Contents

Chapter 1

Week 1

1.1 Monday, 28 Mar 2016

1.1.1 Transition from classical mechanics to QM

Define the variational derivative:

$$\frac{\delta S}{\delta x(t')} = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left\{ S\left[x(t) + \epsilon \delta(t - t')\right] - S[x(t)] \right\}$$

1.1.2 Saddle point method

Consider the integral:

$$I = \int_{-\infty}^{\infty} dy e^{-f(y)/\epsilon}$$

which is dominated by the value of the exponential around the minimum value of $f(y)$. That is, we can write:

$$f(y) = f(y_0) + \frac{1}{2}(y - y_0)^2 f''(y_0) + \dots$$

$$\begin{aligned} \implies I &\approx \int_{-\infty}^{\infty} dy e^{-[f(y_0) + \frac{1}{2}(y-y_0)^2 f''(y_0)]/\epsilon} \\ &= e^{-f(y_0)/\epsilon} \sqrt{\frac{2\pi\epsilon}{f''(y_0)}} \end{aligned}$$

1.1.3 The Path Integral

$$U(x_f, t_f; x_i, t_i) = \int_{x(t_i)=x_i, x(t_f)=x_f} \mathcal{D}(t) \exp\left(\frac{i}{\hbar} S[x(t)]\right)$$

1.2 Wednesday, 30 Mar 2016

1.2.1 Free particle path integral formalism

Consider a free particle moving from (t_0, x_0) to (t_N, x_N) and split the time intervals into discrete slices with time interval length $\epsilon = \frac{t_N - t_0}{N}$. Then we write the propagator:

$$\begin{aligned} U(t_N, x_N; t_0, x_0) &= \int_{\text{paths}, x_0 \to x_N} \mathcal{D}[x] \exp\left(\frac{i}{\hbar} S[x]\right) \\ &= \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \mathcal{D}[x] \exp\left(\frac{i}{\hbar} \sum_{i=0}^{N-1} \frac{m}{2} \frac{(x_{i+1} - x_i)^2}{\epsilon}\right) \end{aligned}$$

Move into dimensionless variables:

$$y_i = \sqrt{\frac{m}{2\hbar\epsilon}} x_i$$

Then the exponential factor simplifies to:

$$\exp\left(\frac{i}{\hbar}\sum_{i=0}^{N-1}\frac{m}{2}\frac{(x_{i+1}-x_i)^2}{\epsilon}\right) = \prod_{i=0}^{N-1}\exp\left(\frac{-(y_{i+1}-y_i)^2}{i}\right)$$

Observe that a single Gaussian integral has the form (only including terms that contain y_n):

$$\int_{-\infty}^{\infty} dy_n \exp\left[-\frac{1}{i}\left((y_{n+1}-y_n)^2+(y_n-y_{n-1})^2\right)\right]$$

We use the Gaussian integral identity:

$$\int_{-\infty}^{\infty} e^{ax^2+bx+c}dx = \sqrt{\frac{\pi}{-a}}e^{-b^2/4a+c}$$

so that the single Gaussian integral becomes:

$$\int_{-\infty}^{\infty} dy_n \exp\left[-\frac{1}{i}\left((y_{n+1}-y_n)^2+(y_n-y_{n-1})^2\right)\right] = \sqrt{\frac{i\pi}{2}}\exp\left(-\frac{(y_{n+1}-y_{n-1})^2}{2i}\right)$$

Observe that the integration of a single x_n variable resulted in a pre-factor of $\sqrt{\frac{i\pi}{2}}$ and an additional value of 2 in the denominator of the exponent. It is possible to prove via induction that:

$$\iiint \exp\left(-\sum_{i=0}^{N-1}\frac{(y_{i+1}-y_i)^2}{i}\right)dx_1dx_2\cdots = \frac{(i\pi)^{(N-1)/2}}{N^{1/2}}e^{-(y_N-y_0)^2/Ni}$$

Observe that $N=2$ corresponds to the single Gaussian integral case. We may hence write the propagator as (with normalization constant A):

$$\begin{aligned}U &= A\left(\frac{2\pi\hbar\epsilon i}{m}\right)^{N/2}\left(\frac{m}{2\pi\hbar i N\epsilon}\right)^{1/2}\exp\left(\frac{im(x_N-x_0)^2}{2\hbar N\epsilon}\right)\\ &= A\left(\frac{2\pi\hbar(t_N-t_0)i}{mN}\right)^{N/2}\left(\frac{m}{2\pi\hbar i(t_N-t_0)}\right)^{1/2}\exp\left(\frac{im(x_N-x_0)^2}{2\hbar(t_N-t_0)}\right)\end{aligned}$$

Recall that the free particle propagator was obtained previously as:

$$U = \sqrt{\frac{m}{2\pi\hbar i(t_N-t_0)}}\exp\left(\frac{im(x_N-x_0)^2}{2\hbar(t_N-t_0)}\right)$$

which has the same exponential dependence. We hence observe that the normalization coefficient is:

$$A = \left(\frac{2\pi\hbar\epsilon i}{m}\right)^{-N/2}$$

1.2.2 1D path integral mathematical representation

We may hence define the normalized interpretation of the "sum over paths":

$$\iiint \mathcal{D}[x] \equiv \lim_{\epsilon\to 0}\frac{1}{B}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\frac{dx_1}{B}\frac{dx_2}{B}\cdots\frac{dx_{N-1}}{B}$$

where $B = \sqrt{\frac{2\pi\hbar\epsilon i}{m}}$.

1.2.3 Soluble systems using path integrals

Consider systems with Lagrangians of the form:

$$\mathcal{L} = \frac{1}{2}m\dot{x}^2 - V$$

where V is quadratic in x or lower:

$$V(x) = a + bx + cx^2 + d\dot{x} + ex\dot{x}$$

where we merge the $\dot{x}^2$ term into the kinetic term. Then the action can be written in the quadratic plus linear form:

$$S[x] = \sum_{i,j} X_i K_{ij} X_j + \sum_j J_i X_i + \text{constant}$$

K_{ij} is just a matrix made of numbers. Observe that we can also make a change of variables (more specifically: a rotation) such that the coupling matrix K_{ij} is diagonal:

$$X_i = \sum_j R_{ij} Y_j, \quad J'_i = \sum_j J_j R_{ji}$$
$$\sum_{j,k} R^T_{ij} K_{jk} R_{kl} = K_i \delta_{il}$$

The propagator in this basis is easy to calculate since the coupling matrix is diagonal:

$$U \sim \int dy_1 \cdots dy_{n-1} \exp\left[i \left(\sum_i y_i^2 K_i + J'_i y_i + \text{const.} \right) \right] \sim \exp\left(-i \sum_i \frac{(J'_i)^2}{4K_i} \right)$$

The parameters y_i are decoupled, which makes the Gaussian integral trivial.

1.2.4 Relation to stationary phase approximation (saddle point approximation)

Note that the saddle point approximation is exact for Gaussian integrals (exponential is purely quadratic anyway). Taking the analogue of the 1D stationary phase integral, we may write the propagator as:

$$U(x_f, t_f; x_i, t_i) = A' e^{iS[x_{cl}(t)]/\hbar}$$

since the dominant component of the stationary phase approximation was the exponential part $I \sim e^{-f(y_0)}$. Hence it will suffice to find the classical path, calculate the action for that path, then use it to obtain the propagator. Note that this process is only guaranteed to work exactly for quadratic or lower potentials.

We verify this approximation for the free particle. Recall that the classical path can be parametrized:

$$x_{cl}(t) = x_i + \frac{x_f - x_i}{t_f - t_i}(t - t_i)$$

and the action becomes:

$$S[x_{cl}(t)] = \frac{m}{2}\frac{(x_f - x_i)^2}{t_f - t_i}$$

giving the exponential dependence as:

$$U(x_f, t_f; x_i, t_i) = A' \exp\left(\frac{im}{2\hbar}\frac{(x_f - x_i)^2}{t_f - t_i} \right)$$

matching that obtained for the full path integral calculation.

1.3 Friday 1 Apr 2016

1.3.1 Equivalence of Path Integral formalism to Schrodinger's Equation - Forward path

Consider a small timestep ϵ. Then we want to show that (to first order):

$$\psi(x,\epsilon) - \psi(x,0) = -\frac{i\epsilon}{\hbar}\hat{H}\psi(x,0)$$

which is equivalent to the Schrodinger equation upon exponentiation.

Observe that the propagator from x' to x over the timestep can be approximated as:

$$U(x,\epsilon;x',0) = \sqrt{\frac{m}{2\pi\hbar i\epsilon}}\exp\left(\frac{i}{\hbar}\left[\frac{m}{2}\frac{(x-x')^2}{\epsilon} - \epsilon V(\frac{x+x'}{2},0)\right]\right)$$

Changing variables to $\eta = x' - x$, we want to integrate over all possible initial positions to obtain:

$$\psi(x,\epsilon) = \sqrt{\frac{m}{2\pi\hbar i\epsilon}}\int_{-\infty}^{\infty}\exp\left(\frac{i}{\hbar}\left[\frac{m}{2}\frac{\eta^2}{\epsilon} - \epsilon V(x+\frac{\eta}{2},0)\right]\right)\psi(x',0)$$

Proceed by the stationary phase approximation. Note that the phases will add constructively provided $\frac{\eta^2}{\epsilon}$ is of order unity. Hence to expand to order ϵ, we have to do the expansion in η to second order. This gives:

$$\exp\left(-\frac{i\epsilon}{\hbar}V(x+\frac{\eta}{2},0)\right) \approx 1 - \frac{i\epsilon}{\hbar}V(x,0), \quad \text{to order } \epsilon$$

and:

$$\psi(x,\epsilon) = \sqrt{\frac{m}{2\pi\hbar i\epsilon}}\int_{-\infty}^{\infty}d\eta\exp\left(\frac{i}{2\hbar\epsilon}m\eta^2\right)\left[\psi(x',0) + \eta\frac{\partial\psi}{\partial x} + \frac{\eta^2}{2}\frac{\partial^2\psi}{\partial x^2}\right] - \frac{i\epsilon}{\hbar}V(x',0)\psi(x',0)dx'$$

After doing the Gaussian integrals, we obtain the first order representation of the TDSE:

$$\frac{i\hbar}{\epsilon}\left[\psi(x,\epsilon) - \psi(x,0)\right] = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,0)\right)\psi(x,0)$$

1.3.2 Reverse process - Schrodinger equation to Path Integrals

Recall that the propagator is the position representation of the unitary evolution operator and using the Schrodinger equation, we can write it as an operator exponential. Do an expansion of the exponential operator:

$$e^{-i\hat{H}t/\hbar} = \left(e^{-i\hat{H}t/N\hbar}\right)^N$$

and define $\epsilon = \frac{t}{N}$. Do a first order approximation:

$$\hat{H} = \frac{p^2}{2m} + V(x) \implies e^{-iH\epsilon/\hbar} \approx \exp\left(\frac{-ip^2\epsilon}{2m\hbar}\right)\exp\left(-\frac{i}{\hbar}V(x)\epsilon\right)$$

where we recall that:

$$e^Ae^B = e^{A+B}e^{\alpha/2} = e^Be^Ae^\alpha$$

if $\alpha = [A,B] \in \mathbb{C}$. If the time interval ϵ is small enough, then the commutator is negligible and we can neglect it. Now insert position basis resolutions of the identity in between pairs of exponentials:

$$U(x,t;x',0) = \langle x|e^{-ip^2\epsilon/2m\hbar}e^{-iV\epsilon/\hbar}\int dx''|x''\rangle\langle x''|e^{-ip^2\epsilon/2m\hbar}e^{-iV\epsilon/\hbar}\cdots|x'\rangle$$

We let the potential exponential (written in the position basis) act on the position eigenstate so that we can replace the position operator with the eigenvalue. We are hence interested in the momentum term:

$$\langle x_n | e^{-ip^2\epsilon/2m\hbar} | x_{n-1} \rangle$$

which we realize is just the free particle propagator between the two positions. This can be calculated by the usual means.

$$\langle x_n | e^{-ip^2\epsilon/2m\hbar} | x_{n-1} \rangle = \sqrt{\frac{m}{2\pi i\hbar\epsilon}} \exp\left(\frac{-im}{2\hbar} \frac{(x_n - x_{n-1})^2}{\epsilon} \right)$$

Combining all the exponentials and noting that the integration is performed over all intermediate positions, we obtain the path integral representation.

Chapter 2

Week 2

2.1 Monday, 4 Apr 2016

2.1.1 Imaginary Time Formalism

This is the analytic continuation of the time parameter:

$$t \to -i\tau$$

where τ is called the imaginary time/Euclidean time. Note that this just rotates time clockwise by a right angle so that the imaginary time runs down the complex axis from positive complex part to negative complex part. The unitary time evolution operator becomes:

$$U(\tau) = e^{-H\tau/\hbar}$$

We can diagonalize the evolution operator as per usual, calling this the **Imaginary Time Propagator**:

$$U(\tau) = \sum_n |n\rangle\langle n| e^{-E_n\tau/\hbar}$$

Note that this propagator is not unitary! $U(\tau)^\dagger U(\tau) \neq \mathbf{1}$. The exponential of a Hermitian matrix (i.e. the Hamiltonian) is just a Hermitian matrix. In the usual propagator, the exponential of a Hermitian matrix *multiplied by* i is unitary.

Consider the late τ propagator, that is $U(\tau \to \infty)$. Observe that the larger E_n is, the more exponentially damped the term in the Imaginary time propagator is. Hence at late imaginary times, the propagator just becomes:

$$U(\tau \to \infty) \propto |0\rangle\langle 0| e^{-E_0\tau/\hbar}$$

This looks like the Boltzmann factor in statistical mechanics. Anyway, this gives a method of finding the ground state of a complicated system. Just take any state then evolve it forward in time to late time with the imaginary time Hamiltonian, which will project that state onto the ground state wavefunction.

2.1.2 Imaginary time and path integrals

Consider the propagator for the imaginary time:

$$U(x, x', \tau) = \langle x|U(\tau)|x'\rangle$$

We want to evaluate the RHS using the path integral. Hence we need to consider what it means to analytically continue the path integral. Recall that time features in the path integral through the action:

$$S[x] = \int dt \mathcal{L}(x, \dot{x}) = \int dt \left[\frac{1}{2}m\dot{x}^2 - V(x)\right]$$

We make the substitution $t \to -i\tau, dt \to -id\tau$. This gives us:

$$S[x] = -i \int d\tau \left[-\frac{1}{2} m \left(\frac{dx}{d\tau} \right)^2 - V(x) \right] = i \int d\tau \left[\frac{1}{2} m \left(\frac{dx}{d\tau} \right)^2 + V(x) \right]$$

Observe that the integrand looks like the Hamiltonian (multiplied by i)! But we will call the action-equivalent the **Euclidean action**:

$$\mathcal{L}_E = \frac{1}{2} m \left(\frac{dx}{d\tau} \right)^2 + V(x)$$
$$\int \mathcal{L} dt = i \int \mathcal{L}_E d\tau$$

Then the path integral terms become:

$$U(x, x', \tau) = \int_{x'}^{x} [dx] \exp\left(-\frac{1}{\hbar} \int d\tau \mathcal{L}_E \right)$$

We should think of $\mathcal{L}_E$ as a Lagrangian with a flipped potential sign.

2.1.3 Example: Quantum Harmonic Oscillator and imaginary time

Transform the QHO propagator using the imaginary time substitution:

$$U(x, x', \tau) = A(\tau) \exp\left[-\frac{m\omega}{2\hbar \sinh \omega\tau} \left[(x^2 + (x')^2 \cosh \omega\tau - 2xx' \right] \right]$$

We expect that at late times, this propagator should be the outer product of two ground state kets $|0\rangle\langle 0|$. Then the hyperbolic exponentials just approach $e^{\omega\tau}$, giving:

$$U(x, x', \tau \to \infty) = A(\tau) \exp\left(-\frac{m\omega(x^2 + (x')^2)}{2\hbar} \right)$$

and indeed it is the product of two harmonic oscillator ground states $\langle x|0\rangle\langle 0|x'\rangle$.

2.1.4 Application to tunneling

Consider the potential $V(x) = \lambda(x^2 - a^2)^2$ which has two minima at $x = \pm a$. We model the system using a two-state system with Hamiltonian:

$$H = \begin{pmatrix} 0 & \Delta \\ \Delta & 0 \end{pmatrix}$$

where we span the space using $|a\rangle, |-a\rangle$, the states where the particle is at $x = a, -a$ respectively. We let their energies be equal. Note that these are not eigenstates of the Hamiltonian since the Hamiltonian contains a small off-diagonal term representing the coupling between the states. The true eigenstates are:

$$|\Omega_\pm\rangle = \frac{1}{\sqrt{2}} \left(|a\rangle \pm |-a\rangle \right)$$
$$H|\Omega_\pm\rangle = E_\pm |\Omega_\pm\rangle, \quad E_\pm = \pm\Delta$$

Δ parametrizes the rate with which the particle transits across the barrier. Note that we can find Δ by calculating the matrix element:

$$\Delta = \langle a|H|-a\rangle$$

We want to use the path integral with imaginary time formalism to compute Δ.

$$\begin{aligned}\langle a|e^{-H\tau/\hbar}|-a\rangle &= \langle a|-a\rangle - \frac{\tau}{\hbar}\langle a|H|-a\rangle + O(\tau^2)\\ &\approx -\frac{\tau}{\hbar}\langle a|H|-a\rangle, \quad \langle a|-a\rangle = 0\end{aligned}$$

We hence want the propagator since we can extract Δ by taking the first order approximation to the propagator at small imaginary time. We proceed using the saddle point approximation, which is exact for potentials of order two and lower. In this case, the potential is of order 4, hence the approximation is not exact. Then:

$$U(a,-a,\tau) \propto e^{-S_{cl,E}/\hbar}$$

where $S_{cl,E}$ is the classical Euclidean action for the transition. But there does not appear to be a classical path across the barrier! But we must remember that the Euclidean action flips the sign of the potential, so the barrier changes sign. There is indeed a classical solution now.

2.2 Wednesday, 6 April 2016

2.2.1 Tunnelling continued - Computing the Euclidean action

Recall that we can invert the sign of the potential to calculate the Euclidean action. We hence want to solve the equation of motion explicitly:

$$\mathcal{L}_E = \frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x)$$

and we proceed by energy methods. The total energy (note that the previous expression was treated as a Lagrangian) is:

$$E = \frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 - V(x)$$

and we consider energies where $E \approx 0$ so that the particle just begins to roll from $x = -a$ to $x = +a$. We hence proceed by quadrature:

$$\begin{aligned}\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 &= V(x)\\ \implies \int_0^\tau d\tau = \int_{-a}^{a}\sqrt{\frac{m}{2V(x)}}dx &= \int_{-a}^{a}\sqrt{\frac{m}{2\lambda(x^2-a^2)^2}}dx\\ \implies \tau &= \frac{1}{a}\sqrt{\frac{m}{2\lambda}}\tanh^{-1}\frac{x}{a}\\ \implies x(\tau) &= a\cdot\tanh\left(\sqrt{\frac{2\lambda}{m}}a(\tau+\text{const.})\right)\end{aligned}$$

Define the characteristic time:

$$\sqrt{\frac{2\lambda}{m}}a \equiv \frac{1}{\Delta\tau}$$

Also pick const.=0. Now we can substitute the trajectory into the Euclidean action and integrate to find S_E and hence $e^{-\frac{1}{\hbar}S_E}$ and hence obtain the imaginary time propagator using the saddle point approximation. However, there is an easier way. Observe that:

$$S_E = \int d\tau(T+V)$$

But we know that $T - V = 0$ using the total energy. Hence:

$$S_E = \int d\tau 2T = \int d\tau 2 \cdot \frac{1}{2} m \left(\frac{dx}{d\tau}\right)^2 = m \int d\tau \frac{dx}{d\tau}\frac{dx}{d\tau} = m \int dx \frac{dx}{d\tau} = \int dx \cdot p(x) = \int dx \cdot \sqrt{2mV(x)}$$

This allows us to write the imaginary time propagator as:

$$\langle a|U|-a\rangle \propto \exp\left(-\frac{1}{\hbar}\int_{-a}^{a} \sqrt{2mV(x)}dx\right)$$

But this is very similar to the (J)WKB approximation for the tunnelling integral!
Note also that the proportionality factor is linear in τ. Then the off-diagonal component, which is the coefficient of the term linear in τ for the propagator, can be calculated as:

$$\Delta = \langle a|H|-a\rangle \propto \exp\left(-\frac{1}{\hbar}\int_{-a}^{a} \sqrt{2mV(x)}dx\right)$$

Justification for the proportionality factor Recall that we can write in the saddle point approximation:

$$I = \int_{-\infty}^{\infty} dy e^{-f(y)/\epsilon} \approx e^{-f(y_0)/\epsilon}\sqrt{\frac{2\pi\epsilon}{f''(y_0)}}$$

Similarly, we write the propagator as:

$$\begin{aligned} U &= \int [dx] e^{-\frac{1}{\hbar}S[x]} \\ &= e^{-\frac{1}{\hbar}S[x_{cl}]} \int [dy] e^{-\frac{1}{\hbar}S[x_{cl}+y]} \end{aligned}$$

where we introduce the small perturbations:

$$y(\tau) = x(\tau) - x_{cl}(\tau)$$

We will find that the integral term will be proportional to τ.

2.2.2 Imaginary Time Formalism and Statistical Mechanics

Recall that the canonical partition function is:

$$Z(\beta) = \sum_n e^{-\beta E_n} = \langle n|e^{-\beta H}|n\rangle = \mathrm{Tr}(e^{-\beta H}) = \int_{-\infty}^{\infty} dx \langle x|e^{-\beta H}|x\rangle$$

which is precisely the imaginary time propagator that has the same start and end points with time interval $\beta\hbar$. Hence we can write:

$$Z(\beta) = \int_{-\infty}^{\infty} dx_0 U(x_0, x_0, \beta\hbar)$$

where x_0 is just a coordinate in space, not a path integral integrand. We can write the propagator in imaginary time path integral notation:

$$Z = \int_{-\infty}^{\infty} dx_0 \int_{x_0}^{x_0} [dx] \exp\left(-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + V(x)\right]\right)$$

Verifying classical limit Note that the higher temperature limit corresponds to $\beta\hbar \to 0$, which is the short time limit in this path integral case. We may hence approximate the integral as the value of the integrand multiplied by the short time interval:

$$\exp\left(-\frac{1}{\hbar}\int_0^{\beta\hbar}\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 d\tau\right) \approx \exp\left(-\frac{1}{\hbar}\frac{m}{2}\frac{\Delta x^2}{\Delta\tau}\right) = e^{-(\frac{\Delta x}{\sqrt{\beta/m\hbar}})^2}, \quad \Delta\tau = \beta\hbar/2$$

Define the thermal wavelength:

$$\Delta x_{th} \equiv \sqrt{\frac{\beta}{m}}\hbar$$

Assume that the potential does not vary much over the thermal wavelength so that we can replace it with the potential value at x_0.

Chapter 3

Week 3

3.1 Monday, 11 Apr 2016

3.1.1 EPR Paradox

Consider a spinless particle that decays into two spin-half particles which go off into opposite directions. The state of the system (which has total angular momentum zero) can be written as the singlet spin state:

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

Suppose Alice measures either σ_x or σ_z. Then let Bob measure either σ_x or σ_z. Proceed in absolute generality. Let the combined wavefunction be written as the superposition of product kets:

$$|\psi\rangle = \sum_{a,b} \psi_{ab} |a\rangle |b\rangle$$

Let Alice measure along an arbitrary axis (or more generally, observe an arbitrary observable). Let an eigenstate of that observable be written as:

$$|\alpha\rangle = \sum_a U_{\alpha a} |a\rangle$$

where U is a unitary transformation relating the representation of the observable eigenstates in terms of the initial eigenstates. Define $P(b, \alpha)$ as the probability that B measures b and A measures α. Note that B measures $|b\rangle$, that is, an observable corresponding to the initial eigenstate representation. Then:

$$P(b, \alpha) = \left| \langle \alpha | \langle b | \cdot \sum_{a',b'} \psi_{a'b'} |a'\rangle |b'\rangle \right|^2$$

The individual components are:

$$\langle \alpha | a' \rangle = \sum_a U_{\alpha a} \delta_{aa'} = U_{\alpha a'}$$
$$\langle b | b' \rangle = \delta_{bb'}$$

so that the probability is given by:

$$P(b, \alpha) = \left| \sum_a U_{\alpha a} \psi_{ab} \right|^2$$

Then the EPR paradox stated mathematically is that this probability depends on both b and α. However, the loophole is that Alice cannot pick what the outcome of α is, although she is allowed to pick what observable to measure. Then, we need to sum over all possible outcomes for α. Then:

$$
\begin{aligned}
P(b) &= \sum_{\alpha} P(b,\alpha) \\
&= \sum_{\alpha} \left| \sum_{a} U_{\alpha a}\psi_{ab} \right|^2 \\
&= \sum_{\alpha}\sum_{a}\sum_{a'} \left(U_{\alpha a}\psi_{ab}\right)\left(U_{\alpha a'}\psi_{a'b}\right)^* \\
&= \sum_{\alpha}\sum_{a}\sum_{a'} U_{\alpha a}\psi_{ab}U^*_{\alpha a'}\psi^*_{a'b} \\
&= \sum_{a}\sum_{a'}\left(\sum_{\alpha} U^\dagger_{a'\alpha}U_{\alpha a}\right)\psi^*_{a'b}\psi_{ab} \\
&= \sum_{a}\sum_{a'} \delta_{a'a}\psi^*_{a'b}\psi_{ab} \\
&= \sum_{a} |\psi_{ab}|^2
\end{aligned}
$$

which does not depend on alpha, that is, the probability that B measures any particular eigenstate does not depend on what A has done. This implies that no signal is sent in terms of the choice that A made.

3.2 Wednesday, 13 April 2016

3.2.1 Bell's Inequalities

Let the measurements performed by A and B be represented as:

$$\vec{S}_A \cdot \hat{a}$$
$$\vec{S}_B \cdot \hat{b}$$

2-axis case Consider two axes $\hat{a}, \hat{b}$ where each of these are arbitrary. We want to calculate the expectation value of the product:

$$\langle (\vec{S}_A \cdot \hat{a})(\vec{S}_B \cdot \hat{b}) \rangle$$

By momentum conservation, we know that:

$$\vec{S}_A + \vec{S}_B = 0$$

because the initial particle had zero spin. Hence the expectation can be written as:

$$-\langle (\vec{S}_A \cdot \hat{a})(\vec{S}_A \cdot \hat{b}) \rangle$$

Recall that for Pauli matrices, the following identities hold:

$$(\vec{\sigma}\cdot\vec{v})\cdot(\vec{\sigma}\cdot\vec{w}) = \vec{1}\vec{v}\cdot\vec{w} + i(\vec{v}\times\vec{w})\cdot\vec{\sigma}$$

where $\vec{\sigma}$ is a vector of 2x2 Pauli matrices. Then we simplify the expectation (and take into account the spin-half scaling coefficient):

$$
\begin{aligned}
-\langle (\vec{S}_A \cdot \hat{a})(\vec{S}_A \cdot \hat{b}) \rangle &= -\left[\vec{1}\frac{\hbar^2}{4}\hat{a}\cdot\hat{b} + \frac{i\hbar}{2}(\hat{a}\times\hat{b})\cdot\vec{S}_A\right] \\
&= -\left[\vec{1}\frac{\hbar^2}{4}\hat{a}\cdot\hat{b}\right], \quad \langle\vec{S}_A\rangle = 0
\end{aligned}
$$

Observe that if $\hat{a} = \hat{b}$, then the spins will always be antialigned.

2-axis case, Hidden Local Variable theory Define a hidden classical variable λ such that there is a statistical distribution for λ: $\rho(\lambda)$. Normalization demands:

$$\int d\lambda \rho(\lambda) = 1$$

Let the observers measure in such a way that the result is deterministically dependent on λ with an unknown function S and the axis that they measure along:

$$\text{A result: } \frac{\hbar}{2} S(\hat{a}, \lambda)$$
$$\text{B result: } -\frac{\hbar}{2} S(\hat{b}, \lambda)$$

Then the expectation of the result is given by:

$$\langle (\vec{S}_A \cdot \hat{a})(\vec{S}_B \cdot \hat{b}) \rangle = -\frac{\hbar^2}{4} \int d\lambda \rho(\lambda) S(\hat{a}, \lambda) S(\hat{b}, \lambda)$$

It is possible to construct a $\rho(\lambda)$ such that this expectation is equal to the QM prediction $-\frac{\hbar^2}{4}(\hat{a} \cdot \hat{b})$. Hence for the two axis case, we cannot (by observation or experimentation) distinguish between the hidden local variable theory and the QM prediction. This, however, can be done using 3 axes.

3-axis case Define three axes $\hat{a}, \hat{b}, \hat{c}$. Then the expectation to compute is modified:

$$\langle (\vec{S}_A \cdot \hat{a})(\vec{S}_B \cdot \hat{b}) \rangle - \langle (\vec{S}_A \cdot \hat{a})(\vec{S}_B \cdot \hat{c}) \rangle$$

We want to compute this expectation using QM and the Hidden Local Variable theory. The HLV expectation is:

$$-\frac{\hbar^2}{4} \int d\lambda \rho(\lambda) \left[S(\hat{a}, \lambda) S(\hat{b}, \lambda) - S(\hat{a}, \lambda) S(\hat{c}, \lambda) \right]$$

Observe that $S^2(\hat{b}, \lambda) = 1$ because the function can only spit out ± 1. This allows us to re-write the expectation:

$$-\frac{\hbar^2}{4} \int d\lambda \rho(\lambda) \left[S(\hat{a}, \lambda) S(\hat{b}, \lambda) - S(\hat{a}, \lambda) S(\hat{c}, \lambda) \right] = -\frac{\hbar^2}{4} \int d\lambda \rho(\lambda) \left[S(\hat{a}, \lambda) S(\hat{b}, \lambda) \left(1 - S(\hat{b}, \lambda) S(\hat{c}, \lambda) \right) \right]$$

The following inequality holds:

$$\left| \langle (\vec{S}_A \cdot \hat{a})(\vec{S}_B \cdot \hat{b}) \rangle - \langle (\vec{S}_A \cdot \hat{a})(\vec{S}_B \cdot \hat{c}) \rangle \right| \leq \frac{\hbar^2}{4} \int d\lambda \rho(\lambda) \left(1 - S(\hat{b}, \lambda) S(\hat{c}, \lambda) \right)$$

because $S(\hat{a}, \lambda) S(\hat{b}, \lambda) = \pm 1$ in the integral is less than or equal to 1. Then the normalization of $\rho(\lambda)$ gives:

$$\left| \langle (\vec{S}_A \cdot \hat{a})(\vec{S}_B \cdot \hat{b}) \rangle - \langle (\vec{S}_A \cdot \hat{a})(\vec{S}_B \cdot \hat{c}) \rangle \right| \leq \frac{\hbar^2}{4} + \langle (\vec{S}_A \cdot \hat{b})(\vec{S}_B \cdot \hat{c}) \rangle$$

This is the Bell's Inequality satisfied by a Hidden Local Variable theory. Now we consider the expectation value as computed by Quantum Mechanics.

Let $\hat{a} \cdot \hat{b} = 0$ and let $\hat{c} = \frac{\hat{a} + \hat{b}}{\sqrt{2}}$. Then the RHS of the inequality is:

$$\begin{aligned} \frac{\hbar^2}{4} + \langle (\vec{S}_A \cdot \hat{b})(\vec{S}_B \cdot \hat{c}) \rangle &= \frac{\hbar^2}{4} - \frac{\hbar^2}{4} \hat{b} \cdot \hat{c} \\ &= \frac{\hbar^2}{4} \left(1 - \frac{1}{\sqrt{2}} \right) \end{aligned}$$

while the LHS is:

$$\left|\langle(\vec{S}_A\cdot\hat{a})(\vec{S}_B\cdot\hat{b})\rangle-\langle(\vec{S}_A\cdot\hat{a})(\vec{S}_B\cdot\hat{c})\rangle\right|=\left|-\frac{\hbar^2}{4}\hat{a}\cdot\hat{b}+\frac{\hbar^2}{4}\hat{a}\cdot\hat{c}\right|$$
$$=\frac{\hbar^2}{4}\frac{1}{\sqrt{2}}$$

But:

$$\frac{1}{\sqrt{2}}\not\leq\left(1-\frac{1}{\sqrt{2}}\right)$$

Hence Bell's Inequality fails for this combination of $\hat{a},\hat{b},\hat{c}$! This means that the HLV theory cannot explain the QM prediction in this case.

3.2.2 De Broglie - Bohm theory

Also known as pilot wave theory. This theory posits that Schrodinger's equation holds for the evolution of the wavefunction. It also posits a guidance equation for particles:

$$m\dot{x}=\hbar\Im\left(\frac{\partial\psi}{\partial x}\frac{1}{\psi}\right)$$

This theory is nonlocal because the local behavior of the particle depends on the wavefunction (or specifically its normalization) everywhere.

3.3 Friday, 15 April 2016

3.3.1 Decoherence

Explains why we do not see superpositions of many states. We include the environment with a large number of degrees of freedom:

$$|\text{air}\rangle=|m_1\rangle|m_2\rangle\cdots$$

We may consider, $\langle m_1'|m_1\rangle=1-\epsilon$, the inner product of one component of the environment with the state that is slightly offset from the original state. Hence ϵ is small. Let this inner product hold for all other components of the environment state. Then a slightly different condition of the environment made of the primed states satisfies:

$$\langle\text{air}'|\text{air}\rangle=(1-\epsilon)^N$$

where N is the number of subsystems m_i. Then since $\epsilon>0$, we can write:

$$(1-\epsilon)^N\to e^{-N\epsilon}$$

which vanishes exponentially. Then the two environments overlap negligibly even though each primed subsystem is only slightly different from the unprimed subsystem.

Now we write the combined system:

$$|\psi\rangle=(c_1|x_1\rangle+c_2|x_2\rangle)|\text{air}\rangle$$

Under unitary time evolution, we write:

$$|\psi\rangle=c_1|x_1\rangle|\text{air}_1\rangle+c_2|x_2\rangle|\text{air}_2\rangle$$

Now because the environment states are effectively orthogonal under slight perturbations, the time evolved state behaves as if the individual states were independent of each other.

Example Consider an observable O on a chair. The expectation value is:

$$\begin{aligned}\langle O\rangle &= \langle\psi|O|\psi\rangle \\ &= \left(c_1^*\langle x_1|\langle \text{air}_1| + c_2^*\langle x_2|\langle \text{air}_2|\right) O\left(c_1|x_1\rangle|\text{air}_1\rangle + c_2|x_2\rangle|\text{air}_2\rangle\right) \\ &= |c_1|^2\langle x_1|O|x_1\rangle + |c_2|^2\langle x_2|O|x_2\rangle\end{aligned}$$

where we used the effective orthogonality of the environment states. The environment state overlap vanishing implies that the contribution of $\langle x_1|O|x_2\rangle$ is eliminated. Hence the distribution of O results appears to just be a statistical distribution of the system being in either the $|x_1\rangle$ or $|x_2\rangle$ states, without the overlap states. Hence the entanglement of the system with the large environment system eliminates the coherent terms.

3.3.2 Density Matrices

Define the projection operator:

$$\rho(t) = |\psi(t)\rangle\langle\psi(t)|$$

Schrodinger's equation for the density matrix can be obtained:

$$\begin{aligned}\rho(t) &= U(t)|\psi(0)\rangle\langle\psi(0)|U(t)^\dagger \\ &= U(t)\rho(0)U(t)^\dagger\end{aligned}$$

Alternatively, take the outer product of the Schrodinger equation in both directions:

$$\begin{aligned}\left(i\hbar\frac{\partial}{\partial t}|\psi\rangle\right)\langle\psi| &= H|\psi\rangle\langle\psi| \\ |\psi\rangle\left(-i\hbar\frac{\partial}{\partial t}\langle\psi| - \langle\psi|H\right) &= 0\end{aligned}$$

Combining:

$$\frac{\partial\rho}{\partial t} = -\frac{i}{\hbar}[H,\rho]$$

which is called the von Neumann equation.

The density matrix is idempotent:

$$\rho(t)^2 = \rho(t)$$

The trace of the matrix is unity:

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

The expectation value of an observable is:

$$\langle O\rangle = \text{Tr}(\rho O) = \sum_n\langle n|\rho O|n\rangle = \sum_n\langle n|\psi\rangle\langle\psi|O|n\rangle = \sum_n\langle\psi|O|n\rangle\langle n|\psi\rangle = \langle\psi|O|\psi\rangle$$

A density matrix from a pure state has rank 1, which means that it has one nonzero eigenvalue and two zero eigenvalues (for 3-space).

Mixed state density matrix does not have rank 1.

$$\rho = \sum_n P_n |n\rangle\langle n|$$

The expectation value becomes:

$$\langle O \rangle = \sum_n P_n \langle n|O|n\rangle$$

which is a statistical distribution. It is a weighted average.

We can get mixed states from pure states. Consider the composite Hilbert space $S \otimes E$, where S corresponds to the system and E corresponds to the environment. Write a general wavefunction as a superposition:

$$|\psi\rangle = \sum_{n_S, n_E} c_{n_S, n_E} |n_S\rangle |n_E\rangle$$

We can remove the environment from the formulation by replacing its contribution by a partial trace, which takes a pure state into a mixed state, where the latter is known as the reduced density state.

$$\rho_{red} = \mathrm{Tr}_E(\rho) = \sum_{n_E} \langle n_E|\rho|n_E\rangle$$

where we trace over the environment states alone. The reduced density matrix acts on S only.

Chapter 4

Week 4

4.1 Monday, 18 April 2016

4.1.1 Supersymmetric (SUSY) QM

Consider a general Hamiltonian:

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

SUSY tries to write this Hamiltonian as the product of two operators $H = A^\dagger A$. We also define a ground state $|0\rangle$ such that $H|0\rangle = 0$ (constant terms, like the half from the QHO, are subtracted from the Hamiltonian to satisfy this condition). Then in the position basis:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_0(x) + V(x)\psi_0(x) = 0$$
$$\implies V(x) = \frac{\hbar^2}{2m}\frac{\frac{d^2\psi_0}{dx^2}}{\psi_0}$$

The operators we will use are:

$$A = \frac{iP}{\sqrt{2m}} + W'(x)$$
$$A^\dagger = -\frac{iP}{\sqrt{2m}} + W'(x)$$

where $W(x)$ is called the superpotential. Expanding the product:

$$\begin{aligned} A^\dagger A &= \frac{p^2}{2m} - \frac{i}{\sqrt{2m}}[P, W'(x)] + (W'(x))^2 \\ &= \frac{p^2}{2m} - \frac{\hbar}{\sqrt{2m}}W''(x) + (W'(x))^2, \quad [P, W'(x)] = -i\hbar W''(x) \end{aligned}$$

Hence comparing with the Hamiltonian,

$$V(x) = (W'(x))^2 - \frac{\hbar}{\sqrt{2m}}W''(x)$$

Hence this method only works for potentials that can be written in terms of a certain W function.

Solving for the ground state Proceed by definition:

$$
\begin{aligned}
A\left|0\right\rangle &= 0 \\
\implies \left(\frac{iP}{\sqrt{2m}} + W'\right)\left|0\right\rangle &= 0 \\
\implies \psi_0(x) &\propto \exp\left(-\frac{\sqrt{2m}}{\hbar}W(x)\right)
\end{aligned}
$$

Hence $W(x)$ contains information about the shape of the ground state.

Nomenclature Define the previous construction as System 1:

$$H_1 = A^\dagger A = \frac{p^2}{2m} + V_1(x), \quad V_1(x) = (W')^2 - \frac{\hbar}{\sqrt{2m}}W''$$

We can define a second system:

$$H_2 = AA^\dagger = \frac{p^2}{2m} + V_2(x), \quad V_2(x) = (W')^2 + \frac{\hbar}{\sqrt{2m}}W''$$

Label the eigenkets accordingly:

$$
\begin{aligned}
H_1\left|n,1\right\rangle &= E_{n,1}\left|n,1\right\rangle \\
H_2\left|n,2\right\rangle &= E_{n,2}\left|n,2\right\rangle
\end{aligned}
$$

The Key Observation Consider the operation of H_2 on the eigenkets of H_1. Then:

$$H_2(A\left|n,1\right\rangle) = AA^\dagger A\left|n,1\right\rangle = AE_{n,1}\left|n,1\right\rangle$$

This implies that $E_{n,1}$ is an eigenvalue of H_2 with eigenket $A\left|n,1\right\rangle$. The same thing applies to H_1:

$$H_1(A^\dagger\left|n,2\right\rangle) = E_{n,2}(A^\dagger\left|n,2\right\rangle)$$

We may now relate the eigenkets of each system to that of the other system, suitably normalized:

$$
\begin{aligned}
\left|n,2\right\rangle &= (E_{n+1,1})^{-1/2}A\left|n+1,1\right\rangle \\
\left|n+1,1\right\rangle &= (E_{n,2})^{-1/2}A^\dagger\left|n,2\right\rangle
\end{aligned}
$$

This means that the energy levels of system 1 and system 2 are identical, with the exception that the ground state of system 2 is the first excited state of system 1. The A operator takes an energy level of system 1 to that of system 2 with the same energy, and the $A^\dagger$ operator returns the energy eigenvectors of system 2 to that of system 1. Note that since A is chosen to annihilate the ground state of system 1, A does not map the ground state of 1 to that of system 2. Note that these two energy spectrums are very similar even though their generating potentials in the Hamiltonian can be very different.

The bottom line is that we can map some systems to another system with a very similar energy spectrum by constructing the A operator.

Combining the two systems Construct a combined Hamiltonian from the tensor product of the system Hamiltonians:

$$\boldsymbol{H} = \begin{pmatrix} \boldsymbol{H}_1 & \mathbf{0} \\ \mathbf{0} & \boldsymbol{H}_2 \end{pmatrix}$$

Construct the matrices:

$$\boldsymbol{Q} = \begin{pmatrix} \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{A} & \boldsymbol{0} \end{pmatrix}$$
$$\boldsymbol{Q}^\dagger = \begin{pmatrix} \boldsymbol{0} & \boldsymbol{A}^\dagger \\ \boldsymbol{0} & \boldsymbol{0} \end{pmatrix}$$

Consider the anticommutators:

$$\{\boldsymbol{Q}, \boldsymbol{Q}\} = 2\boldsymbol{Q}^2 = \boldsymbol{0}$$
$$\{\boldsymbol{Q}^\dagger, \boldsymbol{Q}^\dagger\} = 2(\boldsymbol{Q}^\dagger)^2 = \boldsymbol{0}$$
$$\{\boldsymbol{Q}, \boldsymbol{Q}^\dagger\} = \boldsymbol{H}$$

Hence the anticommutator behaves like the squaring operator to achieve the target Hamiltonian. The physical interpretation of $\boldsymbol{Q}$ is that of a symmetry generator. Recall that we can determine if an operator is a symmetry by computing the commutator with the Hamiltonian:

$$[\boldsymbol{Q}, \boldsymbol{H}] = \boldsymbol{0}$$

$\boldsymbol{Q}, \boldsymbol{Q}^\dagger$ are called SUSY generators. Important bottom line: the presence of a degeneracy in eigenvalue spectrums implies a symmetry.

Features of SUSY systems SUSY systems have non-negative energy:

$$\langle H \rangle = \langle \psi | H | \psi \rangle = \langle \psi | \{\boldsymbol{Q}, \boldsymbol{Q}^\dagger\} | \psi \rangle = \langle \psi | \boldsymbol{Q}\boldsymbol{Q}^\dagger | \psi \rangle + \langle \psi | \boldsymbol{Q}^\dagger \boldsymbol{Q} | \psi \rangle = |\boldsymbol{Q}^\dagger | \psi \rangle|^2 + |\boldsymbol{Q} | \psi \rangle|^2 \geq 0$$

More about the ground state Consider the full ground state by constructing the vector in the combined Hilbert space of the two systems:

$$|0\rangle = \begin{pmatrix} |0,1\rangle \\ |0,2\rangle \end{pmatrix}$$
$$\boldsymbol{H} |0\rangle = 0$$

Now taking the product of this expression with $\langle 0|$, and noting that equality for the energy expectation requires that each squared term vanishes, we require that:

$$\boldsymbol{Q} |0\rangle = 0 \implies A |0,1\rangle = 0$$
$$\boldsymbol{Q}^\dagger |0\rangle = 0 \implies A^\dagger |0,2\rangle = 0$$

Substituting the position basis representation and solving the DE,

$$\psi_{0,1}(x) \propto e^{-\sqrt{2m}W(x)/\hbar}$$
$$\psi_{0,2}(x) \propto e^{\sqrt{2m}W(x)/\hbar}$$

Now wavefunctions have to be normalizable. Hence you cannot have both ground states at the same sign since the exponential sign changes. This gives only one ground state between the two systems.

4.2 Wednesday, 20 Apr 2016

More supersymmetric quantum mechanics
Recall the two systems defined in the last lecture:

$$H_1 = A^\dagger A = \frac{p^2}{2m} + V_1(x) = \frac{p^2}{2m} + W'^2 - \frac{\hbar}{\sqrt{2m}} W''$$
$$H_2 = AA^\dagger = \frac{p^2}{2m} + V_2(x) = \frac{p^2}{2m} + W'^2 + \frac{\hbar}{\sqrt{2m}} W''$$

which had the same energy spectrum, with the exception of the system 1 ground state. One example of such a system is the Harmonic Oscillator. System 2 corresponds to the System 1 state offset by one energy spacing (so that System 1 has one more low-energy state).

4.2.1 Particle in a box using SUSY

Let V_1 be the infinite square well potential. Note that in the definition of System 1, we set the ground state to be at zero energy. Hence we set the value of the potential in the square well to be:

$$V_1(x) = -\frac{\hbar^2\pi^2}{2ma^2}, \quad \text{inside}$$

We will supersymmetrize this by finding a System 2 corresponding to this System 1. Recall that the ground state of System 1 can be written as:

$$\psi_{0,1}(x) = \sqrt{\frac{2}{a}}\sin\frac{\pi x}{a} \propto e^{-\sqrt{2m}W(x)/\hbar}$$

We can re-write this and solve for $W(x)$:

$$W'(x) = -\frac{\hbar}{\sqrt{2m}}\frac{\frac{d}{dx}\psi_{0,1}}{\psi_{0,1}} = -\frac{\hbar}{\sqrt{2m}}\frac{\pi}{a}\cot\frac{\pi x}{a}$$

This gives us a means of calculating the potential $V_2 = W'^2 + \frac{\hbar}{\sqrt{2m}}W''$:

$$V_2(x) = \frac{\hbar^2\pi^2}{2ma^2}(2\csc^2\frac{\pi x}{a} - 1)$$

Note that even though V_2 looks very different from V_1, they have the same energy spectrum! (up to the ground state of system 1). Note that V_2 blows up at the same position as V_1, $x = 0, a$. The energy spectrum of V_1 can be indexed from $n = 0$:

$$E_{n,1} = \frac{((n+1)^2 - 1)\hbar^2\pi^2}{2ma^2}$$

The ground state of system 2 has the same energy as the first excited state for system 1.

4.2.2 Generalizing the SUSY process

Note that we can write System 2 as a new product of raising and lowering operators to create a System 3, where System 3 has a ground state corresponding to the first excited state of System 2. This process can be repeated to achieve a sequence of systems. We obtain the wavefunction for the nth system by acting on the corresponding System 1 wavefunction using the sequence of lowering operators $\{A_n\}$.

Now there is no guarantee that this process will work. However, we may define a property of certain potentials called shape invariance. Consider a superpotential that can generate two potentials V_1, V_2. Let V_1, V_2 also depend on parameters a that determine the wavefunction shape (examples of parameters are the charge of the electron, angular frequency of harmonic oscillator etc.):

$$V_1(x;a)$$
$$V_2(x;a)$$

Shape invariance deals with how the wavefunctions depend on a. **Shape invariance** is the property that $V_2(x;a) = V_1(x;a') + R(a)$ so that they have the same shape up to a constant piece $R(a)$ that does not depend on x. Let $a' = f(a)$, where the prime is just a label, not a derivative. Note that $R(a)$ and $f(a)$ are assumed to hold no matter which system in the sequence you are in. If this condition holds, we may repeat this procedure indefinitely:

$$
\begin{aligned}
H_1 &= \frac{p^2}{2m} + V_1(x; a_1) \\
H_2 &= \frac{p^2}{2m} + V_1(x; f(a_1)) + R(a_1) \\
H_3 &= \frac{p^2}{2m} + V_1(x; f(f(a_1))) + R(f(a_1)) + R(a_1)
\end{aligned}
$$

Including the parameter dependence in the eigenstates:

$$
\begin{aligned}
H_1 \left|0, 1, a_1\right\rangle = 0 \implies \left(\frac{p^2}{2m} + V_1(x; a_1)\right) \left|0, 1, a_1\right\rangle = 0 \\
H_2 \left|0, 2, a_2\right\rangle = \left(\frac{p^2}{2m} + V_1(x; a_2) + R(a_1)\right) \left|0, 1, a_2\right\rangle
\end{aligned}
$$

But comparing the two equations, we observe that the first two terms in the eigenvalue equation for H_2 must vanish due to the first statement. Then the second statement is equivalent to:

$$
H_2 \left|0, 1, a_2\right\rangle = R(a_1) \left|0, 1, a_2\right\rangle
$$

Hence $R(a_1)$ gives the energy offset from system 1 to system 2. Specifically,

$$
\begin{aligned}
E_{0,1} &= 0 \\
E_{0,2} &= R(a_1) \\
E_{0,3} &= R(a_1) + R(a_2) \\
E_{0,n} &= \sum_{i=1}^{n-1} R(a_i)
\end{aligned}
$$

But the nth system ground state must correspond to the $n-1$st excited state of system 1:

$$
E_{m-1,1} = E_{0,m}
$$

Hence the functions R give the energy spectrum of System 1:

$$
E_{n,1} = \begin{cases} 0, & n = 0 \\ \sum_{i=1}^{n} R(a_i), & n > 0 \end{cases}
$$

Hence for a shape invariant system, it will suffice to find the functions R and f to find the energy spectrum.

4.2.3 Solving the hydrogen atom

We will use the fact that the hydrogen atom potential is supersymmetric and shape invariant to solve for the energy spectrum. The Coulomb potential is:

$$
V_{coulomb} = -\frac{e^2}{4\pi\epsilon_0} \frac{1}{r}
$$

Note that although the problem is in 3D, we can consider the radial component as a 1D problem:

$$
-\frac{\hbar^2}{2m} \frac{d^2u}{dr^2} + \left[V_{coulomb}(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} - E_0\right] u(r) = 0
$$

We subtract E_0 to fix the ground state at zero energy. We define the relevant system 1 potential:

$$V_1(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} - E_0$$

We want to know if we can write this in the supersymmetric form:

$$V_1(r) = W'(r)^2 - \frac{\hbar}{\sqrt{2m}}W''(r)$$

We make the ansatz:

$$W'(r) = C - \frac{D}{r}$$

which works.

4.3 Friday 22 Apr 2016

4.3.1 Hydrogen atom continued

The hydrogen atom superpotential was solved with:

$$C^2 = -E_0$$
$$\frac{e^2}{4\pi\epsilon_0} = 2CD$$
$$D = \frac{\hbar}{2\sqrt{2m}}2(l+1), \quad \text{or} \quad -\frac{\hbar}{2\sqrt{2m}}2l$$

The second solution for D is rejected. why?

The second and third equation give a solution for C and hence E_0:

$$C = \frac{e^2\sqrt{2m}}{4\pi\epsilon_0(l+1)\hbar}$$
$$\implies E_0 = -\frac{me^4}{32\pi^2\epsilon_0^2(l+1)^2\hbar^2}$$

and this energy E_0 is the ground state energy *at fixed l*. This is the correct expression for the hydrogen atom energy levels. The hydrogen atom is hence supersymmetric.

Returning to the superpotential generating function,

$$W' = C - \frac{D}{r}$$

we may construct the partner superpotential:

$$V_2 = C^2 - \frac{2CD}{r} + \frac{D^2}{r^2} + \frac{\hbar}{\sqrt{2m}}\frac{D}{r^2}$$

It turns out that V_2 is identical to V_1 with the exception of the last term. The last term is actually the centrifugal term:

$$V_2 = V_1 + \frac{2\hbar}{\sqrt{2m}}\frac{D}{r^2} = V_1 + \frac{\hbar^2}{m}\frac{l+1}{r^2}$$

Hence the superpartner states are states with a different angular momentum.

We investigate shape invariance. Let l be the shape parameter. Explicitly,

$$\begin{aligned}
V_1(l) &= -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + \frac{me^4}{32\hbar^2\pi^2\epsilon_0^2(l+1)^2} \\
V_2(l) &= -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} + \frac{me^4}{32\hbar^2\pi^2\epsilon_0^2(l+1)^2} + \frac{\hbar^2(l+1)}{mr^2} \\
&= V_1(l+1) + \frac{me^4}{32\pi^2\hbar^2\epsilon_0^2}\left(\frac{1}{(l+1)^2} - \frac{1}{(l+2)^2}\right) \\
&= V_1(l+1) + E_{Ry}\left(\frac{1}{(l+1)^2} - \frac{1}{(l+2)^2}\right)
\end{aligned}$$

Comparing this to the form of the shape invariance condition:

$$\begin{aligned}
f(l) &= l+1 \\
R(l) &= E_{Ry}\left(\frac{1}{(l+1)^2} - \frac{1}{(l+2)^2}\right)
\end{aligned}$$

The series of supersymmetric potentials correspond to the excited state energies of the original system corresponding to different angular momentum values.

4.3.2 Scattering

Consider two superpartner potentials V_1, V_2 that do not go to infinity at $x \to \pm\infty$. This implies that the superpotential generator $W(x)$ must grow as fast as or slower than linear dependence on x. Hence the second derivative of $W(x)$ vanishes at $\pm\infty$. Hence the superpotentials, which only differ in the sign of the $W''(x)$ term, must asymptote to the same shape at $\pm\infty$. Write the asymptotic form as:

$$\begin{aligned}
W(x \to \infty) &= W_+ \\
W(x \to -\infty) &= W_-
\end{aligned}$$

where $W_\pm$ are constants. The asymptotic form of the scattering eigenfunctions in System 1 are:

$$\begin{aligned}
\psi_1(x \to -\infty) &= e^{ikx} + R_1 e^{-ikx} \\
\psi_1(x \to \infty) &= T_1 e^{ik'x}
\end{aligned}$$

and since the potentials are the same at infinity, the same form (and same k, k' values) hold for ψ_2 in System 2 as well.

Note further that since the scattering eigenmodes (parametrized by k) are continuous (as opposed to discrete for bound states), we may ignore the ground state offset that we had to consider in the bound state case. Then for eigenmodes of the same energy $E_1 = E_2$:

$$|\psi_1\rangle = NA^\dagger |\psi_2\rangle$$

where N is a normalization constant. Moving into the x-basis and evaluating at negative infinity (note that the LHS and RHS refer to different wavefunctions and hence have different relation coefficients),

$$\begin{aligned}
e^{ikx} + R_1 e^{-ikx} &= N\left(-\frac{\hbar}{\sqrt{2m}}\frac{d}{dx} + W_-\right)\left(e^{ikx} + R_2 e^{-ikx}\right) \\
&= N\left[\left(-\frac{i\hbar k}{\sqrt{2m}} + W_-\right)e^{ikx} + R_2\left(\frac{i\hbar k}{\sqrt{2m}} + W_-\right)e^{-ikx}\right]
\end{aligned}$$

and similarly at $x \to \infty$,

$$T_1 e^{ik'x} = NT_2\left(-\frac{i\hbar k'}{\sqrt{2m}} + W_+\right)e^{ik'x}$$

Comparing coefficients of the exponentials,

$$
\begin{aligned}
N &= \frac{1}{-\frac{i\hbar k}{\sqrt{2m}} + W_-} \\
R_1 &= R_2 \frac{\frac{i\hbar k}{\sqrt{2m}} + W_-}{-\frac{i\hbar k}{\sqrt{2m}} + W_-} \\
T_1 &= T_2 \frac{\frac{i\hbar k'}{\sqrt{2m}} + W_+}{-\frac{i\hbar k'}{\sqrt{2m}} + W_+} \\
&\implies |R_1|^2 = |R_2|^2
\end{aligned}
$$

but the transmission coefficients are:

$$
|T_1|^2 = |T_2|^2 \left(\frac{\frac{\hbar^2 k'^2}{2m} + W_+^2}{\frac{\hbar^2 k^2}{2m} + W_-^2} \right)
$$

This is consistent because the numerator corresponds to the energy $E(x \to \infty)$ and the denominator corresponds to $E(x \to -\infty)$. By the conservation of energy, these must be the same, so $|T_1|^2 + |T_2|^2$. Hence for these two superpartner potentials, the reflection and transmission coefficients are the same.

Chapter 5

Week 5

5.1 Monday 25 Apr 2016

5.1.1 SUSY WKB for bound states

Let x_i, x_f be the classical turning points for a bound state potential with total energy E_n. WKB says that for an energy eigenvalue, the following formula is quantized:

$$\int_{x_i}^{x_f} \sqrt{2m(E_n - V(x))}dx = (n + 1/2)\hbar\pi, \quad n = 0, 1, 2, \ldots$$

If the potential is supersymmetric, we can write (for System 1):

$$V(x) = W'^2 - \frac{\hbar}{\sqrt{2m}}W''$$

Expand the LHS integral in powers of $\hbar$ (the subscript 1 indicates that this is for the system 1 potential):

$$\begin{aligned}\int_{x_i}^{x_f} \sqrt{2m(E_{n,1} - V)}dx &= \int_{x_i}^{x_f} \sqrt{2m(E_{n,1} - W'^2)}dx + \frac{\hbar}{2}\int_{x_i}^{x_f} \frac{W''(x)dx}{\sqrt{E_{n,1} - W'(x)^2}} + O(\hbar^2) \\ &= \int_{x_i}^{x_f} \sqrt{2m(E_{n,1} - W'^2)}dx + \frac{\hbar}{2}\left[\sin^{-1}\frac{W'(x)}{\sqrt{E_{n,1}}}\right]_{x_i}^{x_f} + O(\hbar^2)\end{aligned}$$

Note that at the endpoints:

$$\begin{aligned}E_{n,1} &= V(x_i) = V(x_f) \\ \implies E_n &= W'(x_i)^2 + O(\hbar) = W'(x_f)^2 + O(\hbar)\end{aligned}$$

Hence at the endpoints, the arcsin becomes:

$$\left[\sin^{-1}\frac{W'(x)}{\sqrt{E_{n,1}}}\right]_{x_i}^{x_f} = \sin^{-1} 1 - \sin^{-1}(-1) = \pi$$

Note that the second term has a negative sign inside because:

$$sgn(W'(x_i)) = -sgn(W'(x_f))$$

because the potential must have opposite signs at the classical turning points (if not we won't have a bound state). We may hence write the WKB integral as:

$$\int_{x_i}^{x_f} \sqrt{2m(E_{n,1} - V)}dx = \int_{x_i}^{x_f} \sqrt{2m(E_{n,1} - W'^2)}dx + \frac{\pi\hbar}{2} + O(\hbar^2)$$

Comparing this to the quantization condition,

$$\int_{x_i}^{x_f} \sqrt{2m(E_{n,1} - W'^2)}dx = n\hbar\pi, \quad n = 0, 1, 2, \ldots$$

We may repeat this process for the superpotential partner V_2:

$$\int_{x_i}^{x_f} \sqrt{2m(E_{n,2} - W'^2)}dx = (n+1)\hbar\pi, \quad n = 0, 1, 2, \ldots$$

Observe that the correspondence between the systems indicate that the energy spectrum for the two systems are identical except for the ground state of system 1.

For shape invariant potentials, the SUSY WKB process is exact.

5.1.2 Total derivatives

Consider a Lagrangian:

$$L = \frac{m\dot{x}^2}{2} + \theta\dot{x}$$

The $\theta\dot{x}$ is a total derivative because it is equal to $\frac{d}{dt}(\theta x)$. In classical physics, terms that are written as total derivatives are not important because when calculating the action, the total derivative can be integrated directly and gives a value just dependent on t_i, t_f, x_i, x_f. Its contribution is not dependent on the path taken. Hence it does not affect the classical path calculated using the action.

More generally, we may add any the total time derivative of an arbitrary function of x to the Lagrangian and not change the dynamics:

$$\Delta L = \frac{d}{dt}f(x)$$
$$\implies \frac{d}{dt}\frac{\partial}{\partial\dot{x}}(\dot{x}f'(x)) - \frac{\partial}{\partial x}(\dot{x}f'(x)) = \frac{df'(x)}{dt} - \dot{x}f''(x) = 0$$

so the Euler-Lagrange equations are satisfied with the same classical path.

Note that although the dynamics are unchanged, the addition of the total derivative can change the definition of the canonical momentum of the system.

5.1.3 Total derivatives in quantum mechanics

Let the Lagrangian be written as:

$$L = L_0 + \Delta L, \quad \Delta L = \theta\dot{x}$$

Computing the propagator:

$$\begin{aligned} U(x_f; x_i, t) &= \int [dx] e^{iS/\hbar} \\ &= \int [dx] \exp\left[\frac{i}{\hbar}\left(\int dt L_0 + \int dt \Delta L\right)\right] \\ &= \int [dx] \exp\left[\frac{i}{\hbar}\left(\int dt L_0 + \theta(x_f - x_i)\right)\right] \\ &= e^{i\theta(x_f - x_i)/\hbar} \int [dx] \exp\left[\frac{i}{\hbar}\left(\int dt L_0\right)\right] \\ \implies U(x_f, x_i, t) &= e^{i\theta(x_f - x_i)/\hbar} U_0(x_f, x_i, t) \end{aligned}$$

where U_0 is the propagator with $\theta = 0$. The pre-factor is a pure phase and does not appear to change the dynamics of the system.

However, if we consider the transition between two general states instead of two position eigenstates,

$$\begin{aligned}\langle\psi_f|e^{-iHt/\hbar}|\psi_i\rangle &= \iint dx_f dx_i \langle\psi_f|x_f\rangle\langle x_f|e^{-iHt/\hbar}|x_i\rangle\langle x_i|\psi_i\rangle \\ &= \iint dx_f dx_i \psi_f^*(x_f) U_0(x_f, x_i, t) e^{i\theta(x_f - x_i)/\hbar}\psi_i(x_i)\end{aligned}$$

Now the integration involves the phase with θ!

5.1.4 Example: QHO and total derivatives

Consider the Lagrangian:

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2 + \theta\dot{x} \equiv L_0 + \theta\dot{x}$$

The canonical parameters are:

$$P = \frac{\partial L}{\partial \dot{x}} = m\dot{x} + \theta \implies \dot{x} = \frac{P - \theta}{m}$$

and we can construct the Hamiltonian:

$$H = p\dot{x} - L = \frac{(P-\theta)^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

We now quantize the system. The TISE gives:

$$\begin{gathered}H\psi_E = E\psi_E \\ \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x} - \theta\right)^2 \psi_E + \frac{1}{2}m\omega^2 x^2\psi_E = E\psi_E\end{gathered}$$

Move into another basis:

$$\psi_E = e^{i\theta x/\hbar}\psi_{E,0}$$

where $\psi_{E,0}$ is the wavefunction in the system with $\theta = 0$. Substituting this into the TISE:

$$\left(-i\hbar\frac{\partial}{\partial x} - \theta\right)\psi_E = e^{i\theta x/\hbar}\left(-i\hbar\frac{\partial}{\partial x}\psi_{E,0}\right)$$

which satisfies the same TISE for $\psi_{E,0}$.

5.2 Wednesday, 27 April 2016

5.2.1 QM and Electromagnetism

CGS Maxwell equations:

$$\begin{gathered}\nabla\cdot\boldsymbol{E} = 4\pi\rho \\ \nabla\times\boldsymbol{E} + \frac{1}{c}\frac{\partial\boldsymbol{B}}{\partial t} = 0 \\ \nabla\cdot\boldsymbol{B} = 0 \\ \nabla\times\boldsymbol{B} - \frac{1}{c}\frac{\partial\boldsymbol{E}}{\partial t} = \frac{4\pi}{c}\boldsymbol{j}\end{gathered}$$

Gauge Invariance

$$\boldsymbol{A} \to \boldsymbol{A} - \nabla\Lambda(x,t)$$
$$\phi \to \phi + \frac{1}{c}\frac{\partial\Lambda(x,t)}{\partial t}$$

which give rise to the fields:

$$\boldsymbol{B} = \nabla \times \boldsymbol{A}$$
$$\boldsymbol{E} = -\frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t} - \nabla\phi$$

EM Lagrangian

$$L = \frac{1}{2}m\dot{\boldsymbol{x}}^2 + \frac{q}{c}\frac{d\boldsymbol{x}}{dt}\cdot\boldsymbol{A}(\boldsymbol{x},t) - q\phi(\boldsymbol{x},t)$$

This Lagrangian is invariant under the gauge transformation above.

$$L \to L - \frac{q}{c}\frac{d\Lambda(\boldsymbol{x},t)}{dt}$$

The second term is a total derivative, hence it does not affect the classical motion.

Action and the gauge transformation Insert the gauge-transformed Lagrangian into the action:

$$S \to S - \frac{q}{c}\left[\Lambda(\boldsymbol{x}(t_f),t_f) - \Lambda(\boldsymbol{x}(t_i),t_i)\right]$$
$$\implies U(x_f,t_f;x_i,t_i) \to U(x_f,t_f;x_i,t_i)e^{-\frac{iq}{\hbar c}[\Lambda(x_f,t_f)-\Lambda(x_i,t_i)]}$$

Recall that we can write the eigenkets of the gauge-transformed system using the basis:

$$|\boldsymbol{x}(t)\rangle \to e^{-iq\Lambda(\boldsymbol{x},t)/\hbar c}|\boldsymbol{x}(t)\rangle$$

which removes the effect of the extra phase term. Classical and Quantum Mechanics appears to be gauge-invariant.

5.2.2 Aharonov-Bohm Interference

Consider the usual double slit experiment. Let the path that passes through the ith slit be P_i. Then the wavefunction at the screen is:

$$\psi(\boldsymbol{r}) = \psi_{P_1}(\boldsymbol{r}) + \psi_{P_2}(\boldsymbol{r})$$

Put a solenoid normal to the plane in between the paths so that it does not physically overlap with the paths. Consider the wavefunction when the magnetic field in the solenoid is nonzero.

Now consider the EM Lagrangian with the resultant vector field (due to the introduction of the solenoid) and no scalar field:

$$L = \frac{1}{2}m\left(\frac{d\boldsymbol{r}}{dt}\right)^2 + \frac{q}{c}\frac{d\boldsymbol{r}}{dt}\cdot\boldsymbol{A}$$

ψ_{P_1}, ψ_{P_2} picks up a phase due to this nonzero $\boldsymbol{B}$ field:

$$
\begin{aligned}
e^{i\theta_1} &= \exp\left(\frac{iq}{c\hbar}\int dt \frac{d\boldsymbol{r}}{dt}\cdot\boldsymbol{A}\right) \\
&= \exp\left(\frac{iq}{\hbar c}\int_{P_1} d\boldsymbol{r}\cdot\boldsymbol{A}\right) \\
e^{i\theta_2} &= \exp\left(\frac{iq}{\hbar c}\int_{P_2} d\boldsymbol{r}\cdot\boldsymbol{A}\right)
\end{aligned}
$$

But P_1 and P_2 are different! This means that there will be a phase difference between these two wavefunctions:

$$
\begin{aligned}
\theta_1 - \theta_2 &= \frac{q}{c\hbar}\left[\int_{P_1} d\boldsymbol{r}\cdot\boldsymbol{A} - \int_{P_2} d\boldsymbol{r}\cdot\boldsymbol{A}\right] \\
&= \frac{q}{c\hbar}\oint d\boldsymbol{r}\cdot\boldsymbol{A} \\
&= \frac{q}{c\hbar}\Phi_B
\end{aligned}
$$

$$
\psi(\boldsymbol{r}) \propto e^{iq\Phi_B/\hbar c}\psi_{P_1}(\boldsymbol{r}) + \psi_{P_2}(\boldsymbol{r})
$$

Note further that if $\frac{q\Phi_B}{c\hbar}$ is quantized in terms of $2\pi n$, then there is no effect of the phase shift. Rearranging,

$$
\Phi_q = \frac{2\pi\hbar c}{q}
$$

where Φ_q is the magnetic flux quantum, the change in magnetic flux such that the phase factor does not have an effect.

5.2.3 Detailed calculations for Aharonov-Bohm effect: particle on a ring with solenoid

Move into cylindrical coordinates. Confine a particle on a ring of radius b and place a solenoid of radius a inside the ring so that there is a magnetic field in the $\hat{z}$ direction threading the surface bounded by the ring. There is no magnetic field at the ring position itself $a < b$. The vector potential everywhere is:

$$
\boldsymbol{A} = \begin{cases} \hat{\phi}\frac{\Phi_M r}{2\pi a^2}, & r < a \\ \hat{\phi}\frac{\Phi_M}{2\pi r}, & r > a \end{cases}
$$

where $\Phi_M = B\pi a^2$, leading to the magnetic field:

$$
\boldsymbol{B} = \begin{cases} B\hat{z}, & r < a \\ 0, & r > a \end{cases}
$$

5.3 Friday, 29 Apr 2016

5.3.1 Particle on a ring continued

The Hamiltonian is:

$$
H = \frac{1}{2}m\left(\frac{d\boldsymbol{r}}{dt}\right)^2 + \frac{q}{c}\frac{d\boldsymbol{r}}{dt}\cdot\boldsymbol{A} = \frac{(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A})^2}{2m}
$$

Note that the effect of the magnetic field is to replace the momentum operator with:

$$
\boldsymbol{p} \to \boldsymbol{p} - \frac{q}{c}\boldsymbol{A}
$$

We want to solve the Schrodinger equation for this Hamiltonian with the given vector potential. Then:

$$H = \frac{1}{2m}\left[-i\hbar\nabla - \frac{q}{c}\boldsymbol{A}\right]^2$$
$$= \frac{1}{2m}\left[-\hbar^2\nabla^2 + \frac{q^2}{c^2}A^2 + 2i\hbar\frac{q}{c}\boldsymbol{A}\cdot\nabla\right], \quad \nabla\cdot\boldsymbol{A} = 0$$

H is an operator, consider its operation on a test function when expanding it! Write the wavefunction as having azimuthal dependence only: $\psi(\phi)$. Then solving for the energy eigenvalues:

$$H\psi_E = \frac{1}{2m}\left[-\frac{\hbar^2}{b^2}\frac{d^2}{d\phi^2} + \left(\frac{q\Phi_B}{2\pi bc}\right)^2 + \frac{i\hbar q\Phi_B}{\pi b^2 c}\frac{d}{d\phi}\right]\psi_E = E\psi_E$$

This looks like a damped harmonic oscillator equation. We re-scale the equation:

$$\frac{d^2\psi_E}{d\phi^2} - 2i\beta\frac{d\phi_E}{d\phi} + \epsilon\psi_E = 0$$
$$\beta \equiv \frac{q\Phi_B}{2\pi\hbar c}, \quad \epsilon = \frac{2mb^2E}{\hbar^2} - \beta^2$$

Now we make the ansatz:

$$\psi_E = Ae^{in\phi}$$

n is an integer so that ψ_E is single-valued. This periodicity condition constraints the values of β, ϵ:

$$-n^2 + 2\beta n + \epsilon = 0$$
$$\implies n = \frac{-2\beta \pm \sqrt{4\beta^2 + 4\epsilon}}{-2} = \beta \pm \frac{b}{\hbar}\sqrt{2mE}$$

Rearranging and solving for E:

$$E_n = \frac{\hbar^2}{2mb^2}\left(n - \frac{q\Phi_B}{2\pi\hbar c}\right)^2, \quad n \in \mathbb{Z}$$

Recall that $\Phi_Q = \frac{2\pi\hbar c}{q}$ was the flux quantum. The energy spectrum is hence displaced in the n direction by the tunable parameter Φ_B/Φ_Q. Note that if $\Phi_B/\Phi_Q \in \mathbb{Z}$, then the energy spectrum remains the same!

5.3.2 Dirac Charge Quantization

Suppose we modify Maxwell's Equations:

$$\nabla\cdot\boldsymbol{B} = 4\pi\rho_m$$
$$\implies \boldsymbol{B} = \frac{q_m\hat{r}}{r^2}$$
$$\implies \Phi_B = 4\pi q_m$$

Note that we can keep the vanishing divergence of $\boldsymbol{B}$ by the following construction: Pretend we have a monopole-antimonopole pair connected by an infinitesimally thin solenoid (Dirac string) that channels a very large amount of flux between the pair so as to ensure that the divergence of B is zero. But the Aharonov-Bohm experiment allows us to measure the effect of the Dirac string by choosing a path that surrounds the string. But we noted that if the flux had an integer number of flux quantums, then the effect of the flux is not observable. Setting the magnetic flux equal to the flux quantum times some integer,

$$4\pi q_m = \frac{2\pi c\hbar n}{q}$$
$$\implies \frac{2q_m q}{c\hbar} = n \in \mathbb{Z}$$

This is a quantization condition that relates charge to magnetic monopole charge. Hence if there is a monopole-antimonopole pair, then charge is quantized.

5.3.3 General vector potential and Aharonov-Bohm

Consider a general $\boldsymbol{A}$. Then the TDSE gives:

$$i\hbar\frac{\partial\psi}{\partial t} = \left[\frac{1}{2m}\left(-i\hbar\nabla - \frac{q}{c}\boldsymbol{A}\right)^2 + V\right]\psi$$

We want to write the eigenfunction solution in the form:

$$\psi(\boldsymbol{r},t) = e^{ig(\boldsymbol{r})}\psi^{(1)}(\boldsymbol{r},t)$$

where:

$$g(\boldsymbol{r}) = \frac{q}{\hbar c}\int^{\boldsymbol{r}} d\boldsymbol{r}'\boldsymbol{A}(\boldsymbol{r}')$$

Note that $\nabla g(\boldsymbol{r}) \propto \boldsymbol{A}$. The gradient of the proposed eigenfunction is:

$$\nabla\psi = e^{ig}i\nabla g\psi^{(1)} + e^{ig}\nabla\psi^{(1)} = e^{ig}\left(\nabla + \frac{iq\boldsymbol{A}}{\hbar c}\right)\psi^{(1)}$$

This looks like the momentum component of the Hamiltonian. Then:

$$\begin{aligned}\left(-i\hbar\nabla - \frac{q}{c}\boldsymbol{A}\right)\psi &= -i\hbar e^{ig}\nabla\psi^{(1)}\\ \left(-i\hbar\nabla - \frac{q}{c}\boldsymbol{A}\right)^2\psi &= \left(-i\hbar e^{ig}\nabla\right)^2\psi^{(1)}\\ \implies -\frac{\hbar^2}{2m}\nabla^2\psi^{(1)} + V\psi^{(1)} &= i\hbar\frac{\partial\psi^{(1)}}{\partial t}\end{aligned}$$

which is the usual TDSE for $\psi^{(1)}$. Hence to find the eigenfunctions of the original system, we just tack on $e^{ig(\boldsymbol{r})}$ onto the eigenfunctions of the system without $\boldsymbol{A}$.

Chapter 6

Week 6

6.1 Monday, 2 May 2016

6.1.1 Superconductivity

For more information, see Feynman lectures Vol 3.

We make several assumptions. Model the metal as a sea of electrons in a fixed lattice of ions/atoms. Assume that there is a small attractive force (a polarization effect) between electrons induced by the lattice atoms. Assume that the electrons form weakly-bound Cooper pairs ($\sim 10^{-3}eV$), which are pairs of electrons joined together by the small attractive force. The Cooper pairs are bosons.

Notation: probability distribution $\rho = \psi^*\psi$. Think of the probability distribution as related to the charge density of electrons. Implement the continuity equation:

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \nabla \cdot \boldsymbol{J} = 0 \\
&\quad \implies \frac{\partial \rho}{\partial t} = \frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t} \\
&\qquad = -\frac{1}{2}\nabla \left[\left(-\frac{i\hbar\nabla - \frac{q}{c}\boldsymbol{A}}{m}\psi \right)^* \psi + \psi^* \left(-\frac{i\hbar\nabla - \frac{q}{c}\boldsymbol{A}}{m}\psi \right) \right] = -\nabla \boldsymbol{J} \\
&\quad \implies \boldsymbol{J} = \frac{1}{2}\left[\left(-\frac{i\hbar\nabla - \frac{q}{c}\boldsymbol{A}}{m}\psi \right)^* \psi + \psi^* \left(-\frac{i\hbar\nabla - \frac{q}{c}\boldsymbol{A}}{m}\psi \right) \right]
\end{aligned}$$

We write the Cooper pairs wavefunction in the following form:

$$\psi(\boldsymbol{r}, t) = \sqrt{\rho(\boldsymbol{r}, t)} e^{i\theta(\boldsymbol{r}, t)}$$

Hence we will just deal with the two functions $\rho(\boldsymbol{r}, t), \theta(\boldsymbol{r}, t)$. Substituting this ansatz into the expression for $\boldsymbol{J}$, we obtain:

$$\boldsymbol{J} = \frac{\hbar\rho}{m}\left(\nabla\theta - \frac{q}{\hbar c}\boldsymbol{A} \right) + O(\nabla\rho)$$

At steady state, we expect that the lattice ions would be able to cancel the effect of electric charge build up. Hence make the assumption that the correction terms in $\nabla\rho$ go to zero. This also implies that $\frac{\partial\rho}{\partial t} = 0 \implies \nabla \cdot \boldsymbol{J} = 0$. Recall that we can also choose the Coulomb gauge to fix $\nabla \cdot \boldsymbol{A} = 0$. Then we have that:

$$\nabla \cdot \boldsymbol{J} = \frac{\hbar\rho}{m}\nabla^2\theta = 0$$

θ constant is one solution. Using this constant θ solution, we have that the probability current density is related to the vector potential:

$$\boldsymbol{J} = -\frac{\rho q}{mc}\boldsymbol{A}$$

Recall Maxwell's equations:

$$\Box \boldsymbol{A} + \nabla(\nabla \cdot \boldsymbol{A}) = \mu_0 \boldsymbol{J}$$
$$\Box = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2$$

Under the Coulomb gauge, and approximating the current density to be the probability current density (perhaps by setting the unit of charge to be unity),

$$\Box \boldsymbol{A} = -\frac{\mu_0 \rho q}{mc}\boldsymbol{A} \implies \Box \boldsymbol{A} = -\lambda^2 \boldsymbol{A}, \quad \lambda = \sqrt{\frac{\mu_0 \rho q}{mc}}$$

λ^2 is related to the effective mass for the photon. Substituting an exponential ansatz for $\boldsymbol{A} \sim e^{i(kx-\omega t)}$, the dispersion relation becomes:

$$\omega \sim \sqrt{k^2 + \lambda^2}$$

Static solutions to $\Box \boldsymbol{A} = -\lambda^2 \boldsymbol{A}$ are given by $\frac{\partial}{\partial t} = 0$. Note that the signs of the ∇^2 and $\boldsymbol{A}$ are the same, so the equation of motion is that of an unstable oscillator with solutions:

$$\boldsymbol{A} \sim e^{\pm \lambda x} \implies \boldsymbol{E}, \boldsymbol{B} \sim e^{\pm \lambda x}$$

The boundary condition at infinity will kill off the exponential blow up. Hence the magnetic field will exponentially decay inside the superconductor with penetration length $\frac{1}{\lambda}$. This gives an account of the **Meissner effect**.

6.1.2 Relation of flux quantum to Meissner effect

Consider a cylinder of superconducting material with a cylindrical hole in it. Start at high temperature with a magnetic field passing through the system. As the temperature is decreased, the magnetic field lines will avoid the material, but will also pass through the center of the cylinder through the hole. When the magnetic field is switched off, the flux lines that pass through the hole will be trapped and will be forced to loop around outside the cylinder to form a closed loop. The flux lines are trapped since the material does not permit a magnetic flux inside the material. Note that since there are no currents flowing, we set $\boldsymbol{J} = 0$ and hence find the relation between the ρ, θ components:

$$\boldsymbol{A} = \frac{\hbar c}{q}\nabla\theta$$
$$\implies \frac{\hbar c}{q}\oint_\Gamma \nabla\theta \cdot d\boldsymbol{s} = \oint_\Gamma \boldsymbol{A} \cdot d\boldsymbol{s}$$

Pick the path Γ that is contained inside the superconducting material and that encircles the cylindrical hole. Apply Stokes' theorem to write:

$$\oint_\Gamma \boldsymbol{A} \cdot d\boldsymbol{s} = \int_{S(\Gamma)} \nabla \times \boldsymbol{A} \cdot d\boldsymbol{n} = \Phi_B$$
$$\implies \frac{\hbar c}{q}(\theta_2 - \theta_1) = \Phi_B$$

We are tempted to claim that $\theta_2 = \theta_1$ since periodicity will set the closed path angular difference to be zero. However, writing the wavefunction at the two points:

$$\psi(\theta_1) = \sqrt{\rho}e^{i\theta_1}$$
$$\psi(\theta_2) = \sqrt{\rho}e^{i\theta_2}$$

Requiring that $\psi(\theta_1) = \psi(\theta_2)$ just requires that $\theta_1 = \theta_2 + 2\pi n, n \in \mathbb{Z}$. This gives us:

$$\Phi_B = \frac{\hbar c}{q}2\pi n, \quad n \in \mathbb{Z}$$

This is the same flux quantum. This statement implies that the trapped magnetic flux is quantized. Note that $q = 2q_e$ in this case because a Cooper pair is made of two electrons.

6.2 Wednesday 4 May 2016

6.2.1 Relationship between superconductors and magnetic monopoles

Consider embedding some magnetic monopoles inside a superconductor. Recall that if we introduce Dirac strings connecting monopoles, then we can retain the vanishing of the divergence of $\boldsymbol{B}$. We want the magnetic fields to be exponentially damped inside the superconductor since the photon has an effective mass. If there is a monopole and an antimonopole inside the superconductor, the best configuration for the magnetic field lines are for them to be squashed into a string connecting the two entities. This string is called the flux tube, which can be thought of as a dynamically formed version of the Dirac string. The energy of the flux tube is proportional to its length:

$$E = LT$$

where L is the length and T is the string tension. Note that if the energy is large enough, new monopole-antimonopole pairs form out of the vacuum. The consequence is that you can't just see an isolated monopole or antimonopole. We can hence think of the monopole-antimonopole structure as a bound state. This system is isomorphic to quark confinement.

6.2.2 Josephson Junctions

Consider two superconductors separated by an insulator. The two superconductor system can be written as a matrix of two Cooper pair wavefunctions:

$$|\psi\rangle = \begin{pmatrix} |\psi_1\rangle \\ |\psi_2\rangle \end{pmatrix}$$

Define the Hamiltonian with interaction terms (all terms are matrices) with a tunneling rate K:

$$\boldsymbol{H} = \begin{pmatrix} U_1 & K \\ K & U_2 \end{pmatrix}$$

Then Schrodinger's equation gives:

$$\begin{aligned} i\hbar\frac{\partial\psi_1}{\partial t} &= U_1\psi_1 + K\psi_2 \\ i\hbar\frac{\partial\psi_2}{\partial t} &= U_2\psi_2 + K\psi_1 \end{aligned}$$

Assume that the difference in energies arises from a voltage difference:

$$U_1 - U_2 = qV$$

Hence we write, taking the zero of the energy to be halfway between U_1 and U_2,:

$$\begin{aligned} i\hbar\frac{\partial\psi_1}{\partial t} &= \frac{qV}{2}\psi_1 + K\psi_2 \\ i\hbar\frac{\partial\psi_2}{\partial t} &= -\frac{qV}{2}\psi_2 + K\psi_1 \end{aligned}$$

The wavefunction ansatz is:

$$\begin{aligned} \psi_1 &= \sqrt{\rho_1}e^{i\theta_1} \\ \psi_2 &= \sqrt{\rho_2}e^{i\theta_2} \end{aligned}$$

The two complex equations in Schrodinger's equation provide four conditions. Hence we may solve for the components of the wavefunction:

$$\dot{\rho_1} = -\dot{\rho_2} = \frac{2}{\hbar} K \sqrt{\rho_1 \rho_2} \sin(\delta), \quad \delta = \theta_2 - \theta_1$$
$$\dot{\theta_1} = \frac{K}{\hbar} \sqrt{\frac{\rho_2}{\rho_1}} \cos\delta - \frac{qV}{2\hbar}$$
$$\dot{\theta_2} = \frac{K}{\hbar} \sqrt{\frac{\rho_1}{\rho_2}} \cos\delta + \frac{qV}{2\hbar}$$

Define the current flow from side 1 to side 2 through the function (which is equal to $\dot{\rho}_1$):

$$J = \frac{2}{\hbar} K \sqrt{\rho_1 \rho_2} \sin\delta$$

Consider connecting the two superconductors together to complete the circuit. Then the charge densities ρ_1, ρ_2 are constant (charges are replenished), even though there are charges hopping through the junction (nonzero J). Call $\rho_1 = \rho_2 = \rho_0$. The time derivatives give the current that would flow if the replenishment did not occur. Then the current is given by:

$$J = J_0 \sin\delta, \quad J_0 \equiv \frac{2K\rho_0}{\hbar} = \text{constant}$$

We may solve for $\delta = \theta_2 - \theta_1$ by combining the equations for the angles, and noting that $\rho_1 = \rho_2 = \rho_0$ since the charges are replenished:

$$\dot{\delta} = \dot{\theta}_2 - \dot{\theta}_1 = \frac{qV(t)}{\hbar}$$
$$\implies \delta(t) = \delta(0) + \frac{q}{\hbar} \int_0^t V(t) dt$$
$$\implies J(t) = J_0 \sin\left[\delta(0) + \frac{q}{\hbar} \int_0^t V(t) dt\right]$$

We consider the leading order term in $\hbar$. Since the integral term is of order $\frac{1}{\hbar}$, is a classical effect that does not disappear as $\hbar \to 0$. The constant $\delta(0)$ term, on the other hand, is a quantum effect. Even if the potential difference is zero, there is still a current due to $\delta(0)$.

Suppose the potential difference is constant. Then in the limit of large time:

$$J \sim \sin\frac{qV_0 t}{\hbar}$$

which is a rapidly oscillating function. Hence the time integrated current through the junction will zero out. Hence if V_0 is nonzero, the Josephson effect will be washed out.

It is possible to obtain a current by applying a very high frequency voltage: $V(t) = V_0 + v\cos\omega t$. Then:

$$\delta(t) = \delta_0 + \frac{q}{\hbar} V_0 t + \frac{qv}{\hbar\omega} \sin\omega t$$

To first order, the sine can be written:

$$\sin(x + \Delta x) \approx \sin x + \Delta x \cos x$$
$$\implies J(t) = J_0 \left[\sin\left(\delta_0 + \frac{qV_0 t}{\hbar}\right) + \frac{qv}{\hbar\omega} \sin\omega t \cos\left(\delta_0 + \frac{qV_0 t}{\hbar}\right)\right]$$

The first term averages to zero. If we pick $\omega = \frac{qV_0}{\hbar}$, then the second term is:

$$J_2 = J_0 \frac{qv}{\hbar\omega} \sin\frac{qV_0 t}{\hbar} \cos\left(\delta_0 + \frac{qV_0 t}{\hbar}\right)$$
$$= J_0 \frac{qv}{\hbar\omega} \frac{1}{2} \left[\sin\left(\delta_0 + \frac{2qV_0 t}{\hbar}\right) - \sin\delta_0\right]$$

and the $\sin\delta_0$ term does not average to zero. This can be considered a resonance effect.

Including the effect of the vector potential If there is a vector potential across the junction, the formula for the current is modified:

$$J = J_0 \sin\left(\delta_0 + \frac{2q_e}{\hbar}\int \boldsymbol{A}\cdot d\boldsymbol{s}\right)$$

where the integral is taken across the junction. This results from the value of K being modified in phase by the vector potential. Note that q_e is the charge of a single electron.

6.2.3 Double Josephson Junction

Consider a donut topology with two Josephson junctions between the two contacts at opposite sides of the ring. Put a solenoid in the empty space at the center. Then there are two paths for the electrons to take, which we call Γ_1 and Γ_2. The presence of the magnetic field threading the center creates a phase shift between the paths due to the Aharanov-Bohm effect. Then by measuring the current, we can determine the magnetic field threading the donut center. Recall that δ in the previous discussion of the Josephson function was the phase difference across each junction. Since we now have two junctions, we write down two phase shifts for each of the junctions δ_1, δ_2. Then the phase shift along each of the paths is ($q = 2q_e$):

$$\phi(\Gamma_1) = \frac{q}{\hbar}\int_{\Gamma_1} \boldsymbol{A}\cdot d\boldsymbol{r} + \delta_1$$
$$\phi(\Gamma_2) = \frac{q}{\hbar}\int_{\Gamma_2} \boldsymbol{A}\cdot d\boldsymbol{r} + \delta_2$$

Now we know that the difference between the vector potential contributions of the two paths is related to the magnetic flux:

$$\phi(\Gamma_1) - \phi(\Gamma_2) = \frac{q}{\hbar c}\Phi_B + \delta_1 - \delta_2$$

But this total phase shift must vanish (why?):

$$\frac{q}{\hbar c}\Phi_B = \delta_2 - \delta_1$$

Write each of the phase shifts as:

$$\delta_1 = \delta_0 - \frac{q}{2\hbar c}\Phi_B, \quad \delta_0 = \frac{\delta_1 + \delta_2}{2}$$
$$\delta_2 = \delta_0 + \frac{q}{2\hbar c}\Phi_B$$

The total current flowing through the loop is:

$$\begin{aligned} J_{tot} &= J_1 + J_2 \\ &= J_0 \sin\left(\delta_0 - \frac{q\Phi_B}{2\hbar c}\right) + J_0 \sin\left(\delta_0 + \frac{q\Phi_B}{2\hbar c}\right) \\ &= 2J_0 \sin\delta_0 \cos\frac{q\Phi_B}{2\hbar c} \end{aligned}$$

This maximum current is bound above by $\sin\delta_0 \leq 1$:

$$|J_{max}| = 2J_0 \cos\frac{q\Phi_B}{2\hbar c}$$

so that the maximum current oscillates as the magnetic field is increased. In particular, the current is maximized when the flux is an integer multiple of the flux quantum:

$$\Phi = n\frac{\pi\hbar}{q_e}$$

6.3 Friday, 6 May 2016

6.3.1 Crystals

Consider a 1D crystal with the potential:

$$V(x) = \begin{cases} V_0, & -b \leq x \leq 0 \\ 0, & 0 \leq x \leq a \\ V_0, & a \leq x \leq a+b \\ 0, & a+b \leq x \leq 2a \end{cases}$$

so that the spacing between potential maxima is a and the peaks are of width b. The periodicity of the potential implies:

$$V(x+c) = V(x)$$

We write the wavefunction in a piecewise manner:

$$\psi_E(x) = \begin{cases} \psi_{1E}(x), & 0 \leq x \leq a, V = 0 \\ \psi_{2E}(x), & -b \leq x \leq 0, V = V_0 \end{cases}$$

where E is the energy of the eigenstate. Let E be such that $0 < E < V_0$. The wavefunction satisfies the TISE:

$$\frac{d^2\psi_{1E}}{dx^2} + \frac{2mE}{\hbar^2}\psi_{1E} = 0$$
$$\frac{d^2\psi_{2E}}{dx^2} + \frac{2m(E-V_0)}{\hbar^2}\psi_{2E} = 0$$

Make the ansatz:

$$\psi_{1E} = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}, \quad k_1 = \frac{\sqrt{2mE}}{\hbar}$$
$$\psi_{2E} = A_2 e^{k_2 x} + B_2 e^{-k_2 x}, \quad k_2 = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

Define the discrete translation operator:

$$T[\psi(x)] = \psi(x+c)$$

The symmetry of the Hamiltonian about discrete translation implies:

$$[T, H] = 0$$

We can write the translation operator as a unitary operator:

$$T = e^{ipc/\hbar}$$

where p is the momentum operator. Since H and T commute, then $T\psi_E$ is also an energy eigenfunction with the same eigenvalue. Since the translation operator is unitary,

$$T\psi_E = t\psi_E$$

where t has unit magnitude (pure phase), since the eigenvalues of unitary matrices are phases. Then we can write:

$$t = e^{ikc}$$

where k is a new quantum number. Then we have:

$$\psi_E(x+c) = e^{ikc}\psi_E(x)$$

Applying the shift N times:

$$T^N\psi_E(x) = \psi_E(x+Nc) = e^{ikNc}\psi_E(x)$$

We hence parametrize our wavefunctions:

$$\psi_E(x) = u_k(x)e^{ikx}$$

where $u_k(x)$ is a periodic function of period c and k is the same variable as defined in the eigenvalue of the translation operator.

Proceed to match the wavefunction boundary conditions:

$$\psi_{1E}(0) = \psi_{2E}(0) \tag{6.1}$$

$$\left.\frac{\partial\psi_{1E}}{\partial x}\right|_{x=0} = \left.\frac{\partial\psi_{2E}}{\partial x}\right|_{x=0} \tag{6.2}$$

Substituting the ansatz equations:

$$A_1 + B_1 = A_2 + B_2$$
$$ik_1A_1 - ik_1B_1 = k_2A_2 - k_2B_2$$

The periodicity condition requires:

$$u_k(a) = u_k(-b) \implies e^{-ika}\psi_{1E}(a) = e^{ikb}\psi_{2E}(-b) \tag{6.3}$$

$$u_k'(a) = u_k'(-b) \tag{6.4}$$

which can be explicitly written as:

$$A_1e^{i(k_1-k)a} + B_1e^{-i(k_1+k)a} = A_2e^{(ik-k_2)b} + B_2e^{(ik+k_2)b}$$
$$i(k_1-k)A_1e^{i(k_1-k)a} - i(k_1+k)B_1e^{-i(k_1+k)a} = (k_2-ik)A_2e^{-(k_2-ik)b} - (k_2+ik)B_2e^{(k_2+ik)b}$$

We hence have 4 linear equations for A_1, A_2, B_1, B_2. This systems is actually overconstrained. For all the equations to hold simultaneously, we require that the determinant of the linear algebra system in terms of the unknowns to vanish:

$$\boldsymbol{M}\cdot\begin{pmatrix} A_2 \\ B_2 \\ -A_1 \\ -B_1 \end{pmatrix} = 0$$

$$\boldsymbol{M} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ k_2 & -k_2 & ik_1 & -ik_1 \\ e^{(ik-k_2)b} & e^{(ik+k_2)b} & e^{i(k_1-k)a} & e^{-i(k_1+k)a} \\ k_2e^{(ik-k_2)b} & -k_2e^{(ik+k_2)b} & ik_1e^{i(k_1-k)a} & -ik_1e^{-i(k_1+k)a} \end{pmatrix}$$

Now we know that $\boldsymbol{M}$ has a zero eigenvalue. Hence the determinant of $\boldsymbol{M}$, which is the product of its eigenvalues, is zero. Taking the determinant and setting it to zero, we find the expression:

$$\left(\frac{k_2^2-k_1^2}{2k_1k_2}\right)\sinh(k_2b)\sin(k_1a) + \cosh(k_2b)\cos(k_1a) = \cos kc$$

Recall that k_1, k_2 depend on the energy E. The RHS depend on an unknown k. Hence not every value of the energy will satisfy the above equation, and not every value of E will be allowed. Since the periodicity is $c = a + b$, we can write:

$$\left(\frac{k_2^2 - k_1^2}{2k_1k_2}\right)\sinh(k_2b)\sin(k_1a) + \cosh(k_2b)\cos(k_1a) = \cos[k(a+b)]$$

Both sides of the equation are bounded between -1 and 1. Hence a necessary condition for E to satisfy the equation above is that the LHS expression is bounded between -1 and 1. Consider plotting the LHS and RHS as functions of energy E/V_0. There will only be energy eigenstates in regions of the graph where the LHS function takes values between -1 and 1. There are gaps between the energy bands. Hence the energy spectrum is discrete.

Chapter 7

Week 7

7.1 Monday, 9 May 2016

7.1.1 More on crystals

Consider the dispersion relation around the minimum point of a particular energy band. Approximate it using a quadratic function:

$$E = E_{min} + \alpha k^2$$

Call the curvature term:

$$\alpha = \frac{\hbar^2}{2m_{eff}}$$

7.1.2 Electron-hole statistics

Recall the Fermi-Dirac distribution:

$$f_{FD} = \frac{1}{e^{(\epsilon-\mu)/k_B T} + 1}$$

The Fermi energy is defined as the energy where the occupancy is half. The actual number of occupied states as a function of energy level is hence:

$$N(E) = g(E) f_{FD}(E)$$

where $g(E)$ is the density of states.

7.2 Wednesday, 11 May 2016

7.2.1 Classical Hall Effect

Describes the motion of electric charges in a material under the application of a magnetic field. A current-carrying conductor under a transverse electric field creates a transverse (orthogonal to the magnetic field) potential due to the deflection of the moving charged particles. The natural frequency of a charged particle in a magnetic field is:

$$\omega_0 = \frac{qB}{mc}$$

7.2.2 Quantum Hall Effect

Recall that a constant magnetic field can be associated with a vector potential:

$$\boldsymbol{B} = B\hat{z}$$
$$\boldsymbol{A} = \frac{B}{2}(-y, x, 0)$$

and the Hamiltonian becomes:

$$H = \frac{(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A})^2}{2m} = \frac{(P_x + \frac{qYB}{2c})^2}{2m} + \frac{(P_y - \frac{qXB}{2c})^2}{2m}$$

Perform the gauge transformation:

$$P = P_y - \frac{qXB}{2c}$$
$$Q = \left(cP_x + \frac{qYB}{2}\right)\frac{1}{qB}$$
$$[Q, P] = i\hbar$$

Then the Hamiltonian becomes:

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega_0^2 Q^2, \quad \omega_0 = \frac{qB}{mc}$$

which we can write in terms of raising and lowering operators:

$$a = \sqrt{\frac{m\omega_0}{2\hbar}}Q + i\sqrt{\frac{1}{2m\omega_0\hbar}}P$$
$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$$

The energy quantum numbers are indexed $a^\dagger a = n = 0, 1, 2, 3, \ldots$, and these are called the Landau levels.

There is an infinite degeneracy in the Landau levels. That is, each level n has infinite degeneracy. To see this explicitly, define:

$$P' = \frac{cP_x - \frac{qYB}{2}}{qB}$$
$$Q' = P_y + \frac{qXB}{2c}$$

These new set of parameters are canonical and commute with the Hamiltonian (since they commute with Q, P).

Ground state degeneracy The ground state (Lowest Landau Level LLL) is defined as:

$$a\,|0\rangle = 0$$

This can be written in the position basis by replacing a by Q, P, and then writing Q and P in terms of the original physical X, Y, P_x, P_y variables. We obtain:

$$\left[\sqrt{\frac{mqB}{2\hbar mc}}\frac{cP_x + \frac{qYB}{2}}{qB} + i\sqrt{\frac{c}{2\hbar qB}}\left(P_x - \frac{qXB}{2c}\right)\right]\phi_0 = 0$$
$$\implies \sqrt{\frac{c}{2\hbar qB}}\left[(P_x + iP_y) - i\frac{qB}{2c}(X + iY)\right]\phi_0 = 0$$

Hence we can write the 2D momenta and positions as the real and imaginary parts of a complex coordinate z:

$$a = \sqrt{\frac{c}{2\hbar qB}}\left[-2i\hbar\frac{\partial}{\partial z^*} - i\frac{qB}{2c}z\right]$$

where the complex derivatives are:

$$\frac{\partial}{\partial z^*} = \frac{1}{2}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)$$

The LLL hence satisfies (ignoring the constant coefficients):

$$\left(\frac{\partial}{\partial z^*} + \frac{qB}{4\hbar c}z\right)\psi_0(z, z^*) = 0$$

Make the ansatz:

$$\psi_0(z, z^*) = e^{-qB|z|^2/4\hbar c}u(z, z^*)$$

where $|z|^2 = X^2 + Y^2$.

Then we require:

$$\frac{\partial}{\partial z^*}u(z, z^*) = 0 \implies u(z, z^*) = u(z)$$

This implies that $u(z)$ is just an arbitrary analytic function in z. $u(z)$ hence is infinite dimensional:

$$u(z) = \sum_n c_n z^n$$

The physical origin of this degeneracy can be seen by moving to a different gauge. Pick:

$$\boldsymbol{A} = B(0, x, 0), \quad \boldsymbol{B} = \nabla \times \boldsymbol{A} = B\hat{z}$$
$$\implies H = \frac{P_x^2}{2m} + \frac{1}{2m}\left(P_y - \frac{qXB}{c}\right)^2 = \frac{P_x^2}{2m} + \frac{1}{2}m\omega_0^2\left(X - \frac{P_y}{m\omega_0}\right)^2$$

The Hamiltonian hence looks like a displaced Harmonic oscillator. We can treat P_y as a number because it commutes with the rest of the operators in the Hamiltonian. The system behaves like a harmonic oscillator with a movable origin $X_0 = \frac{P_y}{m\omega_0}$. The infinite degeneracy hence arises because we can displace the entire effective potential by choosing any value for P_y and we will still obtain the same energy spectrum.

7.3 Friday 13 May 2016

7.3.1 Quantum Hall Effect continued

Recall that the LLL was written as:

$$\psi_0(z, z^*) = e^{-qB|z|^2/4\hbar c}U$$

where U was an analytic function in $z = x + iy$. We now want to estimate the size of the degeneracy for a system of fixed size. Note that we could treat the degeneracy in energy by shifting the origin of the potential $V(x)$ by the amount $x_0 = \frac{P_y}{m\omega_0}$.

Consider a box of fixed size $L_x \times L_y$. Now P_y is quantized in terms of the y-length of the box:

$$P_y = \frac{2\pi\hbar N}{L_y}, \quad N \in \mathbb{Z}$$

Similarly, the x-displacement must lie within the x-dimensions of the box:

$$0 \leq x_0 < L_x$$

These two conditions can be combined to write:

$$0 \leq N < \frac{m\omega_0 L_x L_y}{2\pi\hbar} = \frac{BA}{2\pi\hbar c/q}, \quad A = L_x L_y$$

The dimensions of the box hence form an upper bound to the quantum number N. Recall that the magnetic flux quantum is the term in the denominator:

$$0 \leq N < \frac{BA}{\Phi_q}$$

Hence the degeneracy of the ground state corresponds to the number of flux quantums you can fit into the total magnetic flux through the material.

7.3.2 Multiple electron systems

We generalize the wavefunction by writing it in terms of the complex coordinates of each particle:

$$\psi = \psi\left(z_1, z_1^*, z_2, z_2^*, \ldots, z_N, z_N^*\right) = \prod_{i=1}^{N} e^{-qB|z_i|^2/4\hbar c} U(z_1, z_1^*, \ldots)$$
$$\frac{\partial U}{\partial z_i^*} = 0$$

But note further that since the electrons are Fermions, the total wavefunction has to be totally antisymmetric about particle exchange. We can write U as:

$$U = \prod_{i=1}^{N} \prod_{j=1}^{i-1} (z_i - z_j)$$

7.3.3 Dirac Equation

The Schrodinger equation treats time and space on different footing (different number of derivatives). We now try to implement operators in the energy-momentum equation:

$$E = \sqrt{m^2c^4 + p^2c^2}$$

We identify energy with the Hamiltonian. Then we expect:

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = \sqrt{m^2c^4 - \hbar^2 c^2 \frac{\partial^2}{\partial x^2}}\, |\psi\rangle$$

This is still not Lorentz invariant. Consider taking the "square" of the equation:

$$H^2 = m^2c^4 + p^2c^2$$
$$-\hbar^2 \frac{\partial^2 |\psi\rangle}{\partial t^2} = \left(m^2c^4 - \hbar^2 c^2 \frac{\partial^2}{\partial x^2}\right) |\psi\rangle$$
$$\implies \left[\frac{\partial^2}{\partial t^2} - c^2 \frac{\partial^2}{\partial x^2} + \frac{m^2c^4}{\hbar^2}\right] \phi = 0$$

The last equation is called the **Klein-Gordon Equation**. The KG equation is Lorentz invariant. However, it is strange when interpreted as a wavefunction equation. Since it is second order in time, we require information about the first derivative

of the wavefunction as well to specify the system. Also, it admits a negative energy solution for every positive energy solution.

The negative energy solution can be seen by considering a travelling wave ansatz:

$$\begin{aligned} \phi &= e^{-i\omega t}e^{ikx} \\ \implies -\omega^2 + c^2k^2 + \frac{m^2c^4}{\hbar^2} &= 0 \\ \implies \omega &= \pm\sqrt{c^2k^2 + \frac{m^2c^4}{\hbar^2}} \equiv \pm\omega_k \end{aligned}$$

This means that ϕ must be written as a superposition over all positive and negative ω, as well as positive and negative k (4 combinations per ω_k, k set in total)

$$e^{\pm i\omega_k t}e^{\pm ikx}$$

The Dirac equation tries to make a set of first order equations by taking the "square root" of the KG equation. Explicitly, we want to write:

$$H^2 = m^2c^4 + (p_x^2 + p_y^2 + p_z^2)c^2 = \left[\beta mc^2 + c(\alpha_x P_x + \alpha_y P_y + \alpha_z P_z)\right]^2$$

and solve for β, α_i. Combine the α_i terms into a vector $\boldsymbol{\alpha}$:

$$m^2c^4 + (p_x^2 + p_y^2 + p_z^2)c^2 = \left[\beta mc^2 + c\boldsymbol{\alpha}\cdot\boldsymbol{P}\right]^2$$

Matching coefficients, and not making the assumption that α_i terms are commuting scalars (in fact, they are 4x4 matrices)

$$\begin{aligned} \beta^2 &= 1 \\ \alpha_x^2 = \alpha_y^2 &= \alpha_z^2 = 1 \\ \alpha_i\alpha_j + \alpha_j\alpha_i = 0 &\implies \{\alpha_i, \alpha_j\} = 0 \\ \alpha_i\beta + \beta\alpha_i = 0 &\implies \{\alpha_i, \beta\} = 0 \end{aligned}$$

Chapter 8

Week 8

8.1 Monday, 16 May 2016

8.1.1 Dirac Equation Continued

Recall that the conditions on the coefficients of the Dirac Equation was:

$$\begin{gathered}\beta^2 = 1 \\ \alpha_x^2 = \alpha_y^2 = \alpha_z^2 = 1 \\ \{\alpha_i, \alpha_j\} = 0 \\ \{\alpha_i, \beta\} = 0\end{gathered}$$

The matrices that satisfy this condition are:

$$\begin{gathered}\boldsymbol{\beta} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \\ (\boldsymbol{\alpha})_i = \begin{pmatrix} \mathbf{0} & \boldsymbol{\sigma}_i \\ \boldsymbol{\sigma}_i & \mathbf{0} \end{pmatrix}, \quad i = x, y, z \\ \boldsymbol{\alpha} = \begin{pmatrix} \mathbf{0} & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & \mathbf{0} \end{pmatrix}\end{gathered}$$

where the Pauli matrices are:

$$\begin{gathered}\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\end{gathered}$$

Hence the Dirac equation acts on wavefunctions that are represented by four-component vectors. We end up with the symmetric equation:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} |\psi\rangle &= (c\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta mc^2) |\psi\rangle \\ i\hbar \frac{\partial \psi}{\partial t} &= -ic\hbar \boldsymbol{\alpha} \cdot \nabla \psi + \beta mc^2 \psi \end{aligned}$$

8.1.2 Dirac Fermion in EM field

Recall that to introduce an electromagnetic field, we just make the substitutions:

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

The Dirac equation is hence:

$$i\hbar\frac{\partial}{\partial t}\left|\psi\right\rangle = (c\boldsymbol{\alpha}\cdot(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}) + \beta mc^2 + q\phi)\left|\psi\right\rangle$$

Define:

$$\boldsymbol{\pi} = \boldsymbol{p} - \frac{q}{c}\boldsymbol{A}$$

We want to consider a time-independent form of the Dirac Equation. Ignore the electric field for now. Then we define energy eigenfunction ψ_E that satisfies:

$$\begin{aligned} i\hbar\frac{\partial\psi_E}{\partial t} &= E\psi_E = H\psi_E \\ \implies E\psi_E &= \left(c\boldsymbol{\alpha}\cdot\boldsymbol{\pi} + \beta mc^2\right)\psi_E \end{aligned}$$

Write the eigenfunction as a two-component vector made out of two-component vectors (total 4 components):

$$\psi_E = \begin{pmatrix} \boldsymbol{\chi} \\ \boldsymbol{\Phi} \end{pmatrix}$$

The time-independent equation is actually four equations (E is a scalar multiplied by the 4x4 identity):

$$\begin{aligned} &\begin{pmatrix} (E - mc^2)\mathbf{1} & -c\boldsymbol{\sigma}\cdot\boldsymbol{\pi} \\ -c\boldsymbol{\sigma}\cdot\boldsymbol{\pi} & (E + mc^2)\mathbf{1} \end{pmatrix}\begin{pmatrix} \boldsymbol{\chi} \\ \boldsymbol{\Phi} \end{pmatrix} \\ \implies &\begin{cases} (E - mc^2)\boldsymbol{\chi} - c(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\boldsymbol{\Phi} = 0 \\ (E + mc^2)\boldsymbol{\Phi} - c(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\boldsymbol{\chi} = 0 \end{cases} \end{aligned}$$

Solving using the last expression,

$$\boldsymbol{\Phi} = \frac{c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{E + mc^2}\boldsymbol{\chi}$$

We consider the non-relativistic limit. We expect that the energy behaves as:

$$E = mc^2 + E_s, \quad E_s \ll mc_2$$

where E_s is the non-relativistic energy in the Schrodinger equation.
Then the coefficient relating $\boldsymbol{\Phi}$ and $\boldsymbol{\chi}$ is of order:

$$\frac{c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{E + mc^2} \sim \left(\frac{mvc}{mc^2}\right) \sim \frac{v}{c} \ll 1$$

since we take:

$$E + mc^2 \approx 2mc^2$$

In the non-relativistic limit, the simultaneous equations are:

$$\begin{aligned} E_s\boldsymbol{\chi} = c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\boldsymbol{\Phi} &= \frac{(c\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(c\boldsymbol{\sigma}\cdot\boldsymbol{\pi})}{E + mc^2}\boldsymbol{\chi} \\ \implies E_s\boldsymbol{\chi} &\approx \frac{1}{2m}(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\boldsymbol{\chi} \end{aligned}$$

Hence we observe that $(\boldsymbol{\sigma} \cdot \boldsymbol{\pi})$ takes the role of the momentum.

Recall that the product of Pauli matrices with vectors $\boldsymbol{A}, \boldsymbol{B}$ can be written:

$$(\boldsymbol{\sigma} \cdot \vec{A})(\boldsymbol{\sigma} \cdot \vec{B}) = (\vec{A} \cdot \vec{B})\mathbf{1} + i\boldsymbol{\sigma} \cdot (\vec{A} \times \vec{B})$$

Now $\vec{\pi} = \boldsymbol{\pi}$ contains derivative operates, hence the cross product with itself is nonzero.

$$\vec{\pi} \times \vec{\pi} = \frac{iq\hbar}{c}\boldsymbol{B}$$

Hence in the non-relativistic limit, we have:

$$E_s \boldsymbol{\chi} = \frac{1}{2m}\left[\vec{\pi}^2 - \frac{q\hbar}{c}\vec{\sigma} \cdot \vec{B}\right]\boldsymbol{\chi} = H_{eff}\boldsymbol{\chi}$$

where H_{eff} is the effective Hamiltonian for $\boldsymbol{\chi}$. Explicitly,

$$H_{eff} = \frac{(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A})^2}{2m} - \frac{q\hbar}{2mc}\boldsymbol{\sigma} \cdot \vec{B}$$

The second term corresponds to the potential energy of a magnetic dipole moment in a magnetic field. Note that the magnetic moment is a 2x2 matrix in this case.

$$\vec{\mu} = \frac{q\hbar}{2mc}\boldsymbol{\sigma}$$
$$H_{eff} = \frac{(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A})^2}{2m} - \vec{\mu} \cdot \vec{B}$$

The implication of this derivation is that a Dirac particle possesses a magnetic moment, and this was determined by the overlap of relativity and quantum mechanics!

8.1.3 Wavefunction interpretation of Dirac Equation

Ignore the vector potential for now $\boldsymbol{p} = \boldsymbol{\pi}$. Then we had the equations:

$$\boldsymbol{\chi} = \frac{c\boldsymbol{\sigma} \cdot \boldsymbol{p}}{E - mc^2}\boldsymbol{\Phi}$$
$$\boldsymbol{\Phi} = \frac{c\boldsymbol{\sigma} \cdot \boldsymbol{p}}{E + mc^2}\boldsymbol{\chi}$$
$$\implies \boldsymbol{\chi} = \frac{c^2}{E^2 - m^2c^4}(\boldsymbol{\sigma} \cdot \boldsymbol{p})(\boldsymbol{\sigma} \cdot \boldsymbol{p})\boldsymbol{\chi} = \frac{\boldsymbol{p}^2c^2}{E^2 - m^2c^4}\boldsymbol{\chi}$$
$$\implies E^2 = p^2c^2 + m^2c^4$$

which still admits negative energy solutions.

Dirac's proposal States from negative infinity energy to zero energy are filled with a sea of electrons. Negative energy electrons can be excited to positive energy to leave behind a 'hole' that behaves as an antiparticle.

8.2 Wednesday, 18 May 2016

8.2.1 QM and field theory

Define the d'Alembertian:

$$\Box \equiv \frac{\partial^2}{\partial t^2} - c^2\frac{\partial^2}{\partial x^2}$$

Then the Klein-Gordon equation can be written as:

$$\left[\Box + \frac{m^2c^4}{\hbar^2}\right]\phi = 0$$

The interpretation of the scalar field ϕ solution is the Higgs boson or Higgs field.

8.2.2 Correspondence between classical fields and many classical particles

Consider a classical model of N atoms of a crystal with coordinate $x_n(t)$. Let the spacing between atoms be a and the spring constant between atoms be k. Let the mass of each atom be m. The Lagrangian of the 1D system is:

$$L = \sum_{n=-N/2}^{N/2} \left[\frac{1}{2} m \dot{x}_n^2 - \frac{k}{2} \left(x_{n+1} - x_n - a \right)^2 \right]$$

Note that the equilibrium position of the nth particle is $\bar{x}_n = na$ so we can parametrize the motion by the deviation from the equilibrium:

$$x_n(t) = \bar{x}_n + y_n(t)$$

Then the Lagrangian is:

$$L = \sum_{n=-N/2}^{N/2} \left[\frac{1}{2} m \dot{y}_n^2 - \frac{k}{2} \left(y_{n+1} - y_n \right)^2 \right]$$

Moving into the continuum limit where $a \to 0, N \to \infty$, we let the total length be $Na = L$ and parametrize the location of the particles using the physical position:

$$x = na \in \left\{ \frac{-L}{2}, \frac{L}{2} \right\}$$

Then the displacement of the particles is given by $y_n(t) \to y(x,t)$, where x is defined in the previous equation. Note that $y(x,t)$ is now a field with an additional parameter to time. The Lagrangian can hence be written as an integral:

$$\begin{gathered} y_n(t) \to y(x,t) \\ y_{n+1} - y_n \to a \frac{\partial y(x)}{\partial x} \\ \sum_{n=-N/2}^{N/2} \to \frac{1}{a} \int_{-L/2}^{L/2} dx \\ L = \frac{1}{a} \int_{-L/2}^{L/2} dx \left[\frac{1}{2} m \dot{y}^2 - \frac{k}{2} \left(a \frac{\partial y}{\partial x} \right)^2 \right] \end{gathered}$$

Define the rescaled field:

$$\begin{gathered} \phi = \sqrt{\frac{m}{a}} y \\ \implies L = \int_{-L/2}^{L/2} dx \left[\frac{1}{2} \dot{\phi}^2 - \frac{1}{2} \frac{ka^2}{m} \left(\frac{\partial \phi}{\partial x} \right)^2 \right] \end{gathered}$$

Define the velocity $v^2 = \frac{ka^2}{m}$. Then we have:

$$L = \int_{-L/2}^{L/2} dx \left[\frac{1}{2} \dot{\phi}^2 - \frac{v^2}{2} \left(\frac{\partial \phi}{\partial x} \right)^2 \right]$$

Note that this Lagrangian is relativistic! Write the 3D version of the Lagrangian:

$$L = \int d^3x \left[\frac{1}{2} \dot{\phi}^2 - \frac{v^2}{2} (\nabla \phi) \cdot (\nabla \phi) \right]$$

and the action:

$$S = \int L(t)dt = \int d^4x \left[\frac{1}{2}\dot{\phi}^2 - \frac{v^2}{2}(\nabla\phi)\cdot(\nabla\phi)\right]$$

Note that ϕ is measuring the disturbance away from equilibrium. Think of equilibrium $\phi = 0$ as being the vacuum.

Now consider the Euler-Lagrange equations for the discrete case:

$$m\ddot{y}_n - k(y_{n+1} - y_n) + k(y_n - y_{n-1}) = 0$$

which can be made continuous:

$$\begin{aligned}
\ddot{y}_n - \frac{k}{m}\left[\frac{y_{n+1} - y_n}{a} - \frac{y_n - y_{n-1}}{a}\right]a = 0 \\
\implies \ddot{\phi} - \frac{ka^2}{m}\frac{\partial^2\phi}{\partial x^2}\phi = 0 \\
\implies \ddot{\phi} - v^2\frac{\partial^2\phi}{\partial x^2}\phi = 0
\end{aligned}$$

This is precisely the Klein-Gordon equation in the massive limit where $m \to 0$.

8.3 Friday, 20 May 2016

8.3.1 Quantum Field Theory, continued

Recall that for the linear spring and mass system, the action was a Lorentz invariant and corresponded to the massless Klein-Gordon field:

$$S = \int Ldt = \int d^4x \left(\frac{1}{2}\dot{\phi}^2 - \frac{1}{2}v^2(\nabla\phi)^2\right)$$

which gave the wave equation of motion under the Euler-Lagrange equation:

$$\ddot{\phi} - v^2\nabla^2\phi = 0$$

Recall that we can write the wave equation solutions in 1D by superposing waves travelling in $\pm\hat{x}$ directions:

$$\phi(x,t) = f_R(x - vt) + f_L(x + vt)$$

Now we want to include the effect of mass in the Klein-Gordon equation. Note that the terms $\left(\frac{1}{2}\dot{\phi}^2 - \frac{1}{2}v^2(\nabla\phi)^2\right)$ can be thought of as a kinetic energy since space and time are mixed in different frames. We now consider adding a potential energy to the action:

$$S = \int d^4x \left(\frac{1}{2}\dot{\phi}^2 - \frac{1}{2}v^2(\nabla\phi)^2 - V(\phi(x))\right)$$

where the potential must only depend on $\phi(x)$ since the derivatives of ϕ already enter into the kinetic terms. Consider a Taylor expansion of V:

$$V(\phi(x)) = C + \gamma\phi + \frac{m^2\phi^2}{2} + \dots$$

We can remove the linear term by completing the square and shifting the origin. We want to work at the minimum of the potential. The reason why we chose m^2 for the second derivative coefficient is because it will become the mass upon further calculation. Then the terms in the integral be written as (setting all fundamental constants to unity $v = c = 1, \hbar = 1$):

$$\left[\partial_t^2 - \nabla^2 + m^2\right]\phi(x,t) = 0$$

Make the exponential ansatz:

$$\begin{aligned}\phi(x,t) &= e^{i\vec{k}\cdot\vec{x}-i\omega t}\\ \implies -\omega^2 + k^2 + m^2 &= 0\\ \implies \omega = \pm\omega_k, \quad \omega_k &= \sqrt{k^2+m^2}\end{aligned}$$

Hence we can write the general solution as a superposition of k-modes:

$$\phi(\vec{x},t) = \int d^3k \frac{1}{f(\vec{k})}\left[a(\vec{k})e^{i\vec{k}\cdot\vec{x}-i\omega_k t} + a(\vec{k})^* e^{-i\vec{k}\cdot\vec{x}+i\omega_k t}\right]$$

where we have added the complex conjugate to ensure that the function is real-valued. Note that this can be interpreted as waves moving in different directions as in the massless wave solution. We have also included the real function $f(\vec{k})$.

We write the general solution in a manifestly Lorentz invariant form. Write:

$$-\vec{k}\cdot\vec{x} + \omega t = (\omega, \vec{k})\begin{pmatrix} 1 & 0 \\ 0 & -\mathbf{1}_{3\times 3}\end{pmatrix}\begin{pmatrix} t \\ \vec{x}\end{pmatrix} = k^\mu \eta_{\mu\nu} x^\nu \equiv kx$$

where the 4×4 matrix is the metric tensor. Note that k and x on the RHS are now four-vectors. Hence the general solution becomes:

$$\phi(\vec{x},t) = \int d^3k \frac{1}{f(\vec{k})}\left[a(\vec{k})e^{-ikx} + a(\vec{k})^* e^{ikx}\right]$$

Note that the integration measure is not yet Lorentz invariant. We hence need to choose $f(\vec{k})$ so that $\int \frac{d^3k}{f(\vec{k})}$ is Lorentz invariant. It will turn out that we can write it as:

$$\int \frac{d^3k}{f(\vec{k})} = \int \frac{d^3k}{2\omega_k} = \int \frac{d^3k}{2\sqrt{\vec{k}^2+m^2}}$$

The way we are going to proceed is to integrate over d^4k instead of d^3k (i.e. integrate over the k_0 term) and show that the integration of the k_0 term results in the RHS. Consider the object:

$$\int d^4k \delta(k^2 - m^2)\theta(k_0)$$

Note that $k^2 = k^\mu \eta_{\mu\nu} k^\nu = k_0^2 - (k_1^2 + k_2^2 + k_3^2)$ and θ is the Heaviside step function. Splitting the integration variables:

$$\int d^4k \delta(k^2 - m^2)\theta(k_0) = \int dk_0 d^3k \delta(k_0^2 - \vec{k}^2 - m^2)\theta(k_0)$$

Note that the roots of the argument of the delta function are simply $\pm\omega_k = \pm\sqrt{\vec{k}^2+m^2}$. Hence when we evaluate the delta function, we can write it using two terms and divide by the derivative of the function inside the delta function (Jacobian):

$$\int dk_0 d^3k \delta(k_0^2 - \vec{k}^2 - m^2)\theta(k_0) = \int dk_0 d^3k \frac{\theta(k_0)}{|2k_0|}\left[\delta(k_0-\omega_k) + \delta(k_0+\omega_k)\right]$$

Now the step function ensures that contributions from negative k_0 are removed. This means that the $\delta(k_0+\omega_k)$ term disappears:

$$\int dk_0 d^3k \frac{\theta(k_0)}{|2k_0|}\left[\delta(k_0-\omega_k) + \delta(k_0+\omega_k)\right] = \int dk_0 d^3k \frac{\theta(k_0)}{|2k_0|}\left[\delta(k_0-\omega_k)\right] = \int \frac{d^3k}{2\omega_k}$$

Now we need to show that the proposed object is Lorentz invariant. The main issue is that $\theta(k_0)$ appears to be not Lorentz invariant. But note that k_0 is related to the energy. The sign of the energy cannot change upon Lorentz boosts. This means that $\theta(k_0)$, which is just dependent on the sign of k_0, is invariant under Lorentz boosts. Hence the proposed object is Lorentz invariant.

We hence have the following field that is manifestly Lorentz invariant (adding factors of 2π):

$$\phi(\vec{x},t) = \int d^3k \frac{1}{(2\pi)^3 2\omega_k} \left[a(\vec{k}) e^{-ikx} + a(\vec{k})^* e^{ikx} \right]$$

Define the Lorentz invariant measure of volume in k-space:

$$\int d\tilde{k} = \int d^3k \frac{1}{(2\pi)^3 2\omega_k}$$

8.3.2 Finally moving into QFT

We now want to quantize all the terms in the previous section. Note that we can write the Lagrangian density using the previous section:

$$L = \frac{1}{2}\dot{\phi}^2 - \frac{1}{2}(\nabla\phi)^2 - \frac{1}{2}m^2\phi^2$$

We want the Hamiltonian:

$$H = \sum_i p_i \dot{q}_i - L, \quad p_i = \frac{\partial L}{\partial \dot{q}_i}$$

But now note that the dot derivatives in $\dot{q}$ is different (not just a coordinate time derivative) now because we have placed space and time on the same footing. The analogy to the canonical momentum in QFT is:

$$\pi(\vec{x},t) = \frac{\partial L}{\partial \dot{\phi}(\vec{x},t)} = \dot{\phi}$$

where the dot refers to the time derivative. The Hamiltonian density becomes:

$$H(\pi,t) = \pi\dot{\phi} - L = \frac{\dot{\phi}^2}{2} + \frac{1}{2}(\nabla\phi)^2 + \frac{1}{2}m^2\phi^2$$

The Hamiltonian density is not Lorentz invariant because the sign between time and space is not a negative sign. We break Lorentz invariance by imposing initial conditions along a single time-slice. However, the evolution dynamics from then onwards will be Lorentz invariant.

Chapter 9

Week 9

9.1 Monday, 23 May 2016

9.1.1 Quantum Field Theory

Recall that we wrote the phonon field in Lorentz invariant form:

$$\phi(\vec{x},t) = \int d\tilde{k}\left[a(\vec{k})e^{-ikx} + a^*(\vec{k})e^{ikx}\right]$$
$$\int d\tilde{k} = \int \frac{d^3k}{(2\pi)^3 2\omega_k}, \quad \omega_k = \sqrt{k^2+m^2}$$

and the Hamiltonian was not Lorentz invariant:

$$H(\vec{x},t) = \frac{1}{2}\dot{\phi}^2 + \frac{1}{2}(\nabla\phi)^2 + \frac{1}{2}m^2\phi^2$$

where the first two derivative terms behave like a kinetic energy due to deviations from equilibrium. Consider the integral of the Hamiltonian density:

$$\mathcal{H} = \int d^3x H[\phi]$$

Note that each term involves an integration of $\vec{k}, \vec{k}'$ and $\vec{x}$. First implement the x-integrals because you get delta functions:

$$\int d^3x e^{-i\vec{k}\cdot\vec{x}} e^{-i\vec{k}'\cdot\vec{x}} \sim \delta^3(\vec{k}+\vec{k}')$$

After all the algebra and integrating the delta functions,

$$\begin{aligned}\mathcal{H} &= \frac{1}{2}\int\left[\frac{d^3\vec{k}}{(2\pi)^3 2\omega_k}\right]\omega_k\left(a^*(\vec{k})a(\vec{k}) + a(\vec{k})a^*(\vec{k})\right)\\ &= \frac{1}{2}\int d\tilde{k}\omega_k\left(a^*(\vec{k})a(\vec{k}) + a(\vec{k})a^*(\vec{k})\right)\end{aligned}$$

Note that we have not assumed that $a(\vec{k})$ commutes with each other. In fact, it will be a matrix that will be quantized later. The interpretation of $\mathcal{H}$ is that it is a sum over an infinite number of harmonic oscillators. ω_k is hence proportional to the energy of the oscillator and a^* and a are raising and lowering operators for the field. Replace the complex conjugates with adjoints. We hence proceed to quantize a using the canonical commutation relations for raising and lowering operators:

$$[a(\vec{k}), a(\vec{k}')] = 0$$
$$[a^\dagger(\vec{k}), a^\dagger(\vec{k}')] = 0$$
$$[a(\vec{k}), a^\dagger(\vec{k}')] = (2\pi)^3 2\omega_k \delta^3(\vec{k}-\vec{k}')$$

where the normalization coefficient is just the denominator of the Lorentz invariant integral $(2\pi)^3 2\omega_k$.

The Hamiltonian can hence be written as:

$$\mathcal{H} = \int d\tilde{k}\omega_k a^\dagger(\vec{k})a(\vec{k}) + C$$

where C is actually infinity when the constant is integrated over all $\vec{k}$. However, we can shift the Hamiltonian by any constant and it will not change the dynamics. C is unobservable. We may hence throw C out.

$$\mathcal{H} = \int d\tilde{k}\omega_k a^\dagger(\vec{k})a(\vec{k})$$

Aside Note that in gravity, this is not true! C in this case is known as the cosmological constant, a constant parameter added to every position in spacetime.

We now define the states by building objects out of the raising and lowering operators. The ground state satisfies:

$$a(\vec{k})\,|0\rangle = 0, \quad \forall\vec{k}, \quad \langle 0|0\rangle = 1$$

Consider the following objects:

$$\begin{aligned}
\left|\vec{k}_1\right\rangle &= a^\dagger(\vec{k}_1)|0\rangle \\
\left|\vec{k}_1, \vec{k}_2\right\rangle &= a^\dagger(\vec{k}_1)a^\dagger(\vec{k}_2)|0\rangle \\
\left|\vec{k}_1, \ldots, \vec{k}_N\right\rangle &= a^\dagger(\vec{k}_1)\cdots a^\dagger(\vec{k}_N)\,|0\rangle
\end{aligned}$$

These kets live in the Fock space, which is the Hilbert space that describes the vacuum and all particles.

Consider the normalization condition:

$$\begin{aligned}
\langle\vec{k}_1|\vec{k}_2\rangle &= \langle 0|\, a(\vec{k}_1)a^\dagger(\vec{k}_2)\,|0\rangle \\
&= \langle 0|\, a^\dagger(\vec{k}_2)a(\vec{k}_1) + (2\pi)^3 2\omega_k\delta^3(\vec{k}_1 - \vec{k}_2)\,|0\rangle \\
&= (2\pi)^3 2\omega_k\delta^3(\vec{k}_1 - \vec{k}_2), \quad \langle 0|0\rangle = 1
\end{aligned}$$

Integrating over all $\vec{k}_1$,

$$\int d\tilde{k}_1 \langle\vec{k}_1|\vec{k}_2\rangle = \int d^3\vec{k}_1\delta^3(\vec{k}_1 - \vec{k}_2) = 1$$

9.1.2 Higher order terms in QFT

Let all the previous discussion of QFT be the leading order behavior, indicated with a 0 subscript:

$$\begin{aligned}
\mathcal{L}_0 &= \int L_0 dt \\
&= \int d^4x \left[\frac{1}{2}\dot{\phi}^2 - \frac{1}{2}(\nabla\phi)^2 - \frac{1}{2}m^2\phi^2\right] \\
&= \int d^4x \left[\frac{1}{2}\left(\frac{\partial}{\partial x^\mu}\phi\frac{\partial}{\partial x^\nu}\phi\right)\eta^{\mu\nu} - \frac{1}{2}m^2\phi^2\right] \\
&= \int d^4x \left[\frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2\right]
\end{aligned}$$

Consider the higher powers of ϕ:

$$V(\phi) = \frac{A}{3!}\phi^3 + \frac{\lambda}{4!}\phi^4 + \dots$$

Then the full Lagrangian and Hamiltonian can be written:

$$L = L_0 - V(\phi)$$
$$H = H_0 + V(\phi)$$

The leading order terms just represent uncoupled harmonic oscillators or noninteracting particles. $V(\phi)$ contains information about the interactions between modes.

9.2 Wednesday, 25 May 2016

9.2.1 More Quantum Field Theory

Recall that we wanted to extend the Lagrangian and Hamiltonian in terms of the field ϕ:

$$L = L_0 - V(\hat{\phi})$$
$$H = H_0 + V(\hat{\phi})$$
$$\hat{\phi}(\vec{x}, t) = \int d\tilde{k} \left[a(\vec{k}) e^{-ikx} + a^\dagger(\vec{k}) e^{ikx} \right]$$

9.2.2 Different pictures of QM

Recall that the Schrodinger dependence assigns time dependence to the kets:

$$|\psi(t)\rangle = e^{-iHt/\hbar} |\psi(0)\rangle$$

and observables are constant. The expectation values of the observables are:

$$\langle O \rangle = \langle \psi(t)| O |\psi(t)\rangle = O(t)$$

Heisenburg picture
Examine the expectation value:

$$\langle O \rangle = \langle \psi(t)| O |\psi(t)\rangle = \langle \psi(0)| U^\dagger(t) O U(t) |\psi(0)\rangle \equiv \langle \psi(0)| O(t) |\psi(0)\rangle$$

so that the operators carry the time dependence:

$$O(t) \equiv U^\dagger(t) O(0) U(t)$$

and the time derivative satisfies:

$$\frac{d}{dt} O(t) = \frac{i}{\hbar} [H, O(t)]$$

Application of Heisenburg picture to 1D QHO
Then the position operator satisfies:

$$\begin{aligned} \frac{dx(t)}{dt} &= \frac{i}{\hbar} [H, x(t)] \\ &= \frac{i}{\hbar} U^\dagger [H, x(0)] U \\ &= \frac{i}{\hbar} U^\dagger [\frac{p^2}{2m}, x(0)] U \\ &= \frac{p(t)}{m} \end{aligned}$$

Similarly,

$$\frac{dp(t)}{dt} = -m\omega^2 x(t)$$

We can solve these operator differential equations simultaneously,

$$\begin{aligned} \ddot{x}(t) &= -\omega^2 x(t) \\ \implies x(t) &= x_0 \cos\omega t + \frac{p_0}{m\omega}\sin\omega t \\ \implies p(t) &= p_0 \cos\omega t - m\omega x_0 \sin\omega t \end{aligned}$$

Commutation relations in different pictures Note that in the Schrodinger picture, the commutation relation held:

$$[x, p] = i\hbar$$

because there are no time dependences associated with the operators. With the Heisenburg picture, the time dependence must be specified. Consider the commutation relations for the 1D QHO operators:

$$\begin{aligned} [x(t_1), x(t_2)] &= \frac{i\hbar}{m\omega}\sin\omega(t_2 - t_1) \\ [p(t_1), p(t_2)] &= i\hbar m\omega \sin\omega(t_2 - t_1) \\ [x(t_1), p(t_2)] &= i\hbar\cos\omega(t_2 - t_1) \end{aligned}$$

Note that when $t_1 = t_2$, the usual Schrodinger commutation relations hold. However, when the operators evolve in time, the commutation relations have different values.

Commutation relations for raising and lowering operators In analogy to the previous section, the field operators have commutation relations that depend on time. Recall that we can write:

$$\begin{aligned} X &\propto a + a^\dagger \\ P &\propto a - a^\dagger \end{aligned}$$

and the raising and lowering operators have time dependence governed by:

$$\dot{a}(t) = -i\omega a(t) \implies a(t) = a(0)e^{-i\omega t}$$

Interaction picture We expand the Hamiltonian in terms of a zeroth order piece and a higher order piece:

$$H = H_0 + H_1$$

We assign the time evolution due to H_0 into the operators, then examine the time evolution due to H_1 on the kets.

$$|\psi_I(t)\rangle = e^{iH_0 t/\hbar}|\psi(t)\rangle$$

note that the unitary operator in front of the ket un-does the effect of the H_0 piece. Operators have the time dependence:

$$O_I = e^{iH_0 t/\hbar} O e^{-iH_0 t/\hbar}$$

and the updated Schrodinger equation is:

$$i\hbar\frac{d}{dt}|\psi_I(t)\rangle = e^{iH_0 t/\hbar}H_1 e^{-iH_0 t/\hbar}|\psi_I(t)\rangle = H_1(t)|\psi_I(t)\rangle$$

The propagator for the interaction picture is different now:

$$U(t_f,t_i) = 1 + (-i)\int_{t_i}^{t_f} dt_1 H_1(t) + (-i)^2 \int_{t_i}^{t_f} dt_1 \int_{t_i}^{t_1} dt_2 H_1(t_1)H_1(t_2) + (-i)^3 \int_{t_i}^{t_f} dt_1 \int_{t_i}^{t_1} dt_2 \int_{t_i}^{t_2} dt_3 H_1(t_1)H_1(t_2)H_1(t_3) + \dots$$

We can write down a simpler expression for the nth term using the time ordering operator:

$$\int_{t_i}^{t_f} dt_1 \cdots \int_{t_1}^{t_{n-1}} dt_n H_1(t_1)\cdots H_1(t_n) = \frac{1}{n!}\int_{t_i}^{t_f} dt_1 \cdots dt_n T[H_1(t_1),\dots,H_1(t_n)]$$

where the time ordering operator puts the lowest time arguments on the right. The time ordering removes the double counting in phase space that results from replacing all the upper integration limits by t_f. The resultant U operator is called the S-matrix, for scattering. We can write it in exponential form:

$$U(t_f,t_i) = T\exp\left[-\frac{i}{\hbar}\int_{t_i}^{t_f} dt' H_1(t')\right]$$

We can consider the S-matrix for the universe ($\hbar = 1$):

$$U(\infty,-\infty) = T\left[\exp\left(-i\int d^4x H_1(\vec{x},t)\right)\right]$$

Note that the time evolution of operators in the interaction picture follows:

$$\begin{aligned} i\hbar\frac{d}{dt}O_I(t) &= [O_I(t),H_0] \\ \implies \frac{d}{dt}O_I(t) &= \frac{i}{\hbar}[H_0,O_I(t)] \end{aligned}$$

Interpreting operators in QFT Recall that the field was written:

$$\hat{\phi}(\vec{x},t) = \int d\tilde{k}\left[a(\vec{k})e^{-ikx} + a^\dagger(\vec{k})e^{ikx}\right]$$

Writing the time dependence explicitly,

$$\phi(\vec{x},t) = U_0(t)\phi(\vec{x},0)U_0^\dagger(t)$$