WKB approximation

Wentzel – Kramers – Brillouin

Treat the wavefunction by splitting modulus & phase

$$\psi(\vec{x},t) = \sqrt{\rho(\vec{x},t)}\, \exp\left\{\frac{i}{\hbar} S(\vec{x},t)\right\} \quad \ldots \text{ ansatz}$$

Note prob. density $\psi^*\psi = \rho$

Also note the current density

$$\vec{j} = \frac{\hbar}{2mi}\left(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right) = \frac{\hbar}{m}\,\mathrm{Im}\left(\psi^*\vec{\nabla}\psi\right)$$

Recall that

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0$$

... continuity eqn.

Here,

$$\vec{j} = \frac{\hbar}{m} \, \mathrm{Im}\left(\sqrt{\rho}\, \cancel{e^{-iS/\hbar}} \cdot \left(\frac{1}{2\sqrt{\rho}} \vec{\nabla}\rho + i\sqrt{\rho}\, \frac{\vec{\nabla} S}{\hbar} \right) \cancel{e^{iS/\hbar}} \right)$$

$$= \frac{\hbar}{m} (\sqrt{\rho})^2 \frac{1}{\hbar} \vec{\nabla} S \qquad = \frac{\rho}{m} \vec{\nabla} S$$

current $\sim$ density $\times$ velocity $\Rightarrow$ $v_{eff} = \frac{1}{m} \vec{\nabla} S$

This is reminiscent of Hamilton's Principal Function S which gives $\vec{p} = \vec{\nabla} S$

Now substituting the ψ into Schrödinger eqn.,

$$i\hbar\frac{\partial}{\partial t}\psi = i\hbar\frac{1}{2\sqrt{\rho}}\frac{\partial\rho}{\partial t}e^{iS/\hbar} + i\hbar\sqrt{\rho}\cdot\frac{i}{\hbar}\frac{\partial S}{\partial t}e^{iS/\hbar}$$

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi = \frac{\hbar^2}{2m}\left\{\vec{\nabla}\left(\frac{1}{2\sqrt{\rho}}\vec{\nabla}\rho\right)e^{iS/\hbar} + 2\frac{1}{2\sqrt{\rho}}\vec{\nabla}\rho\cdot\frac{i}{\hbar}\vec{\nabla}S e^{iS/\hbar} + \sqrt{\rho}\,\frac{i}{\hbar}\vec{\nabla}\left(\vec{\nabla}S\,e^{iS/\hbar}\right)\right\}$$

Thus with potential $V(\vec{x})$

$$\left(\frac{i}{2}\frac{\hbar}{\sqrt{\rho}}\frac{\partial\rho}{\partial t} - \sqrt{\rho}\frac{\partial S}{\partial t}\right) = \boxed{-\frac{\hbar^2}{2m}}\left(\vec{\nabla}^2\sqrt{\rho} + \frac{2i}{\hbar}\vec{\nabla}\sqrt{\rho}\cdot\vec{\nabla}S + \frac{i}{\hbar}\sqrt{\rho}\,\nabla^2 S - \frac{\sqrt{\rho}}{\hbar^2}|\vec{\nabla}S|^2\right) + V(\vec{x})\sqrt{\rho}$$

Consider terms in orders of $\hbar$:

$$(\hbar^0) : -\sqrt{\rho}\frac{\partial S}{\partial t} = +\frac{1}{2m}\sqrt{\rho}|\vec{\nabla}S|^2 + \sqrt{\rho}\,V(\vec{x})$$

$$(\hbar^1) : \frac{i}{2\sqrt{\rho}}\frac{\partial \rho}{\partial t} = -\frac{1}{2m}\times 2i\,\vec{\nabla}\sqrt{\rho}\cdot\vec{\nabla}S - \frac{i}{2m}\sqrt{\rho}\,\nabla^2 S$$

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The ansatz (or proposed form of the solution) further assumes that $\rho = \psi^*\psi$ is a "stiff" function i.e. slowly varying w.r.t. t & $\vec{x}$

Further assume $|\vec{\nabla}S|^2 >> \hbar\nabla^2 S$

Thus, with these assumptions the dominant equation to be solved is

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

This can be thought of as the Hamilton - Jacobi equation for the function $S(\vec{x}, t)$

When energy is conserved, we can simplify

$$S(\vec{x}, t) = W(\vec{x}) - Et$$

[Recall transformed Hamiltonian $K = H + \frac{\partial S}{\partial t}$ was chosen zero. Then using ~~is~~ $H \equiv E$ Then $S \sim -Et$]

Note this split into space + time is equiv. to "separation of variables" in the language of $\psi \sim \varphi(\vec{x}) f(t)$

$$\sim \varphi(\vec{x}) e^{-iEt/\hbar}$$

Thus, $W(\vec{x})$ satisfies ... restricting to 1-dimension

$$\frac{1}{2m}\left(\frac{dW}{dx}\right)^2 + V(x) - E = 0$$

i.e. $$\left(\frac{dW}{dx}\right)^2 = 2m\left(E - V(x)\right)$$

or $$W(x) = \pm \int_{x_0}^{x} dx' \sqrt{2m\left(E - V(x')\right)}$$

Next, note in the continuity eqn.

$$\frac{\partial \rho}{\partial t} = -\vec{\nabla}\cdot\vec{j} \quad \ldots \quad \boxed{\frac{\partial \rho}{\partial t} = 0}$$ if we have a stationary state

Then $0 = \vec{\nabla}\cdot\vec{j} = \frac{1}{m}\vec{\nabla}(\rho\,\vec{\nabla}S)$

Thus in our 1-dim version

$$\rho\frac{dW}{dx} = \text{const.} = \pm\rho\sqrt{2m(E-V(x))}$$

Thus, $\sqrt{\rho} = \dfrac{\text{const.}}{\{E-V(x)\}^{1/4}} \propto \dfrac{1}{\sqrt{v_{\text{eff}}}}$

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$$\psi(x,t) = \frac{\text{const.}}{(E-V(x))^{1/4}} \exp\left[\pm \frac{i}{\hbar}\int^{x} dx' \sqrt{2m(E-V(x'))} - \frac{iEt}{\hbar}\right]$$

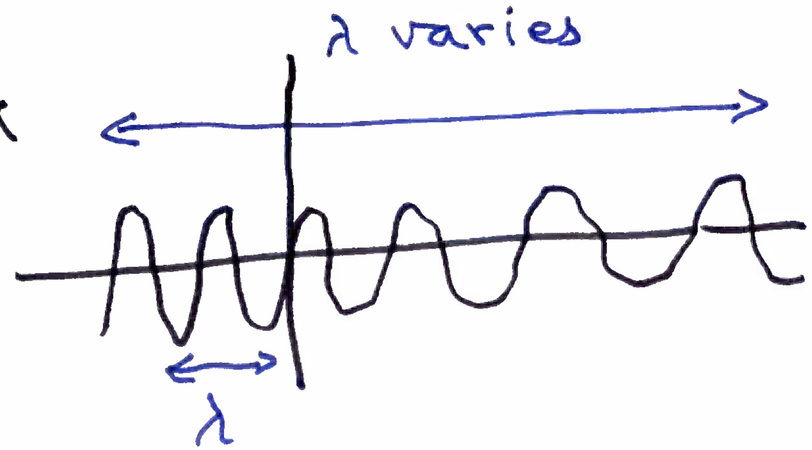
Consistency requirement

$$\hbar \left|\frac{d^2W}{dx^2}\right| << \left|\frac{dW}{dx}\right|^2$$

i.e. $\frac{d}{dx} k_{eff} << k_{eff}^2$

$$\frac{dW}{dx} \sim p \sim \hbar k$$

i.e. roughly $\cancel{\frac{d}{dx}\lambda >> \lambda}$



The scale over which λ may vary is >> λ itself