

The WKB (WENTZEL-KRAMERS-BREITL) APPROXIMATION:

APPROXIMATION:

The WKB approximation is applied to problems in which potential changes slowly with the distance, i.e. potentials which remain almost constant over a region of the order of the de Broglie wavelength. This approximation introduces an expansion in powers of \hbar and terms of order \hbar^2 and higher, are neglected. It is therefore a semi-classical approximation.

If the potential, changes slowly with the distance, then the change in the de-Broglie wavelength is

$$\frac{\delta \lambda}{\lambda} = \frac{d\lambda}{dx} \delta x$$

In one wavelength, we have change

$$\delta \lambda \approx \frac{d\lambda}{dx} \lambda \delta x \approx \lambda$$

In the classical region, $\delta \lambda \ll \lambda$,

we get a condition

$$\left| \frac{\delta \lambda}{\lambda} \right| \approx \left| \frac{d\lambda}{dx} \right| \ll 1$$

called condition for the validity of WKB method.

This means that rate of change of the de-Broglie wavelength is small (i.e. the wavelength of the particle must vary only slightly over distances of the order of its size). This is valid for classical system.

In terms of momentum, this can be expressed as:

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

$$p(x) = \sqrt{2m \cdot (E - V(x))}$$

also

$$\lambda(x) = \frac{h}{p(x)} = \frac{h}{\sqrt{2m(E - V(x))}} \quad (*)$$

So the condition of validity for the WKB method is given by

$$\left| \frac{d\lambda(x)}{dx} \right| = \left| \frac{d}{dx} \left(\frac{h}{p(x)} \right) \right| \ll 1 \quad (**)$$

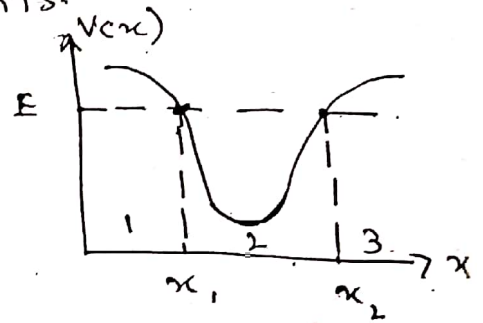
This condition is not valid for classical turning point, i.e. $E = V(x_i)$, since $p(x_i) = 0$. Classically, the particle stops at $x = x_i$ and then moves in the opposite direction.

As $p(x)$ becomes small, the wavelength in eq. (*) becomes large and hence violates the requirement that it remains small and

varies only slightly, when $p(x)$ is too small, the condition in eqn (**), breaks down.

So the WKB approximation is valid in both the allowed and forbidden regions but not at the classical turning points.

In fig, the points x_1 and x_2 are classical turning points.



The WKB Expansion:

Consider the one-dimensional time-independent Schrödinger equ:

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

or

$$\frac{d^2 \psi}{dx^2} + k^2 \psi = 0 \quad \text{--- (1)}$$

where

$$k(x) = \frac{\sqrt{2m(E - V(x))}}{\hbar}$$

If the potential $V(x)$ is slowly varying, then the wavefn. is expected to be approximately the free particle wavefn.

$$\psi(x) = A e^{\pm i K x}$$

So we will look for the solution of form

$$\psi(x) = A e^{i W(x)}$$

where $W(x)$ has an expansion in powers of \hbar , i.e.

$$W(x) = W_0(x) + \hbar W_1(x) + \hbar^2 W_2(x) + \dots$$

Now

$$\frac{d\psi}{dx} = i \psi \frac{dW}{dx}$$

where $\psi = A e^{i W(x)}$

$$\frac{d\psi}{dx} = A e^{i W} i \frac{dW}{dx}$$

$$\frac{d\psi}{dx} = \psi i \frac{dW}{dx}$$

$$\frac{d^2\psi}{dx^2} = i \psi \frac{d^2W}{dx^2} + i^2 \psi \left(\frac{dW}{dx} \right)^2$$

put in equ (1), one gets

$$i \frac{d^2W}{dx^2} - \left(\frac{dW}{dx} \right)^2 + [K(x)]^2 = 0 \rightarrow (2)$$

This can be solved using certain approximation.

In the limit in which $V(x)$ is approximately constant; then

$$W = \pm K x \quad (K \text{ also independent of } x)$$

$$\frac{dW}{dx} = \pm K.$$

$$\frac{d^2W}{dx^2} = 0.$$

When K has certain dependence of on x , we approximate

$$\frac{dW}{dx} \approx \pm K(x). \quad \text{--- (3)}$$

$$\frac{d^2W}{dx^2} \approx \pm K'(x). \quad \text{--- (4)}$$

Integration ^{of} gives

$$W \approx \pm \int K(x) dx + X_0.$$

Let us write this as first approximation

$$W_0 = \pm \int K(x) dx + X_0.$$

For the second approximation, we write the Schrodinger equation, from (2)

$$\left(\frac{dW}{dx}\right)^2 = [K(x)]^2 + i \frac{d^2W}{dx^2}$$

$$\frac{dW}{dx} = \pm \left\{ [K(x)]^2 + 2 \frac{d^2 W}{dx^2} \right\}^{1/2}$$

or we may write

$$W_1(x) = \pm \int_x \left\{ [K(x)]^2 + 2 \frac{d^2 W_0}{dx^2} \right\}^{1/2} dx + X_1$$

This can be used to find $W_2(x)$

as

$$W_2(x) = \pm \int_x \left\{ [K(x)]^2 + 2 \frac{d^2 W_1}{dx^2} \right\}^{1/2} dx + X_2$$

In general

$$W_{n+1}(x) = \pm \int_x \left\{ [K(x)]^2 + 2 W_n''(x) \right\}^{1/2} dx + X_{n+1}$$

We know that

$$W_0' = \pm K(x)$$

$$W_0'' = \pm K'(x)$$

\Rightarrow

$$W_1(x) = \pm \int_x \left\{ [K(x)]^2 + 2 W_0''(x) \right\}^{1/2} dx + X_1$$

(4)
A. Comparison of $W_0''(x)$ and $W_1(x)$ fields.

$$|K'(x)| \ll |[K(x)]^2|$$

(WKB approximation condition)

This can also be expressed as

$$\left| \frac{dP}{dx} \right| \ll \left| P \left(\frac{2\pi}{\lambda} \right) \right|$$

or

as

$$K'(x) \approx \frac{d}{dx} \left(\frac{P}{\hbar} \right)$$

$$\left| \frac{dP}{dx} \right| \ll \left| 2\pi P \right|$$

$$[K(x)]^2 = \frac{P}{\hbar} \cdot \frac{P}{\hbar}$$

$$= \frac{\hbar K}{\hbar} \cdot \frac{P}{\hbar}$$

$$= \frac{P}{\hbar} \left(\frac{2\pi}{\lambda} \right)$$

Systems of Identical Particles

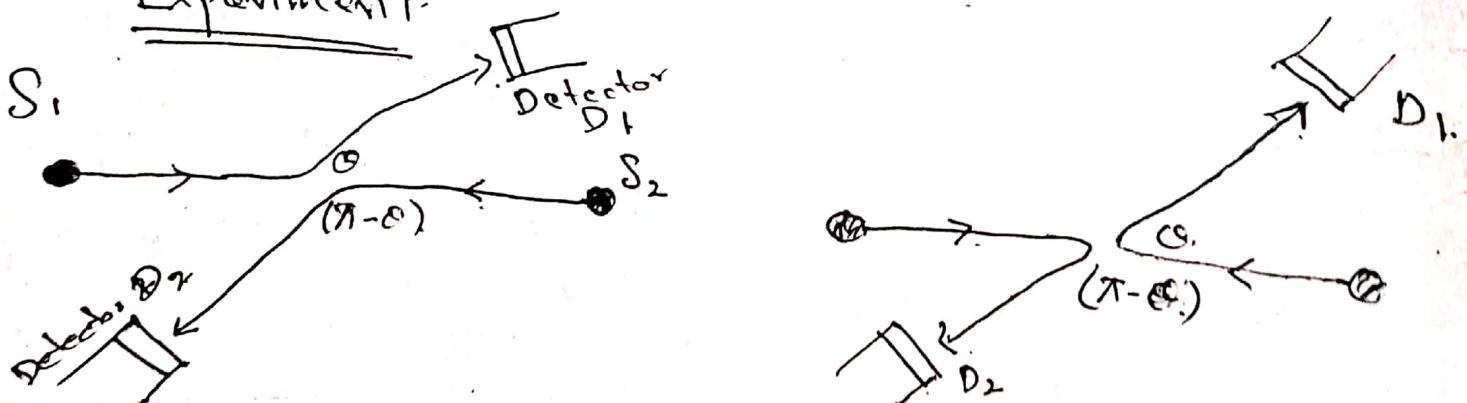
Identical Particles in Classical and Quantum M.

In classical mechanics, when a system is made of identical particles, it is possible to identify and distinguish each particle from the other. Although, all particles have the same physical properties i.e. same spin and space degrees of freedom.

One can "tag" each classical particle and follow its motion along a path. For instance, each particle can be colored differently from the rest, hence we can follow the trajectory of each particle separately at each time. Hence, identical classical particles do not lose their identity; they are distinguishable.

In quantum mechanics, identical particles are truly indistinguishable. First, in particular, there exists no mechanism to tag the particles as in classical mechanics. Second, due to the uncertainty principle, the concept of the path of a particle becomes meaningless. Even if the position of a particle is exactly determined at a given time, it is not possible to specify its coordinates at the next instant. Thus, identical particles lose their identity in quantum mechanics.

Experiment



So far, we have discussed systems of particles which are distinguishable from one another i.e. different particles in different states e.g. a proton and an electron in a hydrogen atom. However, when we study Helium atom, there are two electrons revolving round the nucleus and there is no way of telling which electron is in which state.

One important aspect of quantum mechanics is the indistinguishability of identical particles.

The identical particles are those which have the same mass, charge, spin etc. and behave the same way under same physical conditions.

Consider a system of 2 identical particles. The Hamiltonian of the system is

$$H = H(1, 2).$$

$1 \equiv x_1, \tau_1$ — i.e. particle 1 has both space and spin degrees of freedom. The Hamiltonian is symmetric with respect to a permutation of the labels attached to identical particles.

$$H(1, 2) = H(2, 1).$$

Let $\psi(1,2)$ be the two-particle state,
then its time evolution is given by

$$H(1,2) \psi(1,2) = i\hbar \frac{\partial}{\partial t} \psi(1,2).$$

If we interchange particles 1 and 2,
we get

$$\Rightarrow H(1,2) \psi(2,1) = i\hbar \frac{\partial}{\partial t} \psi(2,1).$$

i.e. if $\psi(1,2)$ is the solution of
Schrodinger wave equation, then $\psi(2,1)$
is also a solution. From superposition
principle, every linear combination of the
functions $\psi(1,2)$ and $\psi(2,1)$ is also
a solution of the same Schrodinger
equation. The states of the system can
have two categories.

The identity

$$\psi(1,2) = \frac{1}{\sqrt{2}} [\psi(1,2) + \psi(2,1)] \\ + \frac{1}{\sqrt{2}} [\psi(1,2) - \psi(2,1)]$$

implies that every state is a
superposition of a symmetric state

$$\Psi_S = \frac{1}{\sqrt{2}} [\Psi(1,2) + \Psi(2,1)]$$

and an anti-symmetric state.

$$\Psi_A = \frac{1}{\sqrt{2}} [\Psi(1,2) - \Psi(2,1)]$$

where $\frac{1}{\sqrt{2}}$ is a normalization factor.

Exchange Degeneracy:

The wave-functions corresponding to all possible electron permutations have the same energy E .

$$\hat{H}\Psi = E\Psi$$

This is known as the exchange degeneracy. For instance, the degeneracy associated with a system of two identical particles is equal to 2, since $\Psi(1,2)$ and $\Psi(2,1)$ correspond to the same energy E .

If \hat{P}_{12} is the exchange operator defined by

$$\hat{P}_{12} \Psi(1,2) = \Psi(2,1)$$

Since $\hat{P}_{12}^2 = 1$, \hat{P}_{12} has eigenvalue of ± 1 (\hat{P}_{12} is an involution).

The corresponding eigenfunctions are.

ψ_S — eigenvalue $+1$

ψ_A — eigenvalue -1 .

$$\hat{P}_{12} \psi_S = \psi_S$$

$$\hat{P}_{12} \psi_A = -\psi_A$$

Since $\psi(1,2)$ and $\psi(2,1)$ are the solutions of the same Schrödinger equations therefore the energy levels are doubly degenerate. This degeneracy is known as exchange degeneracy.

Let us look at \hat{H} is symmetric.

$$\hat{P}_{12} \hat{H}(1,2) \psi(1,2) = \begin{aligned} & \hat{H}(2,1) \psi(1,2) \\ & = \hat{H}(1,2) \psi(1,2) \end{aligned}$$

$$= \hat{H}(1,2) \psi(2,1)$$

↙ interchange
1,2 → 2,1

$$= \hat{H}(1,2) \hat{P}_{12} \psi(1,2)$$

$$\Rightarrow [\hat{P}_{12}, \hat{H}] = 0$$