

The Schrödinger equation

SECTION 2.3

Classical mechanics as the geometrical-optic limit of quantum mechanics

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

$$\psi(\mathbf{x}, t) = A(\mathbf{x}, t)e^{iS(\mathbf{x}, t)/\hbar}. \quad (2.1)$$

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 (??) into the TDSE,

$$i\hbar \frac{\partial}{\partial t} (Ae^{iS/\hbar}) = -\frac{\hbar^2}{2m} \nabla^2 (Ae^{iS/\hbar}) + VAe^{iS/\hbar} \quad (2.2)$$

$$i\hbar (\dot{A}e^{iS/\hbar} + \frac{i}{\hbar} \dot{S}Ae^{iS/\hbar}) = -\frac{\hbar^2}{2m} [\nabla^2 Ae^{iS/\hbar} + 2(\nabla A) \cdot (\nabla e^{iS/\hbar}) + A\nabla^2 e^{iS/\hbar}] + VAe^{iS/\hbar} \quad (2.3)$$

$$(i\hbar \dot{A} - \dot{S}A)e^{iS/\hbar} = -\frac{\hbar^2}{2m} \left[\nabla^2 A + \frac{2i}{\hbar} (\nabla A) \cdot (\nabla S) + \frac{i}{\hbar} A \nabla^2 S - \frac{1}{\hbar^2} A |\nabla S|^2 \right] e^{iS/\hbar} + VAe^{iS/\hbar} \quad (2.4)$$

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.

$$\dot{A} = -(\nabla A) \cdot \frac{\nabla S}{m} - A \frac{\nabla^2 S}{2m} \quad (2.5)$$

$$-\dot{S} = \frac{|\nabla S|^2}{2m} + V - \frac{\hbar^2}{2m} \frac{\nabla^2 A}{A} \quad (2.6)$$

A few extra steps are needed to interpret the first equation (??). 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 $2A$:

$$\begin{aligned} 2A\dot{A} &= \frac{\partial \rho}{\partial t} = -\frac{1}{m} [2A(\nabla A) \cdot \nabla S - A^2 \nabla^2 S] \\ &= -\nabla \cdot \left(A^2 \frac{\nabla S}{m} \right).^1 \end{aligned} \quad (2.7)$$

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,

$$\mathbf{J} = \frac{\hbar}{m} \text{Im}(\psi^* \nabla \psi) \quad (2.8)$$

which we now verify.

$$\psi^* \nabla \psi = (Ae^{-iS/\hbar}) \left(\nabla A e^{iS/\hbar} + \frac{i}{\hbar} A \nabla S e^{iS/\hbar} \right) = A \nabla A + \frac{i}{\hbar} A^2 \nabla S, \quad (2.9)$$

giving, as expected,

$$\mathbf{J} = A^2 \frac{\nabla S}{m}. \quad (2.10)$$

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

$$\boxed{\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}}. \quad (2.11)$$

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

$$\mathbf{p}_{\text{classical}} = \nabla S, \quad (2.12)$$

as we already discussed above.

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

$$-\dot{S} = \frac{|\nabla S|^2}{2m} + V. \quad (2.13)$$

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 $\hbar \approx 1.05^{-34} \text{ J}\cdot\text{s}$ may seem small but we can make it arbitrary large or small by considering units other than Joule-second. What we meant by " $\hbar \rightarrow 0$ ", i.e. that the quantum contribution is negligible, is that

$$\frac{|\nabla S|^2}{2m} \gg \frac{\hbar^2}{2m} \left| \frac{\nabla^2 A}{A} \right|. \quad (2.14)$$

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

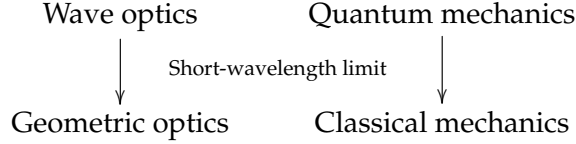
$$\left| \frac{\nabla^2 A}{A} \right| \sim \frac{1}{L^2}. \quad (2.15)$$

Putting these together, we have that

$$\mathbf{p}^2 = \hbar^2 \mathbf{k}^2 \gg \frac{\hbar^2}{L^2} \quad (2.16)$$

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

$$\lambda \ll L. \quad (2.17)$$



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).

$$L \sim \left| V / \frac{dV}{dx} \right| \quad (2.18)$$

Semiclassical (WKB) approximation

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

$$-\hbar^2 \nabla^2 \psi = p^2(x) \psi \quad (2.19)$$

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

$$-\hbar^2 \nabla^2 e^{iS/\hbar} = p^2(\mathbf{x}) e^{iS/\hbar} \quad (2.20)$$

$$\boxed{|\nabla S|^2 - i\hbar \nabla^2 S = p^2(\mathbf{x})}, \quad (2.21)$$

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

$$S = S_0 + \hbar S_1 + \hbar^2 S_2 + \dots \quad (2.22)$$

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

$$\nabla S_0 = p^2(\mathbf{x}), \quad (2.23)$$

$$\hbar \nabla S_0 \nabla S_1 = i \nabla^2 S_0. \quad (2.24)$$

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

$$\boxed{\psi_{\text{WKB}}(x, t) \propto \frac{1}{\sqrt{p(x)}} \exp \left\{ \pm i \int_{x_0}^x dx' k(x') \right\}}. \quad (2.25)$$

This is an approximate wave function in the short-wavelength regime (??), but since we incorporate \hbar to the first order, it is not exactly a classical approxima-

tion 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,

$$\psi_{\text{WKB}}(x, t) \propto \frac{1}{\sqrt{\kappa(x)}} \exp\left\{\pm \int_{x_0}^x dx' \kappa(x')\right\}. \quad (2.26)$$

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 $k \rightarrow 0$ and $\lambda \rightarrow \infty$. 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

$$L \cdot M \approx \int^x dx' p(x') \approx nh, \quad (2.27)$$

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 $L \cdot M$.