Mid-Term Summary

The mid-term examination will cover the following material:

- Theory of relativity: You should have a good general knowledge of the subject, but should particularly understand relativistic four-vectors.
- Wave packets and group velocity:
  - Fourier series and Fourier transforms: These mathematical tools are essential for understanding the evolution of wave packets.
  - Dispersion relation: A dispersion relation for a wave is a functional relationship between the angular frequency of the wave and its wavenumber: $\omega = \omega(k)$.
  - Group velocity: The group velocity is the velocity at which a wave packet moves: $u_g = d\omega/dk$.
  - Wave packet evolution and the propagator: This comes from assuming that a wave packet can be represented as a superposition of plane waves. This expression in turn can be represented as a convolution between the wave packet at $t = 0$ and the *propagator*.
  - Dirac delta function: The propagator invariably takes the form of the Dirac delta function at time $t = 0$.
- Motion of free particles:
  - The Planck-Einstein relationship: Planck hypothesized and Einstein confirmed a relationship between energy and and angular frequency, $E = \hbar\omega$, for photons.
  - De Broglie relationship: Louis de Broglie hypothesized that the Planck-Einstein relation extended also to massive particles. He also showed that the dispersion relation for the quantum mechanical waves associated with massive particles was forced by relativity to be $\omega^2 = k^2c^2 + \mu^2$ where μ is a constant to be determined. If the Planck-Einstein relationship is valid, then there must also be a relationship between momentum and wavenumber: $p = \hbar k$. The above dispersion relation is then seen to be equivalent to the relativistic energy-momentum relation: $E^2 = p^2c^2 + m^2c^4$. The constant $\mu = mc^2/\hbar$.

- Klein-Gordon equation: The wave equation which yields the above dispersion relation is

$$\frac{\partial^2 \psi}{\partial t^2} = c^2 \frac{\partial^2 \psi}{\partial x^2} - \frac{m^2 c^4}{\hbar^2}\psi.$$

- Free particle Schrödinger equation: In the non-relativistic limit in which we consider only positive energy solutions, the dispersion relation becomes $\omega = k^2c^2/(2\mu) + \mu = \hbar k^2/(2m) + mc^2/\hbar$. The second term is usually dropped as it represents a constant additive contribution to the frequency and hence to the energy. The corresponding wave equation is

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}.$$

- Probability interpretation of ψ: The relative probability of finding a particle at position x and time t in non-relativistic quantum mechanics is $P(x,t) = |\psi(x,t)|^2$. For a wave function ψ obeying the Schrödinger equation, there exists a probability flux

$$F(x,t) = \frac{i\hbar}{2m}\left(\frac{\partial \psi^*}{\partial x}\psi - \psi^*\frac{\partial \psi}{\partial x}\right)$$

such that

$$\frac{d}{dt}\int_a^b P\,dx = F(b,t) - F(a,t).$$

Letting $a \to -\infty$ and $b \to \infty$ shows that probability is conserved overall if ψ goes to zero at infinity. *This is not true for the Klein-Gordon equation* unless consideration is restricted to just the positive (or negative) energy states alone.

- Non-relativistic particle in a potential:

  - Schrödinger equation: The total energy is $E = p^2/(2m) + U(x)$ when the particle under consideration has potential energy $U(x)$. The extended Schrödinger equation is

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + U(x)\psi.$$

The solutions to this equation satisfy probability conservation just as do solutions to the free Schrödinger equation.

- Examples of solutions to the 1-D Schrödinger equation:
  * Infinite square well (analytical).
  * Finite square well (analytical development plus graphical solution).
  * Harmonic oscillator (shooting method).
  * One-dimensional scattering and barrier penetration (analytical and numerical).

- Big ideas of quantum mechanics: We need to generalize our ideas of how quantum mechanics works to extend it to systems which don't have classical equivalents.
  - Measurement results and amplitudes: For each possible result A_i of the measurement of a physical quantity A, there is a complex amplitude ψ_i. The probability of finding result A_i in a measurement procedure is $|\psi_i|^2$.
  - Expectation values:
    * Single variable: The expectation value of A is

      $$< A >= \sum_i A_i|\psi_i|^2 = \sum_{i,j} \psi_i^* A_i \delta_{ij} \psi_j \equiv (\psi, A\psi).$$

      The ψ_i are the components of a vector ψ in an abstract vector space called Hilbert space. The $A_i\delta_{ij}$ are the components of a matrix which has the A_i values along the diagonal and zeros elsewhere. (ψ, ϕ) is generalized notation for a dot product between two vectors in Hilbert space. If the Hilbert space vectors have components ψ_i and ϕ_i, then

      $$(\psi, \phi) = \sum_i \psi_i^* \phi_i.$$

      Note that $(A\psi, \phi) = (\psi, A'\phi)$ and $(\psi, \phi) = (\phi, \psi)^*$.
    * Additional incompatible variable: The expectation value of a different physical quantity B can be expressed as

      $$< B >= \sum_{i,j} \phi_i^* B_i \delta_{ij} \phi_j = (\phi, B\phi).$$

The ψ_i and the ϕ_i are related by a unitary transformation

$$\phi_i = \sum_j q_{ij}\psi_j \quad \text{or} \quad \phi = q\psi.$$

Think of the ϕ_i and ψ_i as the vector ψ resolved in two different reference frames rotated relative to each other. Unitary means that $q^{-1} = q'$, where q' is the transposed complex conjugate of q and q^{-1} is the inverse. Thus, $\psi = q^{-1}\phi = q'\phi$.

* Expectation value in non-principal axis coordinate system: Note that

$$< B >= (q\psi, Bq\psi) = (\psi, q'Bq\psi).$$

The matrix $B_t \equiv q'Bq$ is not diagonal. However, it is Hermitian or self-adjoint: $B_t' = B_t$. Think of B_t as the operator B resolved in a different coordinate system.

* If we start with the non-diagonal form of B, we can diagonalize it to get the possible physical values of B (the eigenvalues) and the unit vectors in the principal axis frame (the eigenvectors).

* If two operators commute, i. e., if $[A, B] \equiv AB - BA = 0$, then they share a common principal axis reference frame. A and B are called compatible.

– Degeneracy: If an operator is degenerate, i. e., two or more of its eigenvalues are equal to each other, then there exist one or more additional operators which are compatible with the original operator. The maximal set of compatible operators has been found when each state has a distinct set of operator values associated with it.

– Momentum and energy operators: The momentum and energy operators in the spacetime representation are

$$p = -i\hbar\delta(x - x')\frac{\partial}{\partial x'} \qquad E = i\hbar\delta(t - t')\frac{\partial}{\partial t'}.$$

The application of (say) the momentum operator to a state ψ is

$$\int p(x, x')\psi(x')dx' = -i\hbar\frac{\partial\psi}{\partial x}.$$

Thus, the Dirac delta function is usually dropped and we say

$$p = -i\hbar\frac{\partial}{\partial x} \qquad E = i\hbar\frac{\partial}{\partial t}.$$

– Time evolution: Diagonalizing the energy operator or Hamiltonian allows us to determine the time evolution of a system. Solving

$$H\psi \equiv i\hbar\frac{\partial \psi}{\partial t} = E\psi$$

leads to a set of eigenvalues E_j and eigenvectors $\psi^{(j)}$, with an arbitrary solution taking the form

$$\psi = \sum_j a_j \psi^{(j)} \exp(-iE_j t/\hbar),$$

where the a_j are constants which are determined by the initial conditions.