O. eigenstates
$$\pi_x \propto \hat{a} + \hat{a}^\dagger \text{)}$$

y-direction $\langle \Psi_{nk} | \pi_y | \Psi_{nk} \rangle$

$$\pi_y = -i\hbar \frac{\partial}{\partial y} - \frac{qBx}{c}$$

$\Rightarrow \quad \langle \pi_y \rangle = \hbar k - \frac{qB}{c} \langle x \rangle$

$$= \hbar k - \frac{qB}{c} \left[\frac{c\hbar k}{qB} + \frac{mc^2 E}{qB^2} \right]$$

$$= -\frac{mc E}{B}$$

(Can also calculate group velocity $v_y = \frac{m}{\hbar} \frac{\partial E}{\partial k}$)

This perpendicular velocity is known as
"E x B drift". (Also get this classically—try it!)

Therefore we have a current per particle

$$I_y = \frac{q}{m} \pi_y = \underline{\underline{qc\frac{E}{B}}}$$

Per Landau level, there are $\dfrac{qB}{2\pi\hbar c}$ particles per
unit area (if the Landau level is full).

$\Rightarrow$ total current $\dfrac{qB}{2\pi\hbar c} \cdot \dfrac{qcE}{B} = \dfrac{q^2}{2\pi\hbar} E$

per unit area
per Landau level

The resistivity is $\dfrac{2\pi\hbar}{q^2} \dfrac{1}{\nu} = \dfrac{\Phi_0}{qc} \dfrac{1}{\nu}$.

where ν is the # of Landau levels populated.

We can see this in the transverse resistivity vs. B

ρ_{xy}

plateaus at integer values $\frac{1}{\nu}$ as different numbers of Landau levels are filled.

B
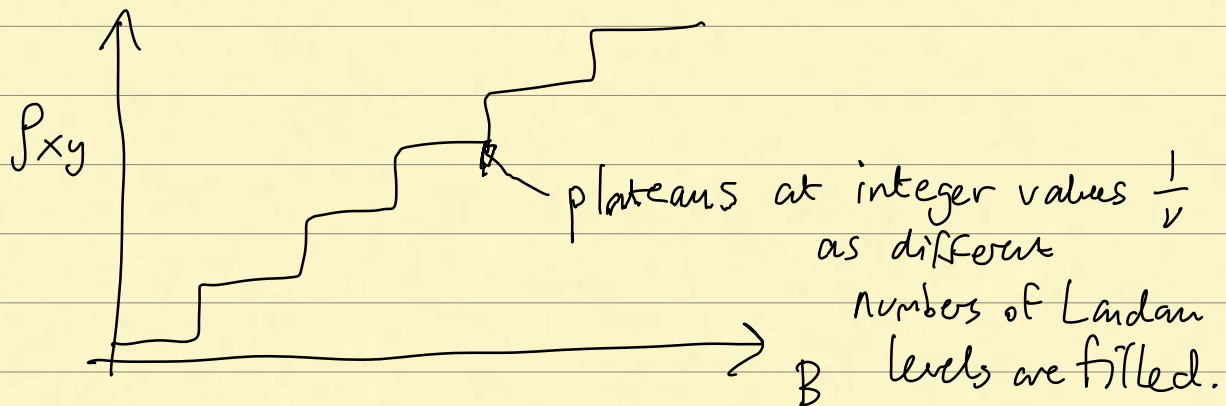
As B increases, each Landau level has more states, so fewer levels are populated — ρ_{xy} goes up.

Whenever a new Landau level is available, there is a discrete jump in the resistivity.

Lots of physics in this! For a good introduction you can look for the lectures by David Tong.

Radiative transitions in atoms

"Semi-classical" approach — treat the EM wave as a perturbing potential. Then Fermi's Golden Rule gives the rate

$$P = \frac{2\pi}{\hbar} \, g(E_f) \, |\langle f | V_0 | i \rangle|^2$$

where $V(t) = V_0 \, e^{\pm i\omega t}$ perturbing potential

$| i \rangle$ initial state

$| f \rangle$ final state

EM wave:

$$\underline{A} = A_0 \, \hat{\underline{n}} \, e^{-i\omega t} \, e^{i\underline{k} \cdot \underline{r}} \qquad |\underline{k}| = \omega / c$$

$$\underline{k} \cdot \hat{\underline{n}} = 0$$

Introduce $\underline{A}$ as a perturbation

$$\frac{p^2}{2m} \rightarrow \frac{(p + eA/c)^2}{2m} = \frac{p^2}{2m} + \frac{e\underline{A} \cdot p}{mc} + \frac{e^2 A^2}{2mc^2}$$

1st order term is $\quad V_0 \simeq \dfrac{eA_0}{mc}\, \underline{p} \cdot \underline{\hat{n}}\, e^{ikx}$

For atomic transitions, $\quad \lambda \gg a_0$

$$\Rightarrow \quad kx \ll 1$$
$$\Rightarrow \quad e^{ikx} \simeq 1.$$
(electric dipole approximation)

$\Rightarrow$ matrix element is

$$\boxed{\; \langle f | V_0 | i \rangle \simeq \dfrac{eA_0}{mc}\, \underline{\hat{n}} \cdot \langle f | \underline{p} | i \rangle \;}$$

Rewrite this using $\quad [H, x_j] = -\dfrac{i\hbar}{m} p_j \quad :$

$$\langle f | \underline{p} | i \rangle = \dfrac{im}{\hbar} \langle f | [H, \underline{x}] | i \rangle$$

$$= \dfrac{im}{\hbar} (E_f - E_i) \langle f | \underline{x} | i \rangle$$

$$= im\omega \langle f | \underline{x} | i \rangle$$

$$\Rightarrow \quad \boxed{\; \langle f | V_0 | i \rangle \simeq ie A_0\, \omega\, \underline{\hat{n}} \cdot \langle f | \underline{x} | i \rangle \;}$$

Often we want a cross-section (cm^2)

$$= \frac{rate \ \Gamma \ (s^{-1})}{photon \ flux \ (cm^{-2} s^{-1})} .$$

Two examples:

1) Atomic absorption

Choose $g(E_f) \approx \delta(E-E_f)$

$$\Gamma = \frac{2\pi}{\hbar} \ \delta(E-E_f) \ e^2 \frac{A_0^2}{c^2} \omega^2 \ |\langle f|x|i\rangle|^2$$

Photon flux in the wave is $\underline{S} = \frac{c}{4\pi} \underline{E} \times \underline{B} \cdot \frac{1}{\hbar\omega}$

$$= \frac{2A_0^2 \omega^2}{4\pi c} \frac{1}{\hbar\omega}$$

$\Rightarrow \ \sigma_{if} = \frac{2\pi\hbar c}{A_0^2 \omega} \times \frac{2\pi}{\hbar} \delta(E-E_f) \ e^2 \frac{A_0^2}{c^2} \omega^2$

$$\times |\langle f|x|i\rangle|^2$$

$$\Rightarrow \quad \sigma_{if} = 4\pi^2 \, \alpha \, \hbar\omega \; \delta(E - E_f) \left| \langle f | x | i \rangle \right|^2.$$

$$\left(\alpha = \frac{e^2}{\hbar c} = \frac{1}{137} \right).$$

Rough size $\quad \sigma \sim \left(\dfrac{\hbar\omega}{\text{energy width}} \right) \times \; a_o^2$

Can be $\gg \left(\text{size of atom.} \right)^2$

Selection rules arise from the matrix elements
— only certain choices of $|i\rangle$ and $|f\rangle$ give a
non-zero $\langle f | x | i \rangle$.

eg. H atom wavefunctions we need $\Delta \ell = \pm 1$
since parity of each state is $(-1)^\ell$.

$\qquad$ 1s $\rightarrow$ 2p $\quad$ allowed

$\qquad$ 1s $\rightarrow$ 2s $\quad$ not allowed.

2) **Photoelectric effect**

$$|i\rangle = \psi_{n\ell m}$$

$$|f\rangle = e^{i\underline{p}\cdot\underline{x}/\hbar}$$

$$g(E_e)\, dE_e = V \frac{p^2\, dp\, d\Omega}{(2\pi\hbar)^3}$$

$$= V \frac{p^2}{\hbar^3} \frac{dp}{dE}\, dE\, d\Omega$$

$$\left(\frac{d\bar{E}}{dp} = \frac{p}{m}\right) \qquad = V \frac{mp}{\hbar^3}\, d\Omega$$

$$\longrightarrow \quad \frac{d\sigma_{bf}}{d\Omega} = \frac{2\pi\hbar c}{A_0^2\, \omega} \times \frac{2\pi}{\hbar} \times \frac{V\, mp}{\hbar^3}$$

"bound-free"
cross-section

$$\times \frac{e^2 A_0^2}{m^2 c^2}\; \left|\langle f|\,\hat{\underline{n}}\cdot\underline{p}\,|i\rangle\right|^2$$

use the momentum version
since $|f\rangle = |p\rangle$

The final result looks like

$$\frac{d\sigma_{bf}}{d\Omega} = \frac{\alpha \hbar}{2\pi m \omega} \frac{P_e (\hat{n} \cdot P_e)^2}{\hbar^3}$$

$$\times \left| \int d^3\underline{r} \; e^{-i\underline{p} \cdot \underline{r}/\hbar} \; \Psi(\underline{r}) \right|^2$$

(see Sakurai §5.8.3 for evaluation of this
for a K shell electron).

Helium atom

The helium atom is interesting as an example of a two-fermion system with interactions.

A reminder about hydrogen. The stationary states $\psi_{n\ell m}(\boldsymbol{r})$ of a hydrogen-like (single electron) atom are labelled by n, ℓ and m, where n tells you the energy of the state,

$$E_n = -\frac{1}{2}\alpha^2 Z^2 m_e c^2 \frac{1}{n^2}$$

and ℓ and m specify the orbital angular momentum (the angular part of the wavefunction is $\propto Y_{\ell,m}(\theta,\phi) \propto e^{im\phi}P_\ell(\cos\theta)$). The ground state wavefunction is

$$\psi_{100}(\boldsymbol{r}) = \frac{1}{\pi^{1/2}a_Z^{3/2}}e^{-r/a_Z},$$

where $a_Z = a_0/Z$ and $a_0 = \hbar/(\alpha m_e c)$ is the Bohr radius. Another way to write the energy is in terms of $e^2/4\pi\epsilon_0 a_0 = \alpha^2 m_e c^2$.

- Plug numbers into the formulae above for E_n and a_0 and check that they give the values you expect. (If you know the electron rest mass in keV that will give you a useful starting point).

- A useful number to remember is $m_e c^2 = 511$ keV, which gives the binding energy of hydrogen as $(1/2) \times (1/137)^2 \times 511$ keV $= 13.6$ eV.

- For the size, the lengthscale $h/m_e c$ is the Compton wavelength of the electron. Putting numbers gives $a_0 = \alpha^{-1}(\hbar/m_e c) = 0.53 \times 10^{-10}$ m $= 0.53$ Å. Another useful quantity to remember is that $\hbar c = 197$ MeV fm, so we can also compute this as

$$a_0 = \frac{\hbar c}{\alpha m_e c^2} = \frac{197 \text{ MeV fm}}{\alpha \text{ } 511 \text{ keV}} = \frac{197 \times 137}{0.511} = 5.3 \times 10^4 \text{ fm}.$$

Ground state. We can construct the Hamiltonian for helium by taking two copies of the hydrogen Hamiltonian and adding the Coulomb interaction between the two electrons:

$$H = H_1 + H_2 + \frac{e^2}{4\pi\epsilon_0|\boldsymbol{r_2} - \boldsymbol{r_1}|},$$

$$H_i = \frac{p_i^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0|\boldsymbol{r_i}|}$$

where $\boldsymbol{r_1}$ and $\boldsymbol{r_2}$ are the positions of the two electrons, and Z is the charge on the nucleus ($Z = 2$ in the case of helium).

- Assume the electrons are non-interacting. Write down the wavefunction for the ground state in terms of the single-particle hydrogen-like atom wavefunctions $\psi_{n\ell m}$. What are the units of your wavefunction?

- What do you predict for the ground state energy (i.e. the ionization energy of helium) ignoring the electron-electron interaction?

- Estimate the relative size of the interaction term at the "back of the envelope" level. How much do you expect the interaction term to change the ground state energy?

- We can construct the ground state by putting both electrons into ψ_{100}, but then we need an antisymmetric spin state (singlet) so that the wavefunction is overall antisymmetric:

$$\psi(\boldsymbol{r_1}, \boldsymbol{r_2}) = \psi_{100}(\boldsymbol{r_1})\psi_{100}(\boldsymbol{r_2})\frac{1}{\sqrt{2}}\left(\left|\uparrow\right\rangle\left|\downarrow\right\rangle - \left|\downarrow\right\rangle\left|\uparrow\right\rangle\right).$$

Note that it is not possible to write down an antisymmetric spatial wavefunction when both electrons have the same single particle wavefunction, so there is no ground state wavefunction where the electrons are in the spin triplet state.

- The two-particle wavefunction has the normalization integral

$$\int d^3\boldsymbol{r_1} \int d^3\boldsymbol{r_2} \left|\psi(\boldsymbol{r}_1, \boldsymbol{r}_2)\right|^2 = 1$$

from which we can see that ψ has units of $1/\text{length}^3$ (as makes sense since it is the product of two single particle wavefunctions, and single particle wavefunctions have units $1/(\text{length})^{3/2}$.

- Ground state energy:

$$(H_1 + H_2)\psi = E_0\psi.$$

Each term gives a contribution -13.6 eVZ^2, which for $Z = 2$ gives a total ground state energy

$$E_0 = -108.8 \text{ eV}.$$

- Looking at the Hamiltonian and assuming that $1/(r_2 - r_1) \sim 1/r_i$ on average, the interaction term is $1/4$ of the sum of H_1 and H_2. So the correction should be about 20% of the total energy. The interaction term is positive because the electrons repel each other. A guess for the true ground state energy is therefore

$$E_0 \approx -108.8 \text{ eV} \times 0.8 \approx -87 \text{ eV}.$$

The electron interaction term is a significant correction. This guess is not too far from the actual value of ≈ -79 eV.

Excited states.

- Write down all possible wavefunctions for the first excited state.

- Write down the first order perturbation theory estimate of the correction to the first excited state energy due to the electron-electron interaction. Just write down the integral that you would need to do, no need to evaluate it. Does the energy depend on the choice of excited state wavefunction? Explain what is happening physically.

- The first excited state corresponds to having one electron in $n = 1$ and the other in $n = 2$. Because the spatial wavefunctions are now different, it is possible to write down an antisymmetric spatial wavefunction, so the spin triplet state is now an option. The two possible wavefunctions are

$$\psi_s(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{1}{\sqrt{2}} \left[\psi_{100}(\boldsymbol{r}_1)\psi_{2\ell m}(\boldsymbol{r}_2) + \psi_{2\ell m}(\boldsymbol{r}_1)\psi_{100}(\boldsymbol{r}_2) \right]$$

with the electrons in a spin singlet state, or

$$\psi_t(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{1}{\sqrt{2}} \left[\psi_{100}(\boldsymbol{r}_1)\psi_{2\ell m}(\boldsymbol{r}_2) - \psi_{2\ell m}(\boldsymbol{r}_1)\psi_{100}(\boldsymbol{r}_2) \right]$$

with the electrons in a spin triplet state.

- With the four possible combinations $(\ell, m) = (0, 0), (1, -1), (1, 0), (1, 1)$ and the four possible spin states (one singlet, three triplet), we end up with 16 possible wavefunctions.

- The first order correction to the energy is

$$\Delta E = \int d^3\boldsymbol{r_1} \int d^3\boldsymbol{r_2} \; \psi^*(\boldsymbol{r}_1, \boldsymbol{r}_2) \frac{e^2}{4\pi\epsilon_0 |\boldsymbol{r_2} - \boldsymbol{r_1}|} \psi(\boldsymbol{r}_1, \boldsymbol{r}_2).$$

If you substitute ψ_s, there are four terms

$$
\begin{aligned}
\Delta E \;=\;& \frac{1}{2} \int d^3\boldsymbol{r_1} \int d^3\boldsymbol{r_2} \; \psi_{100}^*(\boldsymbol{r}_1)\psi_{2\ell m}^*(\boldsymbol{r}_2) \frac{e^2}{4\pi\epsilon_0 |\boldsymbol{r_2} - \boldsymbol{r_1}|} \psi_{100}(\boldsymbol{r}_1)\psi_{2\ell m}(\boldsymbol{r}_2) \\
+\;& \frac{1}{2} \int d^3\boldsymbol{r_1} \int d^3\boldsymbol{r_2} \; \psi_{100}^*(\boldsymbol{r}_1)\psi_{2\ell m}^*(\boldsymbol{r}_2) \frac{e^2}{4\pi\epsilon_0 |\boldsymbol{r_2} - \boldsymbol{r_1}|} \psi_{2\ell m}(\boldsymbol{r}_1)\psi_{100}(\boldsymbol{r}_2) \\
+\;& \frac{1}{2} \int d^3\boldsymbol{r_1} \int d^3\boldsymbol{r_2} \; \psi_{2\ell m}^*(\boldsymbol{r}_1)\psi_{100}^*(\boldsymbol{r}_2) \frac{e^2}{4\pi\epsilon_0 |\boldsymbol{r_2} - \boldsymbol{r_1}|} \psi_{100}(\boldsymbol{r}_1)\psi_{2\ell m}(\boldsymbol{r}_2) \\
+\;& \frac{1}{2} \int d^3\boldsymbol{r_1} \int d^3\boldsymbol{r_2} \; \psi_{2\ell m}^*(\boldsymbol{r}_1)\psi_{100}^*(\boldsymbol{r}_2) \frac{e^2}{4\pi\epsilon_0 |\boldsymbol{r_2} - \boldsymbol{r_1}|} \psi_{2\ell m}(\boldsymbol{r}_1)\psi_{100}(\boldsymbol{r}_2)
\end{aligned}
$$

We can write this as $\Delta E = I + J$ with

$$I = \int d^3\boldsymbol{r_1} \int d^3\boldsymbol{r_2} \; |\psi_{100}(\boldsymbol{r}_1)|^2 |\psi_{2\ell m}(\boldsymbol{r}_2)|^2 \frac{e^2}{4\pi\epsilon_0 |\boldsymbol{r_2} - \boldsymbol{r_1}|}$$

and

$$J = \int d^3\boldsymbol{r_1} \int d^3\boldsymbol{r_2} \; \psi_{100}^*(\boldsymbol{r}_1)\psi_{2\ell m}^*(\boldsymbol{r}_2) \frac{e^2}{4\pi\epsilon_0 |\boldsymbol{r_2} - \boldsymbol{r_1}|} \psi_{2\ell m}(\boldsymbol{r}_1)\psi_{100}(\boldsymbol{r}_2).$$

- If we instead use ψ_t, corresponding to the spin triplet state, the energy shift is $\Delta E = I - J$. **The spin triplet state has a lower energy than the spin singlet state, even though there is no spin term in the Hamiltonian.** The symmetry of the spin state introduces (anti) correlations in the positions of the two electrons. When the spin state is symmetric, the spatial wavefunction is antisymmetric, giving a low probability that the electrons will be found close together. This leads to less repulsion between the electrons, lowering the overall energy.

- On the next page I've included the energy level diagram for helium, taken from Sakurai and Napolitano:
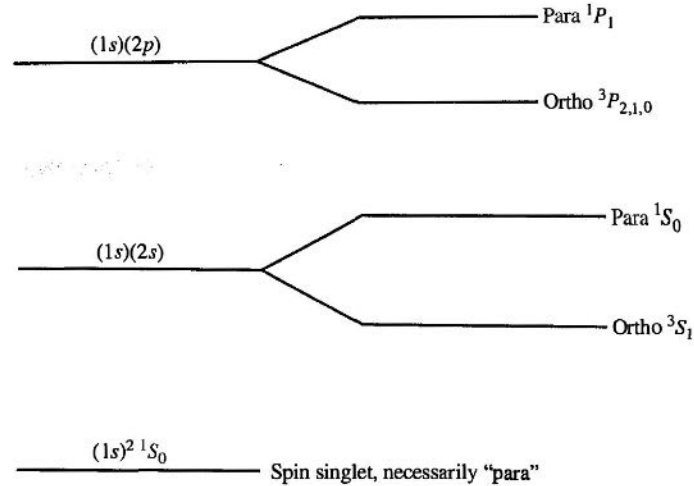
FIGURE 7.6 Schematic energy-level diagram for low-lying configurations of the helium atom.

The terms "para" and "ortho" helium refer to whether the electrons are in a spin singlet or triplet state respectively. Notice that the overall shift depends on the choice of ℓ for the second electron, but not on m – can you see why looking at the integrals?

A more accurate ground state energy

- Try to make a more accurate estimate of the ground state energy using either perturbation theory or the variational method (or both if you have time). Compare your answer with the measured value -78.975 eV. (For the variational method, one example of a trial wavefunction is to replace the charge Z in the hydrogen ground state ψ_{100} with an effective charge Z_{eff} – the argument is that the electron feels a smaller force from the nucleus because of screening from the other electron. The energy can then be minimized with respect to the parameter Z_{eff}. But you can try any trial wavefunction you like.)

To help you avoid doing a lot of integrals, here are some useful formulae. For a wavefunction $\psi(r) \propto e^{-\beta(r_1+r_2)/a_0}$,

$$\left\langle \frac{\partial^2}{\partial r_i^2} \right\rangle = \frac{\beta^2}{a_0^2}, \qquad \left\langle \frac{1}{r_i} \right\rangle = \frac{\beta}{a_0}, \qquad \left\langle \frac{1}{r_{12}} \right\rangle = \frac{5\beta}{8a_0}.$$

You can prove the first two very quickly using the integral

$$\int_0^\infty dr\, r^n e^{-2\beta r/a_0} = n! \left(\frac{a_0}{2\beta}\right)^{n+1} \qquad \text{(positive integer } n\text{)}.$$

The last one is straightforward but a bit more involved – I included the proof on the next page so you can see it.

- Let's use perturbation theory first. As before, the energy shift is

$$\Delta E = \int d^3\mathbf{r}_1 \int d^3\mathbf{r}_2 \; \psi^*(\mathbf{r}_1,\mathbf{r}_2)\frac{e^2}{4\pi\epsilon_0|\mathbf{r}_2-\mathbf{r}_1|}\psi(\mathbf{r}_1,\mathbf{r}_2),$$

  where the wavefunction is $\psi(\mathbf{r}_1,\mathbf{r}_2) \propto e^{-(r_1+r_2)/a_Z}$ (using the expression for ψ_{100} from the beginning of these notes). We can use the integral given above to evaluate this:

$$\Delta E = \frac{e^2}{4\pi\epsilon_0}\frac{5}{8}\frac{1}{a_Z} = \frac{5}{8}Z\frac{\alpha\hbar c}{a_0} = \frac{5}{4}Z\frac{1}{2}\alpha^2 m_e c^2 = \frac{5}{2}\times 13.6 \text{ eV} = 34 \text{ eV}.$$

  This gives the ground state energy as

$$E_0 = (-108.8 + 34) \text{ eV} = -74.8 \text{ eV}.$$

- For the variational principle, we evaluate the expectation value of the full Hamiltonian with a trial wavefunction. If we use the ground state wavefunction above but with $Z \to Z_{\text{eff}}$ as the trial wavefunction, the energy will be

$$\begin{aligned}
E &= 2\frac{\hbar^2}{2m_e}\left\langle\frac{\partial^2}{\partial r_i^2}\right\rangle - 2\frac{Ze^2}{4\pi\epsilon_0}\left\langle\frac{1}{r_i}\right\rangle + \frac{e^2}{4\pi\epsilon_0}\left\langle\frac{1}{r_{12}}\right\rangle \\
&= \frac{\hbar^2}{m_e a_0^2}Z_{\text{eff}}^2 - 2\frac{Ze^2}{4\pi\epsilon_0}\frac{Z_{\text{eff}}}{a_0} + \frac{e^2}{4\pi\epsilon_0}\frac{5Z_{\text{eff}}}{8a_0} \\
&= \frac{e^2}{4\pi\epsilon_0 a_0}\left[Z_{\text{eff}}^2 - 2Z_{\text{eff}}Z + \frac{5}{8}Z_{\text{eff}}\right].
\end{aligned}$$

  Minimizing with respect to Z_{eff}, ie. setting $dE/dZ_{\text{eff}} = 0$ gives

$$Z_{\text{eff}} = 2 - \frac{5}{16} = 1.6875$$

  and

$$E = 2\times 13.6 \text{ eV}\times Z_{\text{eff}}\left[Z_{\text{eff}} - 4 + \frac{5}{8}\right] = -2Z_{\text{eff}}^2 \times 13.6 \text{ eV} = -77.5 \text{ eV}.$$

  This is closer to the correct answer than perturbation theory.

Calculation of electron interaction term

We want

$$I = \int d^3\boldsymbol{r}_1 \int d^3\boldsymbol{r}_2 \; e^{-2\beta(r_1+r_2)/a_0} \frac{1}{|\boldsymbol{r}_2 - \boldsymbol{r}_1|}$$

Choose coordinates such that the z-axis lies along $\boldsymbol{r}_1$. Then $\boldsymbol{r}_1 \cdot \boldsymbol{r}_2 = r_1 r_2 \cos\theta$ and we can write the integral as

$$I = \int d^3\boldsymbol{r}_1 \int 2\pi r_2^2 dr_2 \; e^{-2\beta(r_1+r_2)/a_0} \int \sin\theta d\theta \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta}}$$

The angular part is

$$\int_{-1}^{1} d\mu \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \mu}} = \frac{r_1 + r_2 - |r_2 - r_1|}{r_1 r_2}$$

giving

$$
\begin{aligned}
I &= \int_0^\infty 4\pi r_1^2 dr_1 \left[\int_0^{r_1} 2\pi r_2^2 dr_2 \; e^{-2\beta(r_1+r_2)/a_0} \frac{2}{r_1} + \int_{r_1}^\infty 2\pi r_2^2 dr_2 \; e^{-2\beta(r_1+r_2)/a_0} \frac{2}{r_2} \right] \\
&= 16\pi^2 \int_0^\infty r_1 dr_1 e^{-2\beta r_1/a_0} \left[\int_0^{r_1} r_2^2 dr_2 \; e^{-2\beta r_2/a_0} + \int_{r_1}^\infty r_1 r_2 \, dr_2 \; e^{-2\beta r_2/a_0} \right] \\
&= 16\pi^2 \frac{a_0^3}{4\beta^3} \int_0^\infty r_1 dr_1 e^{-4\beta r_1/a_0} \left(e^{2\beta r_1/a_0} - 1 - \frac{\beta r_1}{a_0} \right) \\
&= 16\pi^2 \frac{a_0^3}{4\beta^3} \left[\frac{a_0^2}{4\beta^2} - \frac{a_0^2}{16\beta^2} - \frac{\beta}{a_0} \frac{2a_0^3}{64\beta^3} \right] \\
&= 16\pi^2 \frac{a_0^5}{16\beta^5} \left[1 - \frac{1}{4} - \frac{1}{8} \right] \\
&= 16\pi^2 \frac{a_0^5}{16\beta^5} \frac{5}{8}.
\end{aligned}
$$

The normalization factor is

$$\int d^3\boldsymbol{r}_1 \int d^3\boldsymbol{r}_2 \; e^{-2\beta(r_1+r_2)/a_0} = 16\pi^2 \int r_1^2 dr_1 r_2^2 dr_2 e^{-2\beta(r_1+r_2)/a_0} = 16\pi^2 \frac{a_0^6}{16\beta^6}.$$

Therefore

$$\left\langle \frac{1}{r_{12}} \right\rangle = \frac{5}{8} \frac{\beta}{a_0},$$

which is the result given on the previous page.

Second quantization

These notes are an introduction to the formalism of second quantization, which is a useful way to deal with systems of multiple, interacting particles.

Part 1 – The harmonic oscillator as a multiply-occupied single state

The significance of $[a, a^\dagger] = 1$ in the harmonic oscillator. We are going to start with a reminder of how we treated the harmonic oscillator in terms of ladder operators. The Hamiltonian for the harmonic oscillator can be written

$$H = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) = \hbar\omega(N + \frac{1}{2})$$

where a and $a^\dagger$ are particular linear combinations of x and p, and $N = a^\dagger a$ is the number operator. The stationary states are also eigenstates of the number operator, and we can label them by the eigenvalue of N:

$$N \ket{n} = n \ket{n}.$$

- Show that $a^\dagger \ket{n}$ is an eigenstate of the number operator with eigenvalue $n+1$, provided that the ladder operators obey $[a, a^\dagger] = 1$. (Similarly you can show that $a \ket{n}$ is an eigenstate of N with eigenvalue $n-1$).

- To show this, act on $a^\dagger \ket{n}$ with the number operator and see what you get:

$$Na^\dagger \ket{n} = a^\dagger a a^\dagger \ket{n} = a^\dagger a^\dagger a \ket{n} - a^\dagger [a^\dagger, a] \ket{n}$$

$$= na^\dagger \ket{n} + a^\dagger [a, a^\dagger] \ket{n}.$$

We see that if the commutator $[a, a^\dagger] = 1$, then $Na^\dagger \ket{n} = (n+1)a^\dagger \ket{n}$

This gives us the spectrum of states of the harmonic oscillator. The ground state $\ket{0}$ is the state that obeys $a \ket{0} = 0$ and then the excited states are constructed by repeatedly operating with $a^\dagger$.

A single state occupied by multiple bosons. Now imagine that we are dealing with a system of bosons that we are putting into the same single

particle state. We can use the machinery of ladder operators to describe this situation. If there are n bosons in the system, we write the state as $|n\rangle$ which is an eigenstate of the number operator $N = a^\dagger a$. We view a and $a^\dagger$ as *annihilation* and *creation* operators that subtract or add particles to the system. The state $|0\rangle$ is the "vacuum" state that has no particles. [Note that we are using N, a and $a^\dagger$ here without assuming a particular Hamiltonian, we will discuss later how to write down the Hamiltonian for the multiparticle system.]

- If the single particle state we are dealing with here is $|\phi\rangle$, write down the state $|n\rangle$ in terms of products of $|\phi\rangle$ (you just have to make sure it has the appropriate exchange symmetry for bosons, and that it is normalized).

- This is straightforward, the idea here is just to emphasize the difference between the new notation $|n\rangle$ which describes the multiparticle state with a single ket, and the state as written as a symmetrized product of single particle states: $|n\rangle = \prod_{i=1}^{n} |\phi\rangle$.

Fermions and the anti-commutator. Now think about putting a fermion into the single particle state. We are only allowed zero or one particles because of the requirement that the state be antisymmetric.

- Show that we can still define a number operator $N = a^\dagger a$ and creation and annihilation operators $a^\dagger$ and a if we take a and $a^\dagger$ to obey the **anti-commutation relation**

$$\{a, a^\dagger\} = aa^\dagger + a^\dagger a = 1.$$

[Hint: follow the first question above and look at the eigenvalue of the state $a^\dagger |n\rangle$ when acted on by the number operator. The difference is that now $\{a, a^\dagger\} = 1$ instead of $[a, a^\dagger] = 1$.] What are the allowed states?

- Repeat the argument from before. Act on $a^\dagger |n\rangle$ with the number operator, but this time when we commute the operators, we write it in terms of the anticommutator:

$$N a^\dagger |n\rangle = a^\dagger a a^\dagger |n\rangle = -a^\dagger a^\dagger a |n\rangle + a^\dagger \{a^\dagger, a\} |n\rangle.$$

Now if the anticommutator is equal to 1, we have

$$N a^\dagger \left| n \right\rangle = (1 - n) a^\dagger \left| n \right\rangle.$$

We then see that $a^\dagger \left| 0 \right\rangle \propto \left| 1 \right\rangle$, so we can put one fermion into the system. But we are not able to add another: $a^\dagger \left| 1 \right\rangle = 0$.

Part 2 – Multi-particle system

In part 1, we were putting particles into a single state (i.e. constructing the multi-particle state from products of a single one-particle state). Now consider the more general case where we have a spectrum of single particle states $\left| k_i \right\rangle$ available (with $i = 1...N$, where N is the dimension of the Hilbert space). We build the state by distributing the particles among the different states $\left| k_i \right\rangle$. In what we have been doing so far, we would write the state of the system as appropriately symmetrized products of the single particle states.

The idea in second quantization is to write the state of the system instead in terms of how many particles are in each of the single particle states, ie.

$$\left| n_1, n_2, ...n_i, ...n_N \right\rangle. \tag{1}$$

- As an example of these two ways of writing down the state of the system, consider a two level system with single particle states $\left| + \right\rangle$ and $\left| - \right\rangle$. What are the possible states for (1) two bosons, or (2) two fermions in this system? Write your answers in two ways: as symmetrized products of two states, and in our new notation of equation (1).

- How would you write down a single particle state $\left| k_i \right\rangle$ in this new notation?

- For fermions, we are only allowed one particle in each state, so the only possible state is the singlet states

$$\left| 11 \right\rangle = 1\sqrt{2} \left(\left| + \right\rangle \left| - \right\rangle - \left| - \right\rangle \left| + \right\rangle \right).$$

For bosons, there are three possible configurations (triplet states)

$$\left| 20 \right\rangle = \left| - \right\rangle \left| - \right\rangle; \quad \left| 11 \right\rangle = 1\sqrt{2} \left(\left| + \right\rangle \left| - \right\rangle + \left| - \right\rangle \left| + \right\rangle \right); \quad \left| 02 \right\rangle = \left| + \right\rangle \left| + \right\rangle.$$

- The single particle state $|k_i\rangle$ has $n_i = 1$ and all other values of n zero, i.e.
$$|k_i\rangle = |0, 0, 0, ...0, 1, 0, ...0\rangle.$$

We move between these states by using particle creation and annihilation operators $a_i^\dagger$ and a_i which add or subtract one particle from the i-th state $|k_i\rangle$, ie.
$$a_i |n_1, n_2, ...n_i, ...n_N\rangle \propto |n_1, n_2, ...n_i - 1, ...n_N\rangle$$
$$a_i^\dagger |n_1, n_2, ...n_i, ...n_N\rangle \propto |n_1, n_2, ...n_i + 1, ...n_N\rangle.$$

If we are dealing with bosons, we set
$$[a_i, a_i^\dagger] = 1,$$

in which case n_i can take any (positive) integer value, or for fermions we set
$$\{a_i, a_i^\dagger\} = 1$$

in which case we are only allowed $n_i = 0$ or 1.

- Start with the vacuum state $|0, 0, 0, ..0\rangle$ and use the particle creation operators to add a particle to each of states i and j. Does it matter which order you do this in? Show that for bosons or fermions, the particle creation operators for different states must commute or anticommute respectively (i.e. either $[a_i^\dagger, a_j^\dagger] = 0$ or $\{a_i^\dagger, a_j^\dagger\} = 0$).

- If we add particle 1 to state i and particle 2 to state j with $a_j^\dagger a_i^\dagger |0\rangle$ this should be the same as adding particle 1 to state j and particle 2 to state i with $a_i^\dagger a_j^\dagger |0\rangle$, except for a minus sign in the case of fermions because the wavefunction is antisymmetric to particle exchange. So therefore $a_j^\dagger a_i^\dagger = a_i^\dagger a_j^\dagger$ for bosons and $a_j^\dagger a_i^\dagger = -a_i^\dagger a_j^\dagger$ for fermions.

Here is a table from Sakurai and Napolitano that summarizes all of the (anti)commutation relations:

TABLE 7.1 The Algebra for Identical Particles in Second Quantization

Bosons	Fermions
$a_i^\dagger a_j^\dagger - a_j^\dagger a_i^\dagger = [a_i^\dagger, a_j^\dagger] = 0$	$a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = \{a_i^\dagger, a_j^\dagger\} = 0$
$a_i a_j - a_j a_i = [a_i^\dagger, a_j^\dagger] = 0$	$a_i a_j + a_j a_i = \{a_i, a_j\} = 0$
$a_i a_j^\dagger - a_j^\dagger a_i = [a_i, a_j^\dagger] = \delta_{ij}$	$a_i a_j^\dagger + a_j^\dagger a_i = \{a_i, a_j^\dagger\} = \delta_{ij}$

Make sure these all make sense to you.

Operators. Now we need to think about how to write down operators that act on the states $|n_1, n_2, ...n_i, ...n_N\rangle$. The simplest case is the single particle operator K whose eigenstates $|k_i\rangle$ are those that we are using to construct the multi-particle states. If the eigenvalues are k_i, that is

$$K |k_i\rangle = k_i |k_i\rangle ,$$

we can write a corresponding operator $\mathcal{K}$ for the multi-particle states

$$
\begin{aligned}
\mathcal{K} |n_1, n_2, ...n_i, ...n_N\rangle &= \sum_i k_i N_i |n_1, n_2, ...n_i, ...n_N\rangle \\
&= \sum_i k_i a_i^\dagger a_i |n_1, n_2, ...n_i, ...n_N\rangle ,
\end{aligned}
$$

ie.

$$\mathcal{K} = \sum_i k_i a_i^\dagger a_i.$$

- Now consider a different single particle operator M with eigenstates $|m_i\rangle$. We could define creation and annihilation operators $b_i^\dagger$ and b_i that add or subtract particles to the state $|m_i\rangle$. Argue that these operators are related to $a_i^\dagger$ and a_i by

$$b_i^\dagger = \sum_j a_j^\dagger \langle k_j|m_i\rangle , \qquad b_i = \sum_j \langle m_i|k_j\rangle a_j.$$

  [Hint: You can use the fact that single particle states can be generated by acting on the vacuum with the creation operator, and use the usual formula for expanding a state in a different basis.]

- Show that the multi-particle version of M can therefore be written

$$\mathcal{M} = \sum_{ij} a_i^\dagger a_j \langle k_i|M|k_j\rangle .$$

- We can expand $|m_i\rangle$ as

$$|m_i\rangle = \sum_j \langle k_j|m_i\rangle |k_j\rangle .$$

If we then write $|m_i\rangle = b_i^\dagger |0\rangle$ and $|k_j\rangle = a_j^\dagger |0\rangle$, the first result follows. Taking the complex conjugate gives the second.

- If we work with the creation and annihilation operators for states $|m_i\rangle$, we have

$$
\begin{aligned}
\mathcal{M} &= \sum_i m_i b_i^\dagger b_i \\
&= \sum_i m_i \sum_j a_j^\dagger \langle k_j | m_i \rangle \sum_\ell \langle m_i | k_\ell \rangle a_\ell \\
&= \sum_{j,\ell} a_j^\dagger a_\ell \langle k_j | \left(\sum_i m_i |m_i\rangle \langle m_i| \right) |k_\ell\rangle \\
&= \sum_{j,\ell} a_j^\dagger a_\ell \langle k_j | M | k_\ell \rangle .
\end{aligned}
$$

So we can write the operator M in any basis by computing its matrix elements in that basis and using the creation and annihilation operators corresponding to that basis.

- As a specific example, write down the kinetic energy operator for a multiparticle state. Do this for both position representation and momentum representation. (This example is using a basis with a continuous eigenvalue spectrum, so the sums above will become integrals)

Interactions between particles. If we have pair-wise interactions between particles, we can represent that as a matrix $V_{ij} = V_{ji}$, where i and j refer to an interaction between particles in states $|k_i\rangle$ and $|k_j\rangle$.

The multiparticle version of this operator is

$$
\mathcal{V} = \frac{1}{2} \sum_{ij} V_{ij} a_i^\dagger a_j^\dagger a_j a_i.
$$

- It is important to note that the specific ordering of the operators is important here. The operator $\mathcal{V}$ does not correspond to $(1/2) \sum_{ij} V_{ij} N_i N_j$ which you might have guessed would be the correct form. Why not?

- If i and j are different, then we can reorder the operators to read $a_i^\dagger a_i a_j^\dagger a_j$ and we do in fact have a sum over $N_i N_j$. The factor of $1/2$ is there because we overcount the interactions when we sum over all pairs of particles twice. The subtlety comes in the terms where $i = j$,

i.e. where we are dealing with an interaction between particles in the same state. For bosons,

$$a_i^\dagger a_i^\dagger a_i a_i = a_i^\dagger a_i a_i^\dagger a_i - a_i^\dagger [a_i, a_i^\dagger] a_i = N_i(N_i - 1).$$

This is the number of ways of choosing two particles from n_i without replacement. For fermions,

$$a_i^\dagger a_i^\dagger a_i a_i = -a_i^\dagger a_i a_i^\dagger a_i + a_i^\dagger \{a_i, a_i^\dagger\} a_i = N_i(1 - N_i).$$

Since $n_i = 0$ or 1 for fermions, we see that the terms with $i = j$ vanish in this case,. There is no chance for two particles in the same state to interact, since only one particle can go into each state for fermions.

- As before, we might not be working in the basis in which V is diagonal. Consider the case where

$$\mathcal{V} = \frac{1}{2} \sum_{ij} V_{ij} b_i^\dagger b_j^\dagger b_j b_i,$$

where the b operators create or annihilate particles in the $|m_i\rangle$ states as above. Show that in terms of the a operators, this is

$$\mathcal{V} = \frac{1}{2} \sum_{ij\ell n} \langle ij|V|\ell n\rangle \, a_i^\dagger a_j^\dagger a_n a_\ell,$$

where

$$\langle ij|V|\ell n\rangle = \sum_{\alpha\beta} V_{\alpha\beta} \, \langle k_i|m_\alpha\rangle \, \langle m_\alpha|k_\ell\rangle \, \langle k_j|m_\beta\rangle \, \langle m_\beta|k_n\rangle \,.$$

- This is straightforward to show if you use the relations we had earlier to write the b operators in terms of the a operators. You just have to keep track of the coefficients and separate out the ones that represent the incoming and outgoing states and those that enumerate the matrix elements of V.

- As a specific example, consider a potential $V(\boldsymbol{r}_i, \boldsymbol{r}_j)$ between particles at positions $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ (this could be a Coulomb interaction for example, $\propto 1/|\boldsymbol{r}_i - \boldsymbol{r}_j|$). Write down the operator $\mathcal{V}$ using momentum representation (ie. where $a^\dagger(\boldsymbol{p})$ acts on the vacuum to create momentum eigenstate $|\boldsymbol{p}\rangle$).

K.E. operator

In the momentum basis, we can write immediately

$$\int d^3p \quad a^\dagger(\underline{p}) \, a(\underline{p}) \quad \frac{p^2}{2m}$$

Position basis

$$\int d^3\underline{x}' \int d^3\underline{x} \quad a^\dagger(\underline{x}) \, a(\underline{x}') \quad \langle x | \frac{\hat{p}^2}{2m} | x' \rangle$$

$$\int d^3\underline{x} \, d^3\underline{x}' \int d^3p \quad a^\dagger(\underline{x}) \, a(\underline{x})$$

$$\langle x | p \rangle \frac{p^2}{2m} \langle p | x' \rangle$$

$$= \int d^3\underline{x} \, d^3\underline{x}' \, a^\dagger(\underline{x}) \, a(\underline{x}) \int \frac{d^3p}{(2\pi\hbar)^3} \, e^{\,i\underline{p}\cdot(\underline{x}-\underline{x}')/\hbar} \quad \frac{p^2}{2m}$$

$$\frac{\hbar^2 \nabla^2}{2m} \int \frac{d^3p}{(2\pi\hbar)^3} \, e^{\,i(\underline{x}-\underline{x}')/\hbar}$$

$$= \frac{\hbar^2}{2m} \int d^3x \; a^\dagger(\underline{x}) \; \nabla^2 \; a(\underline{x})$$

$$\delta(\underline{x} - \underline{x}')$$

Note on the units of a and $a^\dagger$: in the continuous case,

$a^\dagger a$ is the number density operator

$$h(\underline{r}) \; d^3r \; = \; a^\dagger(\underline{r}) a(\underline{r}) \; d^3r.$$

Two body potential $\qquad V(\underline{r}_i, \underline{r}_j)$

$$V = \frac{1}{2} \int d^3p_i \; d^3p_j \; d^3p_n \; d^3p_\ell$$

$$a^\dagger(\underline{p}_i) \; a^\dagger(\underline{p}_j) \; a(\underline{p}_n) \; a(\underline{p}_\ell)$$

$$V_{ijn\ell}$$

$$V_{ijn\ell} = \int d^3 r_1 \, d^3 r_2 \, V(\underline{r}_1, \underline{r}_2)$$

$$\langle p_i | r_1 \rangle \langle r_1 | p_\ell \rangle \langle p_j | r_2 \rangle \langle r_2 | p_n \rangle$$

$$= \int d^3 \underline{r}_1 \, d^3 \underline{r}_2 \, V(\underline{r}_1, \underline{r}_2) \, \frac{1}{(2\pi\hbar)^6}$$

$$e^{\, i \underline{r}_1 \cdot (\underline{p}_\ell - \underline{p}_i)/\hbar} \quad e^{\, i \underline{r}_2 \cdot (\underline{p}_n - \underline{p}_j)/\hbar}$$

assume $V(|\underline{r}_1 - \underline{r}_2|) = V(y)$

$$\underline{r}_2 = \underline{r}_1 + \underline{y}$$

$$\int d^3 \underline{r}_1 \, e^{\, i \underline{r}_1 \cdot (\underline{p}_\ell - \underline{p}_i + \underline{p}_n - \underline{p}_j)/\hbar} \qquad \frac{1}{(2\pi\hbar)^6}$$

$$\int d^3 \underline{y} \, e^{\, i \underline{y} \cdot (\underline{p}_n - \underline{p}_j)/\hbar} \, V(y)$$

$$V_{ijn\ell} = \delta(\underline{p}_\ell + \underline{p}_n - \underline{p}_i - \underline{p}_j)$$

$$\times \underbrace{\int e^{\, i \underline{y} \cdot \underline{q}/\hbar} \, V(y) \, d^3 \underline{y}}$$

$$\tilde{V}(q)$$

$$\underline{q} = \underline{p}_n - \underline{p}_j = \text{momentum transfer.}$$

eg. $V(y) = \dfrac{e^{-\mu y}}{y}$ Screened Coulomb

$\Rightarrow \tilde{V}(q) = \dfrac{4\pi}{q^2 + \mu^2}$

Note that $\underline{p}_n = \underline{p}_j + \underline{q}$

and $\underline{p}_\ell - \underline{p}_i = -\underline{q}$

$\underline{p}_\ell = \underline{p}_i - \underline{q}$

$\Rightarrow V = \dfrac{1}{2} \displaystyle\int d^3 p_i \, d^3 p_j \, d^3 q \; \tilde{V}(\underline{q})$

$$a^\dagger(\underline{p}_i + \underline{q}) \, a^\dagger(\underline{p}_j - \underline{q}) \, a(\underline{p}_j) \, a(\underline{p}_i) \, .$$

Second quantization summary

See notes from last time for solutions.

Particle creation and annihilation operators
$$a, \quad a^\dagger$$

Fermions	Bosons
$\{a_j, a_i^\dagger\} = 1$	$[a_j, a_i^\dagger] = 1$
$\{a_i, a_j\} = 0$	$[a_i, a_j] = 0$

Single particle operator

$$M = \sum_{ij} a_i^\dagger a_j \langle k_i | M | k_j \rangle$$

$\left(a_i^\dagger \text{ adds a particle to } |k_i\rangle \right)$

Pair-wise interaction

$$V = \frac{1}{2} \sum_{ij} V_{ij} \, a_i^\dagger a_j^\dagger a_j a_i$$

The ordering $a_i^\dagger a_j^\dagger a_j a_i$ does the correct accounting —

$i \neq j$ $\qquad \frac{1}{2} a_i^\dagger a_j^\dagger a_j a_i = \frac{1}{2} a_i^\dagger a_i a_j^\dagger a_j$

$$= \frac{1}{2} N_i N_j$$

$i = j$ $\qquad$ bosons $\qquad \frac{1}{2} N_i (N_i - 1)$

$\qquad\qquad$ fermions $\qquad \frac{1}{2} N_i (1 - N_i) = 0$

In a basis where V is not diagonal:

$$V = \frac{1}{2} \sum_{ij\ell n} \underbrace{\langle ij|V|\ell n\rangle}_{V_{ij\ell n}} a_i^\dagger a_j^\dagger a_n a_\ell$$

where

$$V_{ijn\ell} = \sum_{\alpha\beta} V_{\alpha\beta} \langle k_i | m_\alpha \rangle \langle m_\alpha | k_\ell \rangle$$

$$\times \langle k_j | m_\beta \rangle \langle m_\beta | k_n \rangle$$

Continuous examples (see last time)

K.E. $\quad K = \int d^3\underline{p}\; a^\dagger(\underline{p})\, a(\underline{p})\, \dfrac{\underline{p}^2}{2m}$

$$= \int d^3\underline{x}\; a^\dagger(\underline{x})\, a(\underline{x}) \left(\dfrac{-\hbar^2}{2m}\right) \nabla^2$$

units of $\quad a^\dagger(\underline{r})\, a(\underline{r}) \quad$ are $\quad \#$ per unit volume.

Two body potential $\quad V(\,|\underline{r}_2 - \underline{r}_1|\,)$

$$V = \frac{1}{2} \int d^3\underline{p}_i\; d^3\underline{p}_j\; d^3\underline{q}\; \tilde{V}(\underline{q})$$
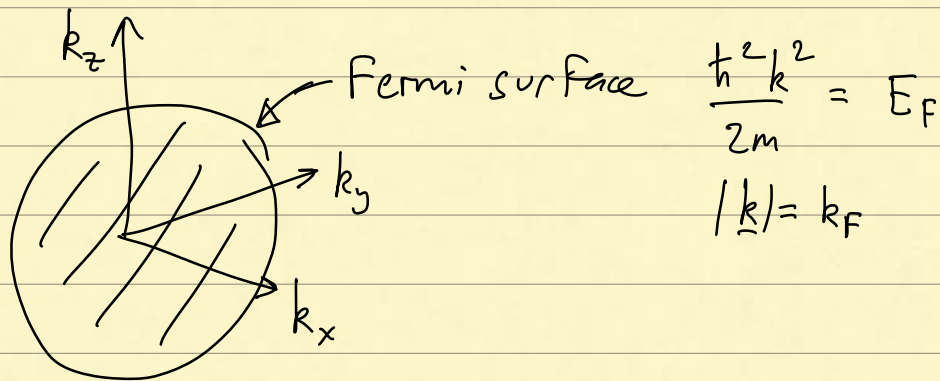
$$a^\dagger(\underline{p}_i + \underline{q})\, a^\dagger(\underline{p}_j - \underline{q})\, a(\underline{p}_j)\, a(\underline{p}_i)$$

eg. Screened Coulomb $\quad V(r) = \dfrac{e^{-\mu r}}{r}$

$$\tilde{V}(\underline{q}) = \dfrac{4\pi}{q^2 + \mu^2}$$

Cooper pairs

Degenerate gas of electrons: fill states up to the Fermi level

Fermi surface $\frac{\hbar^2 k^2}{2m} = E_F$

$|\underline{k}| = k_F$

Consider two electrons just above the fermi surface with an attractive interaction.
(attractive interaction mediated by the positive ions)

Cooper instability — the two electrons have a bound state, no matter how weak the attractive potential!   *

"Cooper pairs" $\longrightarrow$ act as bosons

$\longrightarrow$ macroscopic ground state $\longrightarrow$ Superfluidity
superconductivity

More next time!

* — This is not usually true!

eg. square well has a minimum depth
required for a bound state to exist.

Cooper pairs $\qquad$ (See Tinkham "Introduction to Superconductivity")

Solve the S.E. for a pair of electrons near the Fermi surface with an attractive potential $V(|\underline{r}_2 - \underline{r}_1|)$

$$-\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right)\psi + V\psi = E\psi$$

Take the electrons to have oppositely-directed momenta, since this gives the largest phase space for the outgoing state $\Rightarrow$ strongest interaction.

$\therefore$ with $V = 0$ we would have

$$\psi(\underline{r}_1, \underline{r}_2) \propto e^{i\underline{k}\cdot(\underline{r}_2 - \underline{r}_1)} \propto e^{i\underline{k}\cdot\underline{r}}$$

relative separation

and $E = 2 \times \dfrac{\hbar^2 k^2}{2m} \approx 2E_F$.

With the interaction turned on, write

$$\Psi(\underline{r}_1, \underline{r}_2) = \sum_{\underline{k}} f_{\underline{k}} \, e^{i\underline{k}\cdot\underline{r}}$$

Plug this into the S.E. :

$$\sum_{\underline{k}'} \frac{\hbar^2 k'^2}{m} f_{\underline{k}'} e^{i\underline{k}'\cdot\underline{r}} \quad + \quad V \sum_{\underline{k}'} f_{\underline{k}'} e^{i\underline{k}'\cdot\underline{r}} = E \sum_{\underline{k}'} f_{\underline{k}'} e^{i\underline{k}'\cdot\underline{r}}$$

Now take F.T. :
$$\int e^{-i\underline{k}\cdot\underline{r}} \, d^3\underline{r} \times \left(S.E. \right)$$

giving

$$\frac{\hbar^2 k^2}{m} f_{\underline{k}} \quad + \quad \sum_{\underline{k}'} f_{\underline{k}'} \, \tilde{V}_{\underline{k}\underline{k}'} = E f_{\underline{k}}$$

with $\tilde{V}_{\underline{k}\underline{k}'} = \int e^{i(\underline{k}'-\underline{k})\cdot\underline{r}} \, V(\underline{r}) \, d^3\underline{r}$

$\left(\text{F.T. of the potential} - \text{we also wrote this down} \right.$
$\left. \text{last time, eg. } \tilde{V}(q) = \dfrac{4\pi}{q^2 + \mu^2} \quad \text{for screened Coulomb} \right)$

So we have

$$f_{\underline{k}} = \frac{\sum_{\underline{k}'} V_{\underline{k}\underline{k}'} \, f_{\underline{k}'}}{E - \frac{\hbar^2 k^2}{m}} \qquad \text{——}\circledast$$

Cooper: take $V_{\underline{k}\underline{k}'} = -V_0$

$$\text{for} \quad E_F < \frac{\hbar^2 k^2}{2m} < E_F + \Delta E.$$

eg. electron-phonon interaction

$$V(q, \omega) \sim \frac{e^2}{4\pi\varepsilon_0} \frac{1}{q^2 + p^2} \frac{\omega_q^2}{\omega^2 - \omega_q^2}$$

$V < 0$ for low frequency $\omega < \omega_q$ $\left(\begin{smallmatrix}\text{phonon}\\\text{frequency}\end{smallmatrix}\right)$

The phonon spectrum cuts off at $\omega \sim \omega_D$
$\qquad\qquad\qquad\qquad\qquad$ (Debye frequency)

So we are limited to $\Delta E \lesssim \hbar \omega_D \sim 10^{-3} E_F$.

With $V_{\underline{k}\underline{k}'} = -V_0$, $(\ast) \Rightarrow$

$$\sum_{\underline{k}} f_{\underline{k}} = -V_0 \sum_{\underline{k}} \frac{1}{E - \frac{\hbar^2 k^2}{m}} \cdot \sum_{\underline{k}'} f_{\underline{k}'}$$

$$1 = -V_0 \sum_{\underline{k}} \frac{1}{E - \hbar^2 k^2/m}$$

this is $\approx \int g(E_F) \, d\varepsilon$

$$\Rightarrow \quad \frac{1}{V_0} = \int_{E_F}^{E_F + \Delta E} \frac{g(E_F) \, d\varepsilon}{2\varepsilon - E}$$

$$= \frac{1}{2} g(E_F) \ln \left(\frac{2E_F - E + 2\Delta E}{2E_F - E} \right)$$

$$\Rightarrow \quad E \simeq 2E_F - 2\Delta E \, e^{-2/g(E_F)V_0}$$

$$< 2E_F \quad \Rightarrow \quad \underline{\text{bound state}} \text{ even for}$$

arbitrarily-small V_0.

BCS theory   (Bardeen, Cooper & Schrieffer 1957)

   The argument above shows that the Fermi gas is unstable to the formation of pairs near the Fermi surface. Once pairs condense, the system moves to a new equilibrium. We can explore this using second quantization.

$$H = \sum_{k\sigma} \varepsilon_k \, n_{k\sigma} \quad + \quad \sum_{kk'} V_{kk'} \, c^{\dagger}_{k\uparrow} \, c^{\dagger}_{-k\downarrow} \, c_{-k'\downarrow} \, c_{k'\uparrow}$$

momentum spin

kinetic energy of the electrons

interaction term for pairs with opposite momenta + singlet spin

$$n_{k\sigma} = c^{\dagger}_{k\sigma} \, c_{k\sigma}$$

$\left(\begin{array}{l}\text{Compare what we wrote} \\ \text{last time for the 2-body} \\ \text{potential}\end{array}\right)$

Mean-field approximation:

$$C_{-k\downarrow} \, C_{k\uparrow} \quad = \quad b_k \quad + \quad \left(C_{-k\downarrow} \, C_{k\uparrow} - b_k \right)$$

expectation value
$\langle C_{-k\downarrow} \, C_{k\uparrow} \rangle$

fluctuations
(assume small)

Neglecting quadratic terms in the fluctuations gives the interaction term as

$$\sum_{kk'} V_{kk'} \left(c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger b_{k'} + b_k^\dagger c_{-k'\downarrow} c_{k'\uparrow} - b_k^\dagger b_{k'} \right).$$

Defining the "gap" $\Delta_k = -\sum_{k'} V_{kk'} b_{k'}$

and measuring the energy with respect to the chemical potential μ, $\quad \xi_k = \varepsilon_k - \mu$

gives the "model Hamiltonian"

$$H_M = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma}$$

$$- \sum_k \left(\Delta_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \Delta_k^\dagger c_{-k\downarrow} c_{k\uparrow} - \Delta_k b_k^\dagger \right)$$

Notice that we now have a Hamiltonian that is quadratic only in the c-operators. (We should determine the b_k's self-consistently such that $b_k = \langle c_{-k\downarrow} c_{k\uparrow} \rangle$.)

Bogoliubov – Valatin transformation

Define new operators that are linear combinations
of the c's:

$$\gamma^\dagger_{k_0} = u^*_k\, c^\dagger_{k\uparrow} - v^*_k\, c_{-k\downarrow}$$

$$\gamma^\dagger_{k_1} = u^*_k\, c^\dagger_{-k\downarrow} + v^*_k\, c_{k\uparrow}$$

$$\left(\text{The coefficients satisfy} \quad |u_k|^2 + |v_k|^2 = 1\right)$$

This leads to

$$H_M = \sum_k \left(\xi_k - E_k + \Delta_k\, b^\dagger_k\right) + \sum_k E_k \left(\gamma^\dagger_{k_0}\gamma_{k_0} + \gamma^\dagger_{k_1}\gamma_{k_1}\right)$$

$$\underbrace{\qquad\qquad\qquad}_{\text{g.s.}} \qquad\qquad \underbrace{\qquad\qquad\qquad\qquad}_{\text{excitations}}$$

with $\quad E_k^2 = \xi_k^2 + |\Delta_k|^2 \quad ; \quad \xi_k = \varepsilon_k - \mu$

and $\quad |v_k|^2 = 1 - |u_k|^2 = \dfrac{1}{2}\left(1 - \dfrac{\xi_k}{E_k}\right)$

BCS Ground state

$$|\psi_{GS}\rangle = \prod_k \left(u_k + v_k \, c^\dagger_{k\uparrow} \, c^\dagger_{-k\downarrow} \right) |0\rangle$$

satisfies $\gamma_{k0}|\psi_{GS}\rangle = 0$, $\gamma_{k1}|\psi_{GS}\rangle = 0$.

Notice that this is a sum of terms

$$\left(c^\dagger_{k\uparrow} \, c^\dagger_{-k\downarrow} \right)^n |0\rangle$$

with different numbers of pairs.

More on this next time...

Last time, we ended up with the BCS ground state

$$|\psi_G\rangle = \prod_k \left(u_k + v_k \, c_{k\uparrow}^\dagger \, c_{-k\downarrow}^\dagger \right) |0\rangle$$

Key steps were:
- mean field approximation

$$c_{k\uparrow} \, c_{-k\downarrow} \simeq b_k + \text{fluctuations}$$

self-consistently choose b_k so
that $\langle c_{k\uparrow} \, c_{-k\downarrow} \rangle = b_k$

- Bogliubov transformation

$$\gamma_{k_0}^\dagger = u_k^* \, c_{k\uparrow}^\dagger - v_k^* \, c_{-k\downarrow}$$

$$\gamma_{k_1}^\dagger = u_k^* \, c_{-k\downarrow} + v_k^* \, c_{k\uparrow}$$

Choose u_k and v_k to diagonalise the Hamiltonian.

$$H = \sum_k \left(\xi_k - E_k + \Delta_k \, b_k^\dagger \right) + \sum_k E_k \left(\gamma_{k_0}^\dagger \gamma_{k_0} + \gamma_{k_1}^\dagger \gamma_{k_1} \right)$$
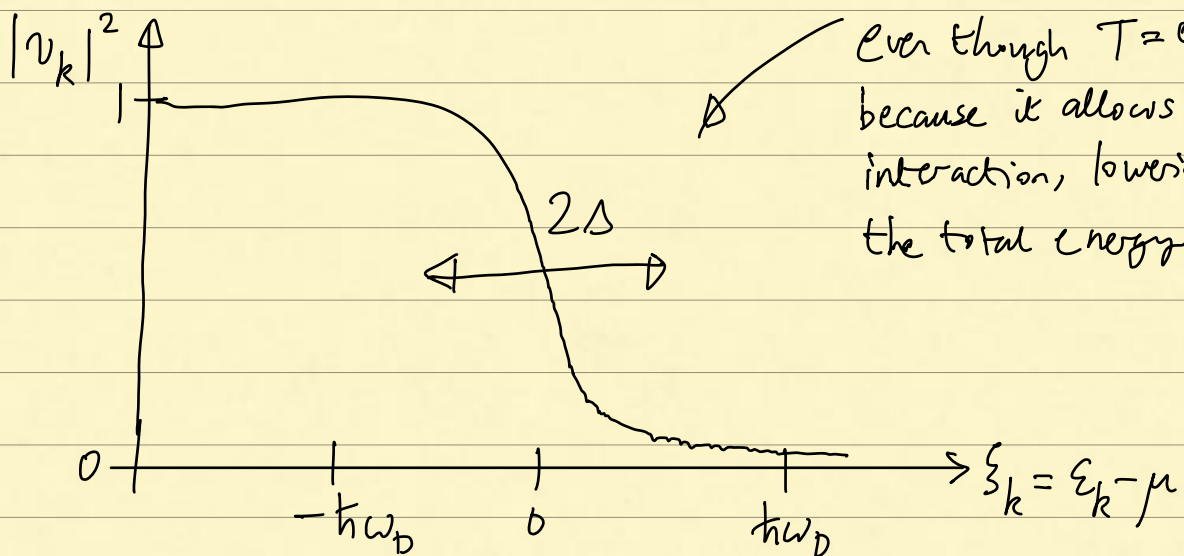
$$|v_k|^2 = 1 - |u_k|^2 = \frac{1}{2}\left(1 - \frac{\xi_k}{E_k}\right) \quad ; \quad \xi_k = \varepsilon_k - \mu$$

$$E_k^2 = \xi_k^2 + |\Delta_k|^2 \quad ; \quad \Delta_k = -\sum_{k'} V_{kk'} b_{k'}$$

The ground state satisfies $\quad \gamma_{k_0} |\psi_G\rangle = 0.$

Occupation numbers:

Fermi surface
is broadened
even though $T=0$
because it allows
interaction, lowering
the total energy

Mean number of paired particles is $\overline{N} = \sum_k 2|v_k|^2$

$$\sigma_N^2 = 4 \sum_k |u_k|^2 |v_k|^2 \quad \Rightarrow \quad \frac{\sigma_N^2}{\overline{N}^2} \sim \left(\frac{\Delta}{E_F}\right)\frac{1}{\overline{N}}$$
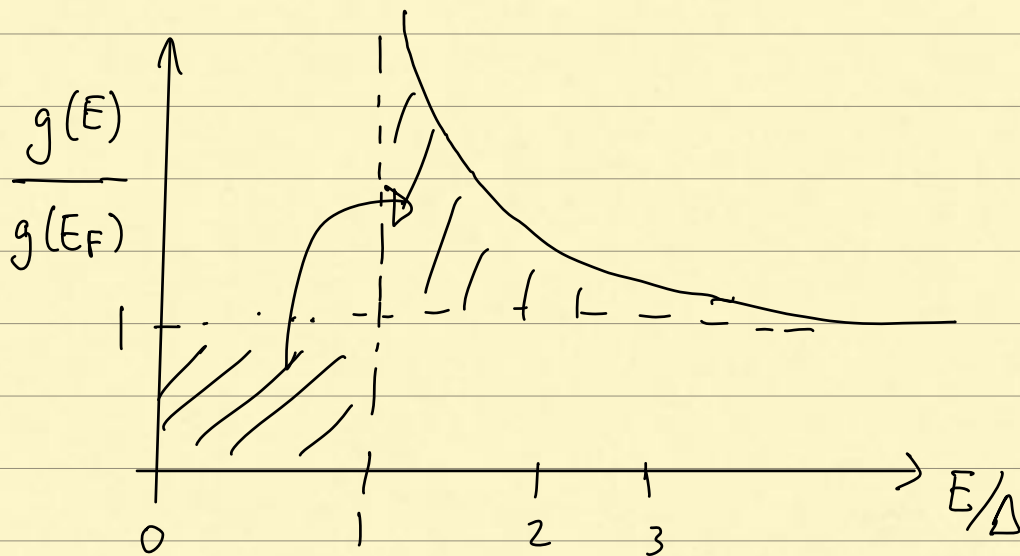
The decrease in energy is

$$-\frac{1}{2}\left(g(E_F)\Delta\right)\Delta \qquad \text{Condensation}$$
$$\text{energy}$$

The pairs overlap with one another

Size of Cooper pair $\sim \dfrac{\hbar}{\Delta p} \sim \dfrac{\hbar}{p}\dfrac{p}{\Delta p}$

$$\sim \dfrac{1}{k_F}\dfrac{E_F}{\Delta} \sim \dfrac{1}{n^{1/3}}\dfrac{E_F}{\Delta}$$

Excited states: minimum excitation energy is Δ
(there is a gap in the energy spectrum)

Klein-Gordon equation

For a non-relativistic free particle,

$$\psi \propto e^{i\underline{p}\cdot\underline{x}/\hbar}\, e^{-iEt/\hbar}$$

then the Schrödinger equation

$$i\hbar\,\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(-i\hbar\underline{\nabla}\right)^2 \psi$$

gives

$$E = \frac{p^2}{2m} \qquad \text{as expected.}$$

For a relativistic particle, we need

$$E^2 = p^2 c^2 + m^2 c^4$$

One option is

$$\left(i\hbar\,\frac{\partial}{\partial t}\right)^2 \psi = c^2\left(-i\hbar\underline{\nabla}\right)^2 \psi + m^2 c^4 \psi$$

$$-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi = -\nabla^2\psi + \left(\frac{mc}{\hbar}\right)^2\psi$$

$$\boxed{\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 + \left(\frac{mc}{\hbar}\right)^2\right]\psi = 0}$$

Klein-Gordon equation.

Points to note:

- this is Lorentz covariant because we can write it in terms of the 4-derivative

$$\partial_\mu = \left(\frac{1}{c}\frac{\partial}{\partial t}, \underline{\nabla}\right)$$

$$g^{\mu\nu}\partial_\nu\partial_\mu = \partial^\mu\partial_\mu = \Box^2 = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2$$

$\Rightarrow$ the Klein-Gordon equation is

$$\left[\partial_\mu\partial^\mu + \left(\frac{mc}{\hbar}\right)^2\right]\psi = 0 \qquad .$$

A reminder about 4-vectors:

contravariant vector   eg. $x^\mu = (ct, \underline{x})$

transforms according to $x'^\mu = \Lambda^\mu_{\ \nu} x^\nu$

$$\Lambda^\mu_{\ \nu} = \begin{pmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

(boost in x-direction)

(if you multiply this out, you'll get the standard Lorentz-transforms for x and t).

covariant vector $x_\mu = g_{\mu\nu} x^\nu$

$g_{\mu\nu}$ = metric tensor

Following Sakurai, we will take
$$g_{\mu\nu} = diag(1, -1, -1, -1)$$

eg. $x_\mu = (ct, -\underline{x})$.

Transforms with $(\Lambda)^{-1}$ rather than Λ.

This means that the inner product $x^\mu x_\mu$ generates a scalar (independent of frame).

eg. energy-momentum $p^\mu = (E/c, \underline{p})$

$$p^\mu p_\mu = g_{\mu\nu} p^\mu p^\nu$$

$$= \frac{E^2}{c^2} - p^2 = (mc)^2.$$

• We can write the free particle plane wave as

$$\psi \propto e^{i\underline{p}\cdot\underline{x}/\hbar} e^{-iEt/\hbar}$$

$$= e^{-ip^\mu x_\mu/\hbar}$$

If you subsititute this into the KG equation, you'll get $E^2 = p^2 c^2 + (mc^2)^2$.

- The lengthscale $\frac{\hbar}{mc}$ is the <u>Compton</u> <u>wavelength</u>

It is the scale on which the confinement energy

$$\frac{p^2}{2m} \sim \frac{\hbar^2}{2mL^2}$$

becomes comparable to the rest mass energy

$$mc^2$$

($\Rightarrow$ potential for particle creation!)

- We can easily incorporate EM fields

$$p^\mu \rightarrow p^\mu - \frac{q A^\mu}{c}$$

where $A^\mu = (\phi, \underline{A})$ $\longleftarrow$ $\begin{bmatrix} \text{cgs units!} \\ \text{In SI} \\ A^\mu = (\phi/c, \underline{A}) \end{bmatrix}$

gives $\frac{E}{c} \rightarrow \frac{E}{c} - \frac{q\phi}{c}$

$$\uparrow$$

electrostatic energy

and $\qquad \underline{p} \longrightarrow \underline{p} - \dfrac{q\underline{A}}{c}$

$\qquad\qquad\qquad\qquad$ canonical momentum.

Furthermore, we can write

$$p_\mu = \left(E/c, -\underline{p} \right)$$

$$= \left(\dfrac{i\hbar}{c} \dfrac{\partial}{\partial t}, + i\hbar \underline{\nabla} \right)$$

$$= i\hbar \left(\dfrac{1}{c} \dfrac{\partial}{\partial t}, \underline{\nabla} \right)$$

$$= i\hbar \, \partial_\mu$$

So if we define $\qquad D_\mu \equiv \partial_\mu + \dfrac{iq}{\hbar c} A^\mu$

then the KG equation is

$$\boxed{ \left[D^\mu D_\mu + \left(\dfrac{mc}{\hbar} \right)^2 \right] \psi = 0 }$$

Last time, we wrote down the Klein-Gordan equation in Lorentz covariant form

$$\left[D^\mu D_\mu + \left(\frac{mc}{\hbar}\right)^2 \right] \psi = 0$$

where

$$D^\mu = \partial^\mu + \frac{iq A^\mu}{\hbar c} \qquad \text{accounts for EM fields.}$$

Free particle $\psi \propto e^{-ip^\mu x_\mu / \hbar}$

This looks promising as a relativistic version of Schrödinger's equation, but there are a number of questions it raises:

1. Negative energy solutions

For a free particle, $E = \pm \sqrt{(pc)^2 + (mc^2)^2}$

$\Rightarrow$ for a given momentum, there are two solutions, one with $E > 0$, one with $E < 0$.

$\left(\text{Compare } E = \frac{p^2}{2m} > 0 \right)$

2. Conservation of probability

In non-relativistic QM,

$$\frac{\partial |\psi|^2}{\partial t} = -\underline{\nabla} \cdot \underline{j}$$

where the probability current

$$\underline{j} = -\frac{i\hbar}{2m} \left[\psi^* \underline{\nabla} \psi - \psi \underline{\nabla} \psi^* \right].$$

Relativistic version: $\quad \partial_\mu j^\mu = 0$

$$j^\mu = \frac{i\hbar}{2m} \left[\psi^* \partial^\mu \psi - \psi \partial^\mu \psi^* \right]$$

Check: $\quad \partial_\mu j^\mu = \frac{i\hbar}{2m} \left[\psi^* \Box^2 \psi - \psi \Box^2 \psi^* \right]$

$$= \frac{i\hbar}{2m} \left[-\psi^* \left(\frac{mc}{\hbar}\right)^2 \psi + \psi \left(\frac{mc}{\hbar}\right)^2 \psi^* \right]$$

$$= 0 \quad \checkmark$$

The time-component gives the probability density

$$\rho = j^0 = \frac{i\hbar}{2mc}\left[\psi^\dagger \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^\dagger}{\partial t}\right].$$

We see that ρ can be negative!

3. The KG equation is second order in time

$\Rightarrow$ we have an initial value problem
where we have to specify both $\psi(t=0)$

and $\dot{\psi}(t=0)$

How to interpret $\dot{\psi}(t=0)$?

The resolution of these questions is to interpret the negative energy solutions as representing <u>antiparticles</u> with opposite charge.

- ρ is charge density

- Specifying ψ and $\dot{\psi}$ at $t=0$ means we have to specify the charge (ie. particle or antiparticle).

ie. there's an extra degree of freedom hiding in the equation that we need to specify.

Looking at the KG equation for a charge q:

$$\frac{1}{c^2}\left(i\hbar\frac{\partial}{\partial t} - \frac{q\phi}{c}\right)^2 \psi = \left(-i\hbar\underline{\nabla} - \frac{q\underline{A}}{c}\right)^2 \psi$$

$$+ m^2 c^2 \psi$$

We see that if ψ is a solution for charge q, then ψ^* '' '' '' '' $-q$.

$$\left[\text{more simply} \quad D_\mu = \partial_\mu - \frac{iqA_\mu}{\hbar c} \quad \text{stays the same}\right.$$

$$\left.\text{if we take} \quad i \rightarrow -i \quad \text{and} \quad q \rightarrow -q \quad\right]$$

It is possible to write the KG equation as two first order equations in time (see Sakurai) which makes explicit the idea that there are two degrees of freedom.

Ultimately, the limitation of a single particle wave equation in relativity is the possibility of particle creation for $E > mc^2$.

$\longrightarrow$ quantum field theory

(relativistic version of second quantization)

We are going to move on to the Dirac equation, which came from attempting to find an equation that is 1st order in time.

As we will see, it contains yet another degree of freedom — particle spin!

Dirac equation

$$\left(i \gamma^\mu \partial_\mu - \frac{mc}{\hbar} \right) \psi = 0$$

- What does γ^μ look like?

$$\left(-i \gamma^\nu \partial_\nu - \frac{mc}{\hbar} \right) \left(i \gamma^\mu \partial_\mu - \frac{mc}{\hbar} \right) \psi = 0$$

$$\Rightarrow \left[\gamma^\nu \partial_\nu \gamma^\mu \partial_\mu + \left(\frac{mc}{\hbar} \right)^2 \right] \psi = 0$$

looks right if $\gamma^\nu \gamma^\mu \partial_\nu \partial_\mu = \partial^\mu \partial_\mu$

$$= \eta^{\mu\nu} \partial_\mu \partial_\nu$$

$$\Rightarrow \left(\gamma^0 \right)^2 = 1 \quad \left(\gamma^i \right)^2 = -1 \qquad (\mu = \nu)$$

$$\gamma^\mu \gamma^\nu = - \gamma^\nu \gamma^\mu \qquad (\mu \neq \nu)$$

A way to write this is

$$\frac{1}{2} \left\{ \gamma^\mu, \gamma^\nu \right\} = \eta^{\mu\nu}$$

The simplest objects that obey this are the set of 4×4 matrices

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad 1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix} \qquad \sigma^i = \text{Pauli matrices}$$

$$\left(\text{ie. } \gamma^0 = \begin{pmatrix} 1 & & & 0 \\ & 1 & & \\ & & -1 & \\ 0 & & & -1 \end{pmatrix}, \quad \gamma^x = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \cdots \right)$$

$\Rightarrow \qquad \psi$ is a 4-component "Spinor"

$$\psi = \begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix} \begin{matrix} \Big\} & \uparrow\downarrow & \text{particle} \\ \\ \Big\} & \uparrow\downarrow & \text{antiparticle} \end{matrix}$$

- Free particle $\qquad P_\mu = i\hbar \partial_\mu$

The Dirac equation becomes

$$(\gamma^\mu P_\mu - mc) \, \psi = 0$$

Components:

$$\gamma^0 \frac{E}{c} - \gamma^i P_i - mc = 0$$

$$E = \underbrace{\gamma^0 \gamma^i}_{\alpha^i} P_i c + \underbrace{\gamma^0}_{\beta} mc^2$$

With the α and β matrices, the Dirac Hamiltonian is

$$H = \underline{\alpha} \cdot \underline{P} \, c + \beta mc^2$$

and we can write

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi \quad \leftarrow \begin{array}{l} (\psi \text{ is a} \\ \text{spinor}) \end{array}$$

- EM fields

As before, we include EM by writing

$$p^\mu \longrightarrow p^\mu - qA^\mu/c$$

eg. $\underline{A} = 0$

$\phi \neq 0$

$$H = \underline{\alpha} \cdot \underline{p} \, c + \beta mc^2 + q\phi$$

eg. relativistic atoms

- Conservation of probability

$$\psi^\dagger \left(i\hbar \frac{\partial \psi}{\partial t} = H\psi \right)$$

$$\psi \left(-i\hbar \frac{\partial \psi^\dagger}{\partial t} = (H\psi)^\dagger \right)$$

$$i\hbar \frac{\partial}{\partial t} (\psi^\dagger \psi) = \psi^\dagger H\psi - \psi (H\psi)^\dagger$$

$$= -\psi^\dagger \underline{\alpha} \cdot i\hbar \underline{\nabla} \psi - \psi \underline{\alpha} \cdot i\hbar \underline{\nabla} \psi^\dagger$$

$$= -i\hbar \underline{\nabla} \cdot (\psi^\dagger \underline{\alpha} \psi)$$

This is in the form

$$\frac{\partial \rho}{\partial t} = -\underline{\nabla} \cdot \underline{j}$$

with

$$\rho = \psi^\dagger \psi$$

$$\underline{j} = \psi^\dagger \underline{\alpha} \psi$$

we are back to a positive-definite probability density!

To write this in covariant form, define

$$\bar{\psi} = \psi^\dagger \gamma^0$$

$$\Rightarrow \quad \rho = \psi^\dagger \psi = \psi^\dagger \gamma^0 \gamma^0 \psi = \bar{\psi} \gamma^0 \psi$$

$$\underline{j} = \psi^\dagger \gamma^0 \gamma^0 \underline{\alpha} \psi$$

$$= \bar{\psi} \gamma^0 \underline{\alpha} \psi = \bar{\psi} \gamma^i \psi$$

So we see that

$$\boxed{j^\mu = \bar{\psi} \gamma^\mu \psi}$$

$$\boxed{\partial_\mu j^\mu = 0} \quad \checkmark$$

Particle in a magnetic field

This is an interesting example, because it reproduces the spin term in the NR Hamiltonian.

Write the wavefunction as

$$\psi = \begin{pmatrix} u \\ v \end{pmatrix}$$

With $\underline{p} - q\underline{A} = \underline{\Pi}$,

the Dirac equation is

$$\begin{pmatrix} mc^2 & c\,\underline{\sigma}\cdot\underline{\Pi} \\ c\,\underline{\sigma}\cdot\underline{\Pi} & -mc^2 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix}$$

lower part: NR limit

$$c\,\underline{\sigma}\cdot\underline{\Pi}\, u - mc^2 v = Ev \approx mc^2 v$$

$$\boxed{\underline{\sigma}\cdot\underline{\Pi}\, u \simeq 2mc\, v}$$

upper part:

$$mc^2 u + c\,\underline{\sigma}\cdot\underline{\pi}\,v = Eu$$

$$mc^2 u + \frac{(\underline{\sigma}\cdot\underline{\pi})^2}{2m} u = Eu$$

We can use the identity
$$(\underline{\sigma}\cdot\underline{\pi})^2 = \left[\pi^2 + i\underline{\sigma}\cdot(\underline{\pi}\times\underline{\pi})\right]$$

(Sakurai Chapter 3)

The cross-product $\underline{\pi}\times\underline{\pi}$ does not vanish because $\underline{\pi}$ contains a gradient:

$$\left(-i\hbar\underline{\nabla} - q\underline{A}\right) \times \left(-i\hbar\underline{\nabla} - q\underline{A}\right) u$$

$$= i\hbar q\left[\underline{\nabla}\times(\underline{A}u) - \underline{A}\times\underline{\nabla}u\right]$$

$$= i\hbar q(\underline{\nabla}\times\underline{A}) u = i\hbar q\,\underline{B}\,u$$

$\Rightarrow$ We arrive at

$$\left(\frac{\pi^2}{2m} - \underline{\mu} \cdot \underline{B} \right) u = (E - mc^2) u$$

$$\underline{\mu} = g \frac{q}{2m} \underline{S}$$

$$2 \qquad \frac{\hbar}{2} \underline{\sigma}$$

The non-relativistic limit knows about spin!

Solutions for a free particle

The Dirac equation is $\qquad \Psi \propto e^{-i p^\mu x_\mu / \hbar}$

$$\begin{pmatrix} mc^2 & \underline{\sigma} \cdot \underline{p} \, c \\ \underline{\sigma} \cdot \underline{p} \, c & -mc^2 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix}$$

First consider a particle at rest $\underline{p} = 0$

then $\quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix}$

has eigenvalues $\quad mc^2, \quad mc^2, \quad -mc^2, \quad -mc^2$

eigenvectors $\qquad \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$

For $\quad \underline{p} = p \, \hat{\underline{z}}$

$$\begin{pmatrix} mc^2 & 0 & pc & 0 \\ 0 & mc^2 & 0 & -pc \\ pc & 0 & -mc^2 & 0 \\ 0 & -pc & 0 & -mc^2 \end{pmatrix} \Psi = E \Psi$$

has eigenvalues $E = +E_p, +E_{p_1}, -E_{p_1}, -E_p$

where $E_p = +\sqrt{(pc)^2 + (mc^2)}$

We can see from the structure of the matrix that the spin up / down components are coupled separately.

eg. look for $\psi = \begin{pmatrix} u \\ 0 \\ v \\ 0 \end{pmatrix}$ with $E = +E_p$

$$mc^2 u + pc\, v = E_p\, u$$
$$pc\, u - mc^2 v = E_p\, v$$
$$pc\, v = (E_p - mc^2) u$$
$$pc\, u = (E_p + mc^2) v$$

set $u = 1$ then $v = \dfrac{E_p - mc^2}{pc} = \dfrac{pc}{E_p + mc^2}$

and $\psi \propto \begin{pmatrix} 1 \\ 0 \\ \dfrac{pc}{E_p + mc^2} \\ 0 \end{pmatrix}$
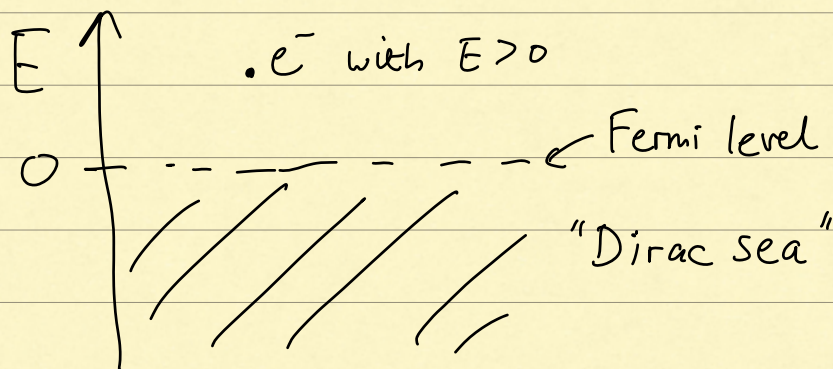
The 4 eigenvectors are

	$E = +E_p$	$E = -E_p$

helicity
$(\underline{\sigma} \cdot \hat{\underline{p}})$

right-handed

$$\begin{pmatrix} 1 \\ 0 \\ \dfrac{pc}{E_p + mc^2} \\ 0 \end{pmatrix} \qquad \begin{pmatrix} \dfrac{-pc}{E_p + mc^2} \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

left-handed

$$\begin{pmatrix} 0 \\ 1 \\ 0 \\ \dfrac{-pc}{E_p + mc^2} \end{pmatrix} \qquad \begin{pmatrix} 0 \\ \dfrac{pc}{E_p + mc^2} \\ 0 \\ 1 \end{pmatrix}$$

$$\left(\text{each has a normalization factor } \frac{2E_p}{E_p + mc^2} \right.$$

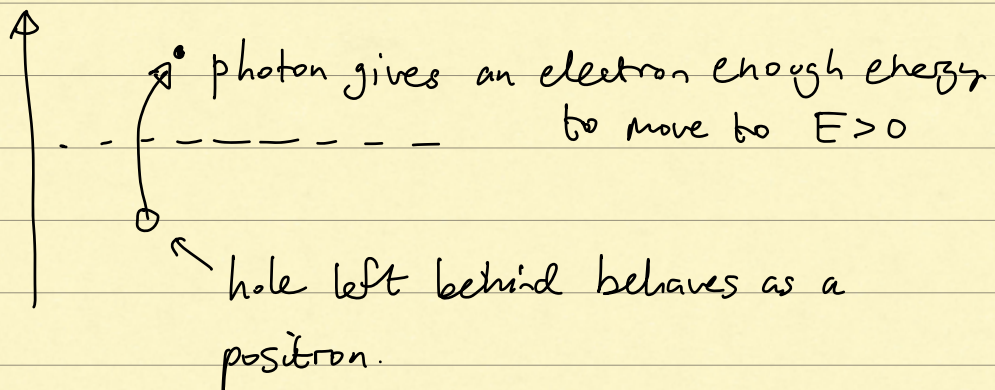$$\left. \text{and is } \propto e^{-ip^\mu x_\mu / \hbar} \right)$$

Measure "spin up / spin down" with respect to the
momentum direction
    "Helicity" $\underline{\Sigma} \cdot \hat{\underline{p}} = \begin{pmatrix} \underline{\sigma} \cdot \hat{\underline{p}} & 0 \\ 0 & \underline{\sigma} \cdot \hat{\underline{p}} \end{pmatrix}$

Dirac's interpretation of negative energy solutions:
they are occupied by a sea of electrons which
prevents electrons with $E > 0$ from lowering their
energy by moving to $E < 0$.

E ↑

. e^- with $E > 0$

0 — — — — — — — ← Fermi level

"Dirac sea"

Positrons are "holes" left by promoted electrons

photon gives an electron enough energy
to move to $E > 0$

hole left behind behaves as a
positron.

This interpretation seems problematic, what about
bosons for example?

Feynman – Stückelberg : interpret negative energy solutions going backwards in time $(\underline{p} \to -\underline{p})$ as equivalent to positive energy antiparticles going forwards in time
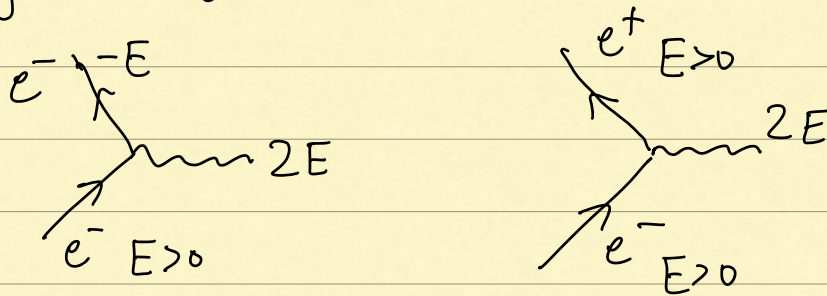
Charge conjugation

$$\gamma^\mu \left(\partial_\mu + \frac{igA_\mu}{\hbar c} \right) \psi + \frac{imc}{\hbar} \psi = 0$$

$$-i\gamma^2 \times (c.c.)$$

$$\overset{R}{\curvearrowleft} \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix}$$

gives

$$-i\gamma^2 \gamma^{\mu*} \left(\partial_\mu - \frac{igA_\mu}{\hbar c} \right) \psi^* - \frac{imc}{\hbar} \left(-i\gamma^2 \psi^* \right)$$

$$= 0$$

But $\gamma^{0*} = \gamma^0$, $\gamma^{1*} = \gamma^1$, $\gamma^{2*} = -\gamma^2$

$\gamma^{3*} = \gamma^3$

and $\gamma^\mu \gamma^\nu = -\gamma^\nu \gamma^\mu$ $\quad \mu \neq \nu$

$\Rightarrow$

$$\gamma^2 \gamma^{\mu*} = -\gamma^\mu \gamma^2$$

$\Rightarrow \quad \gamma^\mu \left(\partial_\mu - \frac{iqA_\mu}{\hbar c} \right) \left(i\gamma^2 \psi^* \right) + \frac{imc}{\hbar} \left(i\gamma^2 \psi^* \right) = 0$

ie.   if ψ satisfies the Dirac equation for a charge q, then $\left(i\gamma^2 \psi^* \right)$ satisfies the Dirac equation for $-q$.

    (particle $\rightarrow$ antiparticle)

Check the free particle solutions:

$$i\gamma^2 = i \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

eg. $\quad i\gamma^2 \begin{pmatrix} 1 \\ 0 \\ \dfrac{pc}{E_p + mc^2} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \dfrac{-pc}{E_p + mc^2} \\ 0 \\ 1 \end{pmatrix}$

changes right-handed $\longrightarrow$ left-handed
particle $\qquad\qquad$ antiparticle

$\propto e^{-ip^\mu x_\mu / \hbar} \qquad\qquad \propto e^{+ip^\mu x_\mu / \hbar}$