SECTION 2.3
Classical mechanics as the geometrical optic limit

We can always write a wave function in the polar form,

$$\psi(\mathbf{x},t) = A(\mathbf{x},t)e^{iS(\mathbf{x},t)/\hbar}. \tag{2.24}$$

A surface of constant S is a wave front, and the vector ∇S normal to the wave front is the propagation direction of the wave. For a particle in a constant potential, the (non-normalizable) stationary state solutions are of the form $\propto e^{\pm i\mathbf{p}\cdot\mathbf{x}/\hbar}$, i.e. $S = \pm\mathbf{p}\cdot\mathbf{x}$, and $\nabla S = \pm\mathbf{p}$. One might expect that for a slowly-varying potential, the solution is *nearly* a plane wave, and we may be able to approximate it with a simple form of the function $S(\mathbf{x},t)$.

Plugging the Ansatz (2.24) into the TDSE,

$$i\hbar\frac{\partial}{\partial t}\left(Ae^{iS/\hbar}\right) = -\frac{\hbar^2}{2m}\nabla^2(Ae^{iS/\hbar}) + VAe^{iS/\hbar} \tag{2.25}$$

$$i\hbar(\dot{A}e^{iS/\hbar} + \frac{i}{\hbar}\dot{S}Ae^{iS/\hbar}) = -\frac{\hbar^2}{2m}\left[\nabla^2 Ae^{iS/\hbar} + 2(\nabla A)\cdot(\nabla e^{iS/\hbar}) + A\nabla^2 e^{iS/\hbar}\right] + VAe^{iS/\hbar} \tag{2.26}$$

$$(i\hbar\dot{A} - \dot{S}A)e^{iS/\hbar} = -\frac{\hbar^2}{2m}\left[\nabla^2 A + \frac{2i}{\hbar}(\nabla A)\cdot(\nabla S) + \frac{i}{\hbar}A\nabla^2 S - \frac{1}{\hbar^2}A|\nabla S|^2\right]e^{iS/\hbar} + VAe^{iS/\hbar} \tag{2.27}$$

After canceling the phase factor $\exp(iS(\mathbf{x},t)/\hbar)$, we obtain two separate equations, one for the real part and another for the imaginary part.

$$\dot{A} = -(\nabla A)\cdot\frac{\nabla S}{m} - A\frac{\nabla^2 S}{2m} \tag{2.28}$$

Imaginary part

$$-\dot{S} = \frac{|\nabla S|^2}{2m} + V - \frac{\hbar^2}{2m}\frac{\nabla^2 A}{A} \tag{2.29}$$

Real part

A few extra steps are needed to interpret the first equation (2.28). Since we know that $\rho = A^2$ is the probability density, observe that we could obtain the rate of change $\dot{\rho}$ by multiplying the LHS by $2A$:

$$\begin{aligned} 2A\dot{A} = \frac{\partial\rho}{\partial t} &= -\frac{1}{m}\left[2A(\nabla A)\cdot\nabla S - A^2\nabla^2 S\right] \\ &= -\nabla\left(A^2\frac{\nabla S}{m}\right).^{6} \end{aligned} \tag{2.30}$$

[6]
$$\begin{aligned} &2A\partial_j A\partial_j S + A^2\partial_j\partial_j S \\ &= \partial_j(A^2)\partial_j S + A^2\partial_j\partial_j S \\ &= \partial_j(A^2\partial_j S) \end{aligned}$$

This has the form of a continuity equation. The quantity in the bracket in the RHS therefore should have the meaning of the probability current,

$$\mathbf{J} = \frac{\hbar}{m}\mathrm{Im}(\psi^*\nabla\psi) \tag{2.31}$$

which we now verify.

$$\psi^* \nabla \psi = (A e^{-iS/\hbar}) \left(\nabla A e^{iS/\hbar} + \frac{i}{\hbar} A \nabla S e^{iS/\hbar} \right) = A \nabla A + \frac{i}{\hbar} A^2 \nabla S, \tag{2.32}$$

giving, as expected,

$$\mathbf{J} = A^2 \frac{\nabla S}{m}. \tag{2.33}$$

So the imaginary part of the TDSE just expresses the local conservation of probability,

$$\boxed{\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}}. \tag{2.34}$$

Note further that, classically since the current is the density times the velocity, we arrive at the relation

$$\mathbf{p}_{\text{classical}} = \nabla S, \tag{2.35}$$

as we already discussed above.

In the formal limit $\hbar \to 0$, the second equation (2.29) becomes the *Hamilton-Jacobi equation* from classical dynamics,

$$-\dot{S} = \frac{|\nabla S|^2}{2m} + V. \tag{2.36}$$

In particular, it is the equation of motion for the generating function S such that $\nabla S = \mathbf{p}$. But in physics, it is meaningless to say that a quantity is large or small by itself. Case in point, the value of $\hbar \approx 1.05^{-34}$ J·s may seem small but we can make it arbitrary large or small by considering units other than Joule-second. What we meant by "$\hbar \to 0$", i.e. that the quantum contribution is negligible, is that

$$\frac{|\nabla S|^2}{2m} \gg \frac{\hbar^2}{2m} \left| \frac{\nabla^2 A}{A} \right|. \tag{2.37}$$

The LHS is nothing but $\mathbf{p}^2/2m$, while the RHS hints at some kind of a characteristic length scale

$$\left| \frac{\nabla^2 A}{A} \right| \sim \frac{1}{L^2}. \tag{2.38}$$

Putting these together, we have that

$$\mathbf{p}^2 = \hbar^2 \mathbf{k}^2 \gg \frac{\hbar^2}{L^2} \tag{2.39}$$

Expressed in terms of the local de Broglie wavelength, we need

$$\lambda \ll L. \tag{2.40}$$

$$\boxed{\begin{array}{ccc} \text{Wave optics} & & \text{Quantum mechanics} \\ \downarrow & \text{Short-wavelength limit} & \downarrow \\ \text{Geometric optics} & & \text{Classical mechanics} \end{array}} \tag{2.41}$$

In the case of a particle moving in a one-dimensional potential, the length scale of the problem is determined by how fast the potential is varying (i.e. the force felt by the particle).

$$L \sim \left| V / \frac{\mathrm{d}V}{\mathrm{d}x} \right| \tag{2.42}$$

Semiclassical (WKB) approximation

In terms of the local momentum $p(\mathbf{x}) = \sqrt{2m(E - V(\mathbf{x}))}$, the TISE becomes

$$-\hbar^2 \nabla^2 \psi = p^2(x)\psi \tag{2.43}$$

The idea of the WKB approximation is to consider plugging only the phase part of the Ansatz (2.24) into (2.43):

$$-\hbar^2 \nabla^2 e^{iS/\hbar} = p^2(\mathbf{x}) e^{iS/\hbar} \tag{2.44}$$

$$\boxed{|\nabla S|^2 - i\hbar \nabla^2 S = p^2(\mathbf{x})}, \tag{2.45}$$

and solve for a series solution in powers of $\hbar$:

$$S = S_0 + \hbar S_1 + \hbar^2 S_2 + \cdots . \tag{2.46}$$

The first two orders ($\hbar^0$ and $\hbar$) give two equations

$$\nabla S_0 = p^2(\mathbf{x}), \tag{2.47}$$

$$\hbar \nabla S_0 \nabla S_1 = i \nabla^2 S_0. \tag{2.48}$$

Solving them in one dimension yields the *WKB wave function*,

$$\boxed{\psi_{\mathrm{WKB}}(x,t) \propto \frac{1}{\sqrt{p(x)}} \exp\left\{ \pm i \int_{x_0}^{x} dx' k(x') \right\}}. \tag{2.49}$$

This is an approximate wave function in the short-wavelength regime (2.47), but since we incorporate $\hbar$ to the first order, it is not exactly a classical approximation but a *semiclassical* approximation.

In the classically forbidden area $p^2 = -\hbar^2 \kappa(x)$. Since $p(x) = i\kappa(x)$, so we can write down the WKB solution,

$$\psi_{\mathrm{WKB}}(x,t) \propto \frac{1}{\sqrt{\kappa(x)}} \exp\left\{ \pm \int_{x_0}^{x} dx' \kappa(x') \right\}. \tag{2.50}$$

We want to match the solutions in the classically allowed region and the classical forbidden areas, but near the turning point where $E \approx V$, the approximation breaks down because $k \to 0$ and $\lambda \to \infty$. Fixing the problem requires a *connection formula*, which is outside the scope of this course, but assuming that there is a fix, we have a following neat application of the WKB approximation to counting the number of bound states.

Application of WKB approximation to bound states

$$L \cdot M \approx \int^{x} dx' p(x') \approx nh, \tag{2.51}$$

where L and M are the characteristic length and momentum scales respectively, and n is the number of allowed energy levels. A pictorial interpretation of this formula is that the number of bound states is roughly equal to the number of cells of area h that can be fit into a phase-space region of dimension L times M.