Lecture 23

Review

Schrödinger equation

The general solution of Schrödinger equation in three dimensions (if V does not depend on time)

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi \equiv H\psi$$

is

$$\psi(\vec{r}, t) = \sum_n C_n \psi_n(\vec{r}) \, e^{-iE_n t/\hbar}$$

where functions $\psi_n(\vec{r})$ are solutions of time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi \qquad (H\psi = E\psi)$$

If potential V is spherically symmetric, i.e. only depends on distance to the origin r, then the separable solutions are

$$\psi(r, \theta, \phi) = R(r) \, Y_\ell^m(\theta, \phi) \quad \text{spherical harmonics}$$

where $R(r) = \frac{1}{r} u(r)$ and $u(r)$ are solutions of radial equation

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left[v(r) + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2} \right] u = Eu$$

Hydrogen-like atom energy levels: $E_n = E_1 \dfrac{Z^2}{n^2}$, $E_1 = -13.6 \, eV$

Identical particles

Bosons and fermions

In classical mechanics, you can always identify which particle is which. In quantum mechanics, you simply can't say which electron is which as you can not put any labels on them to tell them apart.

There are two possible ways to deal with indistinguishable particles, i.e. to construct two-particle wave function from single particle wave functions $\psi_a(\vec{r})$ and $\psi_b(\vec{r})$ that is non committal to which particle is in which state:

Symmetric

$$\psi_+(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \left[\psi_a(\vec{r}_1) \psi_b(\vec{r}_2) + \psi_b(\vec{r}_1) \psi_a(\vec{r}_2) \right]$$

Antisymmetric

$$\psi_-(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \left[\psi_a(\vec{r}_1) \psi_b(\vec{r}_2) - \psi_b(\vec{r}_1) \psi_a(\vec{r}_2) \right].$$

Therefore, quantum mechanics allows for two kinds of identical particles: **bosons** (for the "+" sign) and **fermions** (for the "-" sign). N-particle states are constructed in the same way, antisymmteric state for fermions (which can be easily written as Slater determinant) and symmetric state for bosons; the normalization factor is $1/\sqrt{N}$. In our non-relativistic quantum mechanics we accept the following statement as an axiom:

**All particles with integer spin are bosons,
all particles with half-integer spin are fermions.**

Note that it is **total** wave function that has to be antisymmetric. Therefore, for example if spatial wave function for the electrons is symmetric, then the corresponding spin state has to be antisymmteric. **Note:** make sure that you can add angular momenta and know what are singlet and triplet states.

From the above, two identical fermions can not occupy the same state.
It is called **Pauli exclusion principle**.

Perturbation theory

General formalism of the problem:

Suppose that we solved the time-independent Schrödinger equation for some potential and obtained a complete set of orthonormal eigenfunctions ψ_n^0 and corresponding eigenvalues E_n^0 .

$$H^0 \psi_n^0 = E_n^0 \psi_n^0$$

$$\langle \psi_n^0 | \psi_m^0 \rangle = \delta_{nm}$$

This is the problem that we completely understand and know solutions for.

We mark all these solutions and the Hamiltonian with " ^{0} " label.

Now we slightly perturb the potential: $H = H^0 + H'$

The problem of the perturbation theory is to find eigenvalues and eigenfunctions of the perturbed potential, i.e. to solve approximately the following equation:

$$H \psi_n = E \psi_n \quad ,$$

using the known solutions of the problem $H^0 \psi_n^0 = E_n^0 \psi_n^0$.

Nondegenerate perturbation theory

We expand our solution as follows in terms of perturbation H'

$$\psi_n = \psi_n^0 + \psi_n^1 + \psi_n^2 + \dots$$

$$E_n = E_n^0 + E_n^1 + E_n^2 + \dots$$

The first-order correction to the energy is given by: $E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle$

First-order correction to the wave function is given by

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

Note that as long as m ≠n, the denominator can not be zero as long as energy levels are nondegenerate. If the energy levels are degenerate, we need degenerate perturbation theory (consider later).

The second-order correction to the energy is

$$E_n^2 = \sum_{m \neq n} \frac{|\langle \psi_m^0 | H' | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0}$$

Degenerate perturbation theory

Suppose now that the states $\psi_1^0, \psi_2^0, \ldots \psi_n^0$ are degenerate, i.e. have the same energy E^0.

How to calculate first-order energy correction E^1?

In the case of n-fold degeneracy, E^1 are eigenvalues of n x n matrix

$$W_{ij} = \langle \psi_i^0 | H' | \psi_j^0 \rangle.$$

Variational method

The variational principle let you get an **upper bound** for the ground state energy when you can not directly solve the Schrödinger's equation.

How does it work?

(1) Pick any normalized function ψ.

(2) The ground state energy E_{gs} is

$$\boxed{E_{gs} \leq \langle \psi | H | \psi \rangle \equiv \langle H \rangle}$$

Note: in 1D $\quad H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$

3) Some choices of the trial function ψ will get your E_{gs} that is close to actual value.

If you picked a function with a parameter, minimize the resulting expression for $\langle H \rangle$. Substitute resulting value of the parameter into $\langle H \rangle$ to get lowest upper bound on E_{gs}.

WKB approximation

This method allows to obtain approximate solutions to the time-independent Schrödinger equation in one dimension and is particularly useful in calculating tunneling rates through potential barriers and bound state energies.

"Classical" region, E > V

$$\psi(x) \cong \frac{C}{\sqrt{p(x)}} \; e^{\pm \frac{i}{\hbar} \int p(x)\,dx} \quad ; \quad p(x) = \sqrt{2m(E - V(x))}$$

General solution is the combination of these two.

If E < V (non-classical region), then p is imaginary but we can still write

$$\psi(x) \cong \frac{C}{\sqrt{|p(x)|}} \; e^{\pm \frac{1}{\hbar} \int |p(x)|\,dx}$$

Transmission probability:
$$T = \frac{|F|^2}{|A|^2} \cong e^{-2\gamma}$$

$$\gamma = \frac{1}{\hbar} \int_{x_1}^{x_2} |p(x)|\,dx$$

↳ over non-classical region

Formulas above are derived with the assumption that the potential is slowly varying in comparison with the wavelength λ (or $1/\kappa$ for E<V). This is not the case for the turning points, where "classical" region connects with "non classical" region. In this case WKB approximation breaks down. **Note:** make sure that you know how to apply connection formulas to derive quantization conditions

$$\int_{x_1}^{x_2} p(x)\,dx = (n - a)\pi\hbar \; ,$$

$$a = \begin{cases} 0 & \text{for potential with two vertical walls at } x_1 \text{ and } x_2 \\ 1/4 & \text{for potential with one vertical wall at } x_1 \\ 1/2 & \text{for potential with no vertical walls.} \end{cases}$$

turning points
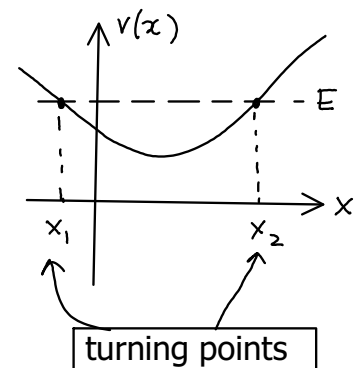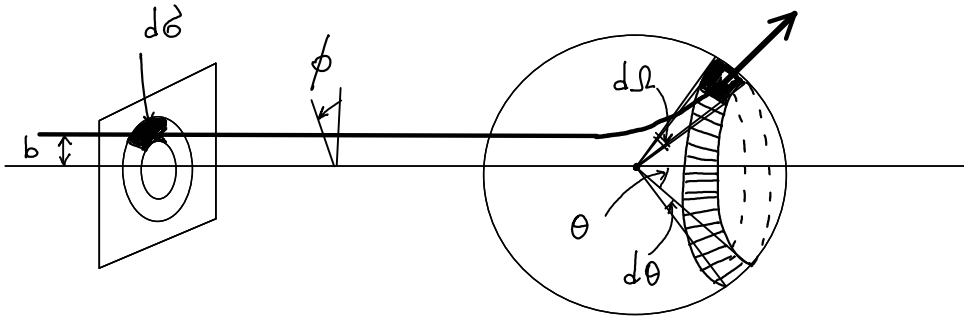
Scattering

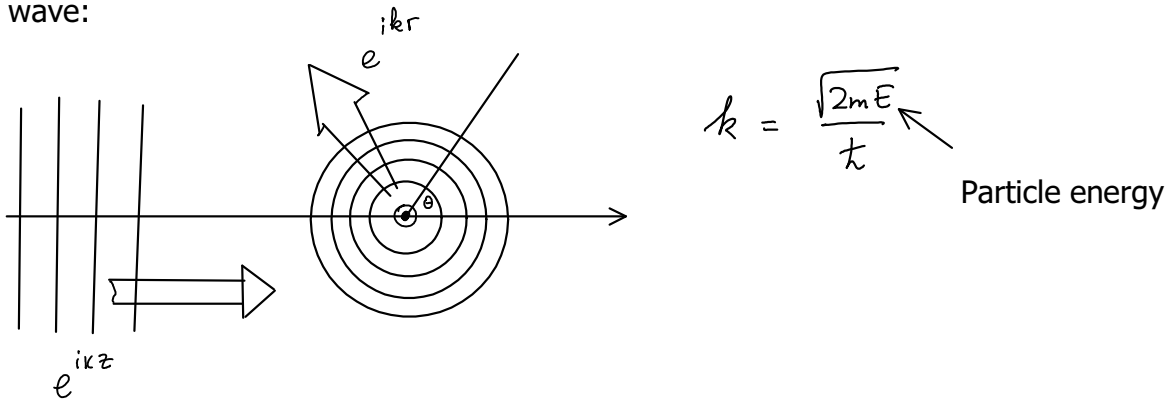Differential (scattering) cross-section: $D(\theta) = \dfrac{d\acute{6}}{d\Omega}$

Total cross section is defined as the integral of $D(\theta)$ over all solid angles: $\acute{6} \equiv \displaystyle\int D(\theta)\, d\Omega$

Quantum scattering theory

Our problem: incident plane wave

$$\psi(z) = A\, e^{ikz}$$

traveling in Z direction encounters a scattering potential that produces outgoing spherical wave:

$$k = \frac{\sqrt{2mE}}{\hbar}$$

Particle energy

Therefore, the solutions of the Schrödinger equation have the general form:

$$\psi(r,\theta) \simeq A\left\{ e^{ikz} + f(\theta)\, \frac{e^{ikr}}{r} \right\} \quad \text{for large } r$$

scattering amplitude

$$D(\theta) = \frac{d\acute{6}}{d\Omega} = |f(\theta)|^2$$

Partial wave analysis

For spherically symmetric potential, the scattering amplitude may be calculated using partial wave analysis formula

$$f(\theta) = \sum_{l=0}^{\infty} (2l+1) \, a_l \, P_l(\cos\theta) \tag{1}$$

The partial wave amplitudes a_l are found by solving the Schrödinger equation for the area where $V \neq 0$ and using the boundary conditions. Substituting the expression for the partial wave scattering amplitude (1) into the formula for the differential cross section and integrating over all solid angles yields simple expression for the total scattering cross-section:

$$\sigma = 4\pi \sum_{l=0}^{\infty} (2l+1) \, |a_l|^2 .$$

Scattering amplitude in Born approximation.

$$f(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \int e^{-i(\vec{k}' - \vec{k})\vec{r}_0} \, V(\vec{r}_0) \, d^3 r_0$$
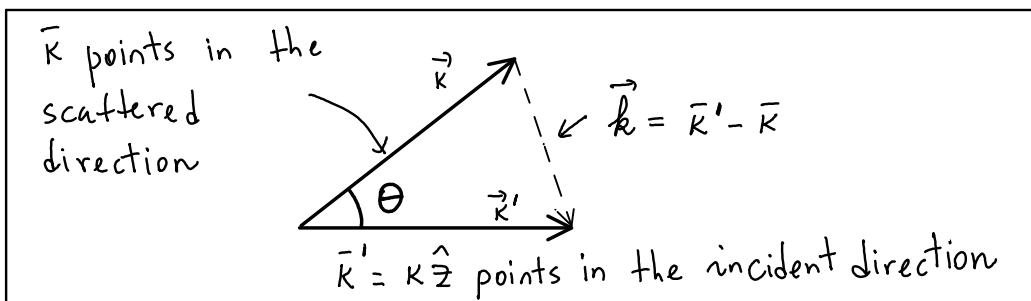
As before, the differential and total cross sections are given by

$$\frac{d\sigma}{d\Omega} = |f|^2 , \qquad \sigma = \int |f|^2 \, d\Omega .$$

(1) Low-energy scattering $f(\theta, \phi) \simeq -\dfrac{m}{2\pi\hbar^2} \int V(\vec{r}) \, d^3 r$

(2) Spherically symmetric potential.

$$f(\theta) = -\frac{2m}{\hbar^2 k} \int_0^{\infty} r_0 V(r_0) \sin(k r_0) \, dr_0 \qquad k = 2\kappa \sin\frac{\theta}{2}$$

$\bar{K}$ points in the scattered direction

$\vec{k} = \bar{K}' - \bar{K}$

$\bar{K}' = \kappa\hat{z}$ points in the incident direction

Notes on the exam preparation & exam taking:

1. Make sure that you know, understand and can use all formulas and concepts from this lecture.

2. Make sure that you can solve on your own and without looking into any notes any problem done in class in Lectures or from homeworks (if integrals are complicated, use Maple, Matematica, etc.)

3. During exam, look through all the problems first. Start with the one you know best and the one that is shortest to write a solution for.

4. Make sure that you read the problem very carefully and understand what is being asked. If you are unsure, ask me.

5. To save time, make sure you are not repeating the same calculations. For example, if you need to do several similar integrals, make sure that you are not redoing the ones you have already done.

If you are out of time and you have not finished, write an outline of what you would do to finish the problem if you had time.