PHY 362K Review Note 1

Xiaohui Chen

February 16, 2015

1 Prerequisite

1.1 One-dimensional Wave Mechanics

The relationship between the particle's energy and the wave's frequency is $E = \hbar\omega = \frac{p^2}{2m}$

The relationship between its momemtum and wavevector is $p = \hbar k$

Therefore, the dispersion relation is $\omega = \frac{\hbar k^2}{2m}$

Time-dependent Schrodinger equation: $\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)$

The wave equation must have an i in it, because that is the only way to construct a wave equation with the correct dispersion relation

When the potential energy V is independent of time, the TDSE can be separated into a time equation and a space equation

For a harmonic oscillator, $c_n = \int_{-\infty}^{\infty} \psi_n^*(x) f(x) dx$ where $f(x)$ is written as $f(x) = \sum_n c_n \psi_x(x)$.

Here $|c_n|^2$ is the probability to measure the particle to be in its nth eigenstate with energy $E_n = \left(n + \frac{1}{2}\right)\hbar\omega$

The wave function at time t is $\Psi(x,t) = \sum_n c_n e^{-\frac{iE_n t}{\hbar}} \psi_n(x)$

1.2 Bra-Ket

$|x\rangle$ represents a state of the particle in which its position is x. That means if you measure the position of the particle you are certain to the the result x

$\langle x|\psi\rangle$ is the probability amplitude that a particle in state $|\psi\rangle$. In other words, it is the wavefunction of the particle $\langle x|\psi\rangle = \psi(x)$

$\langle x|p\rangle$ is the probability amplitude that a particle in an eigenstate of momentum p will be found at position x. In other words, it is the wavefunction of a particle of definite momentum p

$\langle x|p\rangle = Ne^{ikx} = Ne^{\frac{ipx}{\hbar}} = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ipx}{\hbar}}$

The state vector can always be written as $|\psi\rangle = \sum_n s_n|a_n\rangle$ where the values s_n are arbitrary complex constants

$|s_n|^2$ is the probability that you will get result a_n

$\langle\psi| = \sum_n s_n^*\langle a_n|$

If $|\psi\rangle = \sum_n s_n|a_n\rangle$ and $|\phi\rangle = \sum_n p_n|a_n\rangle$, then $\langle\psi|\phi\rangle = \sum s_n^* p_n$. This can be thought as the "degree of overlap" of the state vector $|\phi\rangle$ with the state vector $|\psi\rangle$ and $|\phi\rangle$

$\sum_n |a_n\rangle\langle a_n| = 1$

An operator O is a mapping of the ket space onto itself. e.g $O|\psi\rangle = |\gamma\rangle$. A linear operator is an operator with the property that if $O|\psi_1\rangle = |\gamma_1\rangle$ and $O|\psi_2\rangle = |\gamma_2\rangle$, then $O(c_1|\psi_1\rangle + c_2|\psi_2\rangle) = c_1|\gamma_1\rangle + c_2|\gamma_2\rangle$

If the matrix of O represents an observable, then it must be an Hermitian (the matrix must be equal to its complea-conjugate transpose)

$\langle\phi|O$ is the bra such that $(\langle\phi|O)|\psi\rangle = \langle\phi|(O|\psi\rangle)$ for all possible kets $|\psi\rangle$

Examples of adjoint:

(1) The adjoint of $cA|\psi\rangle$ is $c^*\langle\psi|A^+$

(2) The adjoint of $A|\psi\rangle\langle\phi|B$ is $B^+|\phi\rangle\langle\psi|A^+$

(3) The adjoint of $AB|\gamma\rangle$ is $\langle\gamma|B^+A^+$

If $[A, B] = c$ where c is a complex constant, then A and B are incompatible observables, which means that it is not possible to measure both A and B with perfect precision. $\Delta A \Delta B \geq \frac{1}{2} |\langle[A, B]\rangle|$

2 Time Independent Perturbation

2.1 Non-degenerate Perturbation

We want to solve $H|\psi_n\rangle = E_n|\psi_n\rangle$

$H = H_0 + H'$ where $H_0|\psi_n\rangle = E_n^{(0)}|\psi_n\rangle$

$E_n^{(1)} = \langle\psi_n^{(0)}|H'|\psi_n^{(0)}\rangle$

$E_n \approx E_n^{(0)} + E_n^{(1)}$ (1st order approach for the energy)

$|\psi_n^{(1)}\rangle = \sum_{m\neq n} \frac{\rangle\psi_m^{(9)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)}-E_m^{(0)}}|\psi_m^{(0)}\rangle$

$|\psi_n\rangle \approx |\psi_n^{(0)}\rangle + |\psi_n^{(1)}\rangle$

$E_n \approx E_n^{(0)} + E_n^{(1)} + E_n^{(2)}$

$\langle\psi_{nlm}^{(0)}|z|\psi_{n'l'm'}^{(0)}\rangle = 0$ unless $m = m'$ and $l = l' + 1$ or $l = l' - 1$

2.2 Degenerate Perturbation Theory

$H'_{jk} = \langle\psi_{nj}^{(0)}|H'|\psi_{nk}^{(0)}\rangle$

$$\begin{bmatrix} H'_{11} & H'_{12} & \dots & H'_{1g_n} \\ H'_{21} & H'_{22} & \dots & H'_{2g_n} \\ \dots & \dots & \ddots & \dots \\ H'_{g_n1} & H'_{g_n2} & \dots & H'_{g_ng_n} \end{bmatrix} \begin{bmatrix} c_{i1} \\ c_{i2} \\ \dots \\ c_{ig_n} \end{bmatrix} = E^{(1)}_{ni} \begin{bmatrix} c_{i1} \\ c_{i2} \\ \dots \\ c_{ig_n} \end{bmatrix}$$

More simply as $H'|\phi^{(0)}_{ni}\rangle = E^{(1)}_{ni}|\phi^{(0)}_{ni}\rangle$

$|\phi^{(0)}_{ni}\rangle = c_{i1}|\psi^{(0)}_{n1}\rangle + c_{i2}|\psi^{(0)}_{n2}\rangle + \ldots + c_{ig_n}|\psi^{(0)}_{ng_n}\rangle$

3 Hydrogen-Like Particles

$\frac{1}{\lambda_{n,n'}} = R_H\left(\frac{1}{n^2} - \frac{1}{n'^2}\right)$ where $R_H \approx 1.097 * 10^7 m^{-1}$ is the Rydberg constant for hydrogen

3.1 Bohr Model

$E_n = -\frac{1}{2}\left(\frac{m_e}{\hbar^2}\right)\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\left(\frac{m_p}{m_p+m_e}\right)\frac{1}{n^2}$

Bohr postulated that a photon may be given off only in a Bohr transition between these energy states, with the photon wavelength given by $\frac{hc}{\lambda_{n,n'}} = E_n - E_{n'}$

$R_H = R_\infty\left(\frac{m_p}{m_p+m_e}\right)$ with $R_\infty = \left(\frac{1}{4\pi}\right)\frac{m}{\hbar^3 c}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2$

3.2 Wavenumber or Inverse Centimeter Units

Transition energies can also be measured in wavenumbers by $\bar{v} = \frac{1}{\lambda}$

$1\ cm^{-1} \leftrightarrow 29.979\ GHz$ and $8066\ cm^{-1} \leftrightarrow 1\ eV$

3.3 Schrodinger Equation for the Hydrogen Atom

$H\psi(\vec{r}) = \left[-\frac{\hbar^2}{2m_e}\vec{\nabla}^2 - \frac{Ze^2}{4\pi\epsilon_0 r}\right]\psi(\vec{r}) = E\psi(\vec{r})$

$\psi_{nlm}(\vec{r}) = R_{nl}(r)Y_{lm}(\theta, \phi)$

Let $u(r) = rR(r)$, then $\left[-\frac{\hbar^2}{2m_e}\frac{d^2}{dr^2} + V_{eff}(r)\right]u(r) = Eu(r)$ where $V_{eff}(r) = -\frac{Ze^2}{4\pi\epsilon_0 r} + \frac{l(l+1)\hbar^2}{2m_e r^2}$

Coulomb Potential: $-\frac{Ze^2}{4\pi\epsilon_0 r}$

Centrifugal Potential: $\frac{l(l+1)\hbar^2}{2m_e r^2}$

$n = 1, 2, 3, \ldots$ and $l = 0, 1, 2, \ldots, n-1$

The wave function is normalized in three dimensions

The spherical harmonics are orthonormal on the unit sphere

$\int_0^\infty |R_{nl}|^2 r^2 dr = 1$, where $|R_{nl}|^2 r^2$ is the radial probability density

3.4 Hamiltonian of an Electron Interacting with an Electromagnetic Field

scalar potential: $\Phi(\vec{r}, t)$ and scalar potential $\vec{A}(\vec{r}, t)$

$\vec{E}(\vec{r}, t) = -\vec{\bigtriangledown}\Phi(\vec{r}, t) - \frac{\partial \vec{A}(\vec{r}, t)}{\partial t}$

$\vec{B}(\vec{r}, t) = \vec{\bigtriangledown} \times \vec{A}(\vec{r}, t)$

$H = \frac{1}{2m}(\vec{p} + q\vec{A})^2 + q\Phi = \frac{1}{2m}\left(\vec{p}^2 + q\vec{A}\cdot\vec{p} + q\vec{p}\cdot\vec{A} + q^2|\vec{A}|^2\right) + q\Phi$

If we choose a specific gauge: $\Phi = 0$ and $\vec{A} = \frac{1}{2}\left(\vec{B} \times \vec{r}\right)$

Then $H = \frac{\vec{p}^2}{2m_e} - \vec{\mu}\cdot\vec{B} + \frac{e^2}{8m_e}(x^2 + y^2)$ where $\vec{\mu} = \vec{\mu_l} + \vec{\mu_s} = -\mu_B\left(\frac{\vec{l} + g_e\vec{s}}{\hbar}\right)$