Wentzel - Kramers - Brillouin (WKB) Approximation - Multivariable
(semiclassical)

- Useful for slowly varying potentials (that remain constant over ~ de Broglie wavelength)

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x},t) + V(\vec{x})\psi(\vec{x},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t)$$

If $V(\vec{x}) = \text{const.}$, the solution is of form: $\psi(\vec{x},t) = A e^{\pm i\vec{p}(\vec{x}-\vec{a})/\hbar} e^{-iEt/\hbar}$

If $V(\vec{x})$ ~ slowly varying, then WKB says try:

$$\psi(\vec{x},t) = A(\vec{a},\vec{x},t)e^{iS(\vec{a},\vec{x},t)/\hbar}$$

($\vec{a}$ = initial configuration, $\psi(\vec{x},t=0) = \delta(\vec{x}-\vec{a})$)

Amplitude and phase functions of $\vec{r}$ & t.

by the way, $\hat{S}(x,t) = S(x,t)/\hbar$ is the Eikonal

Greek "Eikon" = "Image"

Substitute into Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\left(Ae^{iS/\hbar}\right) + V(\vec{x})Ae^{iS/\hbar} = i\hbar\frac{\partial}{\partial t}Ae^{iS/\hbar}$$

$$\underbrace{-\frac{\hbar^2}{2m}\nabla^2\left(Ae^{iS/\hbar}\right)}_{\mathrm{I}} + V(\vec{x})Ae^{iS/\hbar} \underbrace{- i\hbar\frac{\partial}{\partial t}\left(Ae^{iS/\hbar}\right)}_{\mathrm{II}} = 0$$

I: $$\nabla^2\left(Ae^{iS/\hbar}\right) = \vec{\nabla}\cdot\left(\vec{\nabla}A\, e^{iS/\hbar} + \frac{i}{\hbar}A\vec{\nabla}S\, e^{iS/\hbar}\right)$$

$$= \nabla^2 A\, e^{iS/\hbar} + (\vec{\nabla}A)\cdot\frac{i}{\hbar}(\vec{\nabla}S)e^{iS/\hbar} + \frac{i}{\hbar}(\vec{\nabla}A)\cdot(\vec{\nabla}S)e^{iS/\hbar} + \frac{i}{\hbar}A\nabla^2 S\, e^{iS/\hbar} + \left(\frac{i}{\hbar}\right)^2 A(\vec{\nabla}S)^2 e^{iS/\hbar}$$

$$= \left(\nabla^2 A + \left(\frac{i}{\hbar}\right)^2 A(\vec{\nabla}S)^2 + \frac{2i}{\hbar}(\vec{\nabla}A)\cdot(\vec{\nabla}S) + \frac{i}{\hbar}A\nabla^2 S\right)e^{iS/\hbar}$$

II: $$-i\hbar\frac{\partial}{\partial t}\left(Ae^{iS/\hbar}\right) = -i\hbar\left(\frac{\partial A}{\partial t}e^{iS/\hbar} + A\frac{i}{\hbar}\frac{\partial S}{\partial t}e^{iS/\hbar}\right)$$

So, Schrödinger equation becomes (dividing through by $e^{iS/\hbar}$)

$$-\frac{\hbar^2}{2m}\left(\nabla^2 A + \left(\frac{i}{\hbar}\right)^2 A(\vec{\nabla}S)^2 + \frac{2i}{\hbar}(\vec{\nabla}A)\cdot(\vec{\nabla}S) + \frac{i}{\hbar}A\nabla^2 S\right) + V(\vec{x})A - i\hbar\left(\frac{\partial A}{\partial t} + A\frac{i}{\hbar}\frac{\partial S}{\partial t}\right) = 0.$$

Rearranging:

$$A\left(-\frac{\hbar^2}{A}\nabla^2 A + \frac{1}{2m}(\vec{\nabla}S)^2 + V(\vec{x}) + \frac{\partial S}{\partial t}\right)$$

$$-\frac{i\hbar}{2A}\left(\frac{A}{m}2(\vec{\nabla}A).(\vec{\nabla}S) + \frac{1}{m}A^2\nabla^2 S + 2A\frac{\partial A}{\partial t}\right) = 0$$

The real and imaginary parts vanish independently:

① Re: $\dfrac{\partial S}{\partial t} + \dfrac{1}{2m}(\vec{\nabla}S)^2 + V(\vec{x}) = \dfrac{\hbar^2}{A}\nabla^2 A$ ← (Classical) Hamilton–Jacobi equation (with $\hbar^2$ q. corr.)

② Im: $2A\dfrac{\partial A}{\partial t} + \dfrac{2A}{m}(\vec{\nabla}A).(\vec{\nabla}S) + \dfrac{1}{m}A^2\nabla^2 S = 0$

Recall: $H\left(q_i; \frac{\partial S}{\partial q_i}\right) + \frac{\partial S}{\partial t} = 0$

$\vec{p}(t) = \vec{\nabla}S(x,t)$

trajectories orthogonal to wave fronts

WKB ASSUMPTION:

$\dfrac{\hbar^2}{A}\nabla^2 A \ll \dfrac{\partial S}{\partial t}$ and $\dfrac{1}{2m}(\vec{\nabla}S)^2$, so neglect it in 1st eqn.

So the phase, $S(\vec{r},t)$ obeys Hamilton–Jacobi equation $\Rightarrow$ decouples from 2nd eqn

The second equation is the continuity equation for probability density:

$$\dot{\rho} + \vec{\nabla}.\vec{J} = 0$$

Put $\rho = A^2$ & $\vec{J} = A^2\dfrac{\vec{\nabla}S}{m}$:

then $2A\dfrac{\partial A}{\partial t} + 2A(\vec{\nabla}A.)\dfrac{\vec{\nabla}S}{m} + A^2\dfrac{\nabla^2 S}{m} = 0$ is eq. ②.

So the multivariable WKB equations are

① $$\frac{\partial S}{\partial t} + \frac{1}{2m}(\vec{\nabla}S)^2 + V(\vec{x}) = 0$$

② $$\frac{\partial \rho}{\partial t} + \vec{\nabla}.\vec{J} = 0, \quad \text{with } \rho = A^2 \ \& \ \vec{J} = \frac{1}{m}A^2\vec{\nabla}S$$

Once ① is solved for $S(\vec{r})$, the amplitude $A(\vec{r})$ can be found by using the continuity equation, ②.

Define $p_i(x,t) = -\dfrac{\partial}{\partial a_i} S(\vec{a},\vec{x},t)$.

n.b.: In Jacobi-Hamilton's formulation, S is the principal function, and its gradient, $\dfrac{\partial S}{\partial a_i}$, is the momentum, p_i.

Differentiate with respect to t

$$\frac{\partial p_i}{\partial t} = -\frac{\partial}{\partial a_i}\frac{\partial S}{\partial t} \quad \Big\downarrow \text{use ①}$$

$$= -\frac{\partial}{\partial a_i}\left(-\frac{1}{2m}(\vec{\nabla} S)^2 - V(\vec{x})\right) \qquad \vec{\nabla} = \frac{\partial}{\partial x_k}$$

$$= \frac{1}{\cancel{2}m}\left(\cancel{2}\left(\frac{\partial}{\partial x_k}\underbrace{\frac{\partial S}{\partial a_i}}\right)\frac{\partial S}{\partial x_k} + 0\right)$$

$$= \frac{1}{m}\frac{\partial}{\partial x_k}(-p_i)\frac{\partial S}{\partial x_k}$$

Differentiate with respect to x_j

$$\frac{\partial}{\partial t}\underbrace{\frac{\partial p_i}{\partial x_j}}_{\text{Define: } \equiv M_{ij}} + \frac{1}{m}\left(\frac{\partial}{\partial x_k}\underbrace{\frac{\partial p_i}{\partial x_j}}_{\equiv M_{ij}}\right)\frac{\partial S}{\partial x_k} + \frac{1}{m}\underbrace{\frac{\partial p_i}{\partial x_k}}_{\equiv M_{ik}}\underbrace{\left(\frac{\partial}{\partial x_k}\frac{\partial S}{\partial x_j}\right)}_{\equiv N_{kj}} = 0$$

$$\frac{\partial}{\partial t}M + \frac{1}{m}(\vec{\nabla}M).(\vec{\nabla}S) + \frac{1}{m}MN = 0 \qquad \text{(matrix eqn)}$$

Multiply at left by M^{-1}, and take trace

$$\mathrm{Tr}\left[M^{-1}\frac{\partial M}{\partial t}\right] + \frac{1}{m}\mathrm{Tr}\left[M^{-1}\vec{\nabla}M\right].\vec{\nabla}S + \frac{1}{m}\underbrace{\mathrm{Tr}\,N}_{\nabla^2 S} = 0$$

$$\mathrm{Tr}\left[M^{-1}\frac{\partial M}{\partial t}\right] + \frac{1}{m}\mathrm{Tr}\left[M^{-1}\vec{\nabla}M\right].\vec{\nabla}S + \frac{1}{m}\nabla^2 S = 0$$

Use identity:

$$\mathrm{Tr}\left[M^{-1}(t) \frac{\partial}{\partial t} M(t) \right] = \frac{\partial}{\partial t} \ln \mathrm{Det}\, M(t) = \frac{1}{\mathrm{Det}\, M(t)} \frac{\partial}{\partial t} \mathrm{Det}\, M(t)$$

Then,

$$\frac{1}{\mathrm{Det}\, M} \frac{\partial}{\partial t} \mathrm{Det}\, M + \frac{1}{m} \frac{1}{\mathrm{Det}\, M} (\vec{\nabla}\, \mathrm{Det}\, M) . \vec{\nabla} S + \frac{1}{m} \nabla^2 S = 0$$

$$\frac{\partial}{\partial t} \mathrm{Det}\, M + \frac{1}{m} \left[(\vec{\nabla}\, \mathrm{Det}\, M) . \vec{\nabla} S + (\mathrm{Det}\, M) \nabla^2 S \right] = 0$$

$$\frac{\partial}{\partial t} \mathrm{Det}\, M + \vec{\nabla} . \left[\frac{1}{m} (\mathrm{Det}\, M)(\vec{\nabla} S) \right] = 0$$

This is the continuity equation. ②, with the identification $A^2 = \mathrm{Det}\, M$,

or

$$A(r) = [\mathrm{Det}\, M]^{1/2} = \left[\mathrm{Det}\, \frac{\partial p_i}{\partial x_j} \right]^{1/2} = \left[\mathrm{Det}\, \frac{-\partial^2 S}{\partial a_i \partial x_j} \right]^{1/2}$$

HENCE, THE many-body wavefunction in the WKB approximation is

$$\psi_{WKB}(x) = \mathcal{N} \left[\mathrm{Det}\, \frac{-\partial^2 S}{\partial a_i \partial x_j} \right]^{1/2} e^{iS} \qquad (?)$$

Not $\frac{1}{\sqrt{\det}}$?