# B7.3 Further Quantum Theory Lecture 13

Our next topic is yet another approximation scheme, this one applies specifically to the case of systems described by wave-functions, and in fact is applied more broadly in the study of differential equations. We will start with the time-dependent version, but will quickly specialize to the study of stationary states, where it is often the most useful

We begin (without loss of generality) by parameterizing a general solution of the time-dependent Schrödinger equation in polar form:

$$\Psi(\underline{x},t) = A(\underline{x},t)e^{\frac{i}{\hbar}S(\underline{x},t)} \quad (\text{for now, } A \geq 0,\ S \in \mathbb{R})$$

It's then useful to compute: $\underline{\nabla}\Psi = \left(\frac{\nabla A}{A} + \frac{i}{\hbar}\nabla S\right)Ae^{\frac{i}{\hbar}S}$

$$\nabla^2\Psi = \left(\frac{\nabla^2 A}{A} + \frac{i}{\hbar}\left(\frac{2\nabla S\cdot\nabla A}{A} + \nabla^2 S\right) - \frac{1}{\hbar^2}|\nabla S|^2\right)Ae^{\frac{i}{\hbar}S}$$

$$\partial_t\Psi = \left(\frac{\partial_t A}{A} + \frac{i}{\hbar}\partial_t S\right)Ae^{\frac{i}{\hbar}S}$$

We can rewrite the time-dependent Schrödinger equation in terms of $A$ & $S$:

$$i\hbar\frac{\partial}{\partial t}\Psi + \frac{\hbar^2}{2m}\nabla^2\Psi - V\Psi = 0 \iff i\hbar\frac{\partial_t A}{A} + \frac{i\hbar}{2m}\left(\frac{2\nabla S\cdot\nabla A}{A} + \nabla^2 S\right) - \partial_t S - \frac{1}{2m}|\nabla S|^2 - V + \frac{\hbar^2}{2m}\left(\frac{\nabla^2 A}{A}\right) = 0$$

So far this looks like a terrible idea. Our beautiful, linear Schrödinger equation is replaced by a complicated, non-linear mess. Still, we proceed!

Taking real and imaginary parts:

$O(1)$ $\qquad$ $O(\hbar^2)$

Real Part: $\partial_t S + \frac{1}{2m}\nabla S\cdot\nabla S + V = \frac{\hbar^2}{2m}\frac{\nabla^2 A}{A}$

$O(\hbar)$

Imaginary Part: $i\hbar\,\partial_t A + \frac{i\hbar}{2m}\left(A\nabla^2 S + 2\nabla S\cdot\nabla A\right) = 0 \rightarrow \partial_t(A^2) + \frac{1}{m}\nabla\cdot\left(A^2\nabla S\right) = 0$

The "semi-classical approximation" (or WKB approximation) is to set to zero the $O(\hbar^2)$ term in the real part. The validity is clearly state dependent, but heuristically it is a "small $\hbar$" approximation.

Recall some definitions: $\rho = |\Psi|^2 = A^2$ "probability density"

$$\underline{j} = \frac{i\hbar}{2m}\left[\Psi\underline{\nabla}\bar{\Psi} - \bar{\Psi}\underline{\nabla}\Psi\right] = \frac{1}{m}A^2\underline{\nabla}S \quad \text{"probability current"}$$

Our semi-classical equations are now:

the Continuity Equation: $\partial_t(A^2) + \underline{\nabla}\cdot\left(\frac{1}{m}A^2\underline{\nabla}S\right) = 0 \quad (\partial_t\rho + \underline{\nabla}\cdot\underline{j} = 0)$

the Hamilton-Jacobi Equation: $\partial_t S + \frac{1}{2m}|\nabla S|^2 + V = 0$

The Hamilton-Jacobi equation governs the behaviour of the action of classical trajectories, so in some sense, the phase is controlled by classical dynamics (though we won't pursue this here).

By far the simplest setting in which to apply the WKB method is that of time-independent, one-dimensional problems. For the time-independent case, we will estimate the wave-function of a state of energy $E$ by writing:

$$\Psi(\underline{x},t) = A(\underline{x})\, e^{\frac{i}{\hbar}W(\underline{x}) - \frac{i}{\hbar}Et}$$

So $S(\underline{x},t) = W(\underline{x}) - Et$. Our equations for $A$ and $S$ become, for $A$ and $W$,

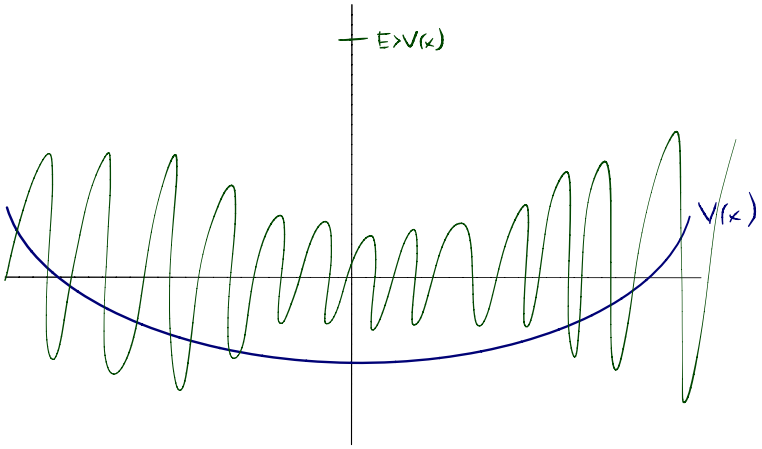
- $\underline{\nabla}\cdot(A^2\underline{\nabla}W) = 0$
- $|\underline{\nabla}W|^2 = 2m(E-V)$

Further specializing to one dimension, (call it $x$) we have

- $(\partial_x W)^2 = 2m(E-V(x)) = p^2(x)$ ← classical momentum at $x$ if energy is $E$: $\frac{p^2}{2m}+V(x)=E$
  - $\rightarrow \partial_x W = \pm p(x)$ (by convention, let $p(x)\geq 0$)
  - $\rightarrow W(x) = \pm\int^x p(x')dx'$

  } for our reality conditions, we must be in classically allowed region, where $E \geq V(x)$.
- $\partial_x\left(A^2(\pm p(x))\right) = 0 \quad \rightarrow A^2 = \frac{\tilde{K}}{p(x)}$
  - $\rightarrow A = \frac{K}{\sqrt{p(x)}} = \frac{K}{(2m(E-V))^{1/4}}$

Putting these together $\Psi_{\pm}^{\text{allowed}}(x) = \frac{K}{\sqrt{p(x)}}\exp\left(\frac{\pm i}{\hbar}\int^x p(x')dx'\right)$. What's the intuition here?



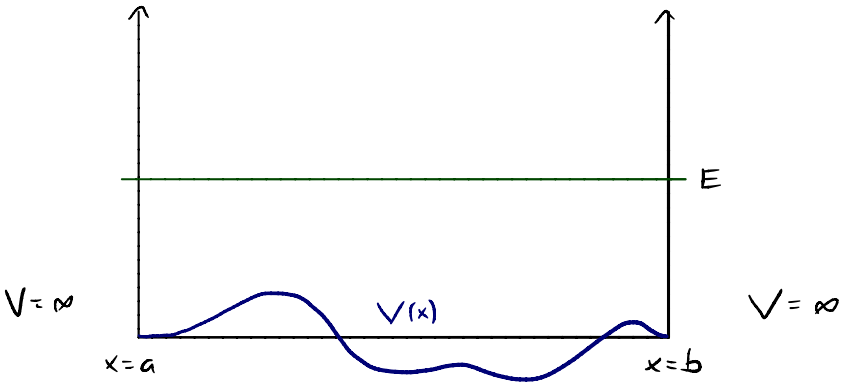

Approximate wave fn by plane wave of frequency determined by energy locally as for constant potential. Should be good approximation if potential is slowly varying compared to wavelength. Can investigate the term we dropped from Schrödinger equation to see this is roughly the case.

$$\frac{\hbar^2}{2m}\frac{A''}{A} = \frac{\hbar^2}{2m}\left\{\frac{3}{4}\frac{(p')^2}{p^2} - \frac{1}{2}\frac{p''}{p}\right\}$$

This should be small compared to leading terms of order $\frac{p^2}{2m}$, and it is then sufficient to have $\left|\frac{p'}{p}\right| \ll \left|\frac{p}{\hbar}\right|$, $\left|\frac{p''}{p'}\right| \ll \left|\frac{p}{\hbar}\right|$. This means relative change in $p$ or $p'$ over a distance [$\hbar/p$ ~wavelength] is very small.

So, for fixed $V(x)$, high energy states should be well-approximated.

# First applications (a bit artificial): particle in a lumpy box




$$\psi_{WKB}(x) = \frac{K_+}{p(x)^{1/2}} \exp\left[\frac{i}{\hbar}\int_a^x p(x')dx'\right] + \frac{K_-}{p(x)^{1/2}} \exp\left[\frac{-i}{\hbar}\int_a^x p(x')dx'\right]$$

Boundary conditions $\psi_{WKB}(a) = \psi_{WKB}(b) = 0$:

B.C. @ $x=a$ $\quad \psi_{WKB}(a) = \dfrac{K_+ + K_-}{p(a)^{1/2}} = 0 \iff K_- = -K_+$

$$\Rightarrow \psi_{WKB}(x) = \frac{2iK_+}{p(x)^{1/2}} \sin\left(\frac{1}{\hbar}\int_a^x p(x')dx'\right)$$

B.C. @ $x=b$ $\quad \psi_{WKB}(b) = \dfrac{2iK_+}{p(b)^{1/2}} \sin\left(\frac{1}{\hbar}\int_a^b p(x')dx'\right) = 0$

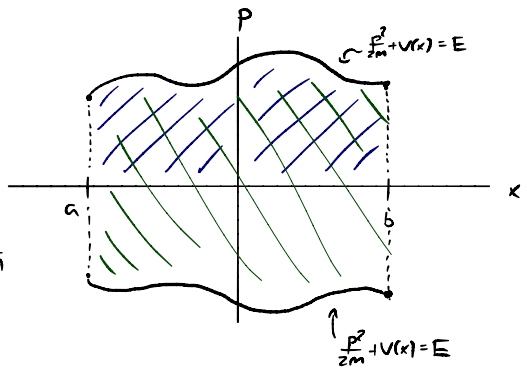
$$\Rightarrow \int_a^b p(x')dx' = \int_a^b \sqrt{2m(E-V(x))}\,dx = n\pi\hbar \quad \text{for } n \in \mathbb{Z}_+$$

(setting $V(x)=0 \Rightarrow E = \frac{\pi^2\hbar^2 n^2}{2m(b-a)^2}$, which is exact)

This quantization condition determines the allowed energies, just like for particle in a box. Note that if we define $p(x)$ as we have done,

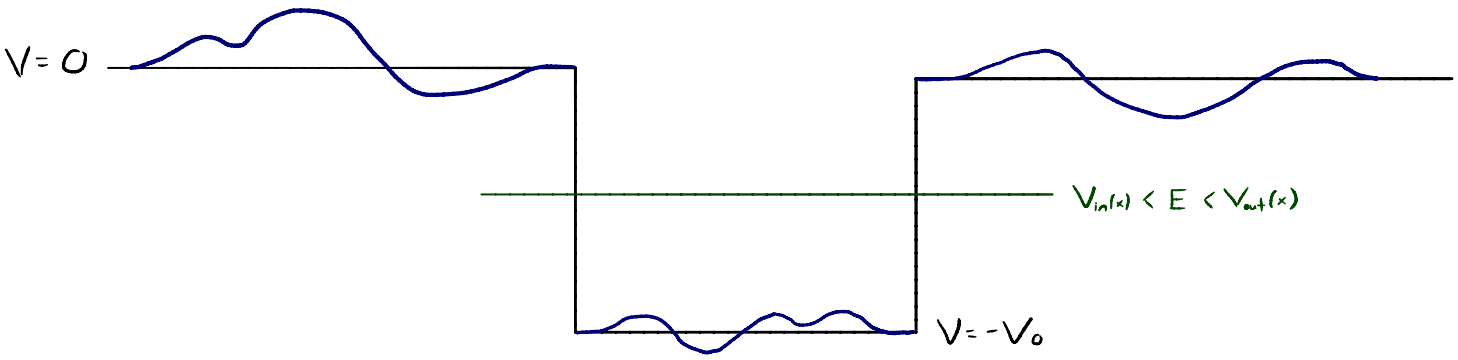
$$\int_a^b p(x)dx = \text{Area under graph of } p(x) \text{ in phase space} = n\pi\hbar$$

$$\int_{\frac{p^2}{2m}+V(x)\le E} dp\,dx = \text{Area enclosed by classical orbit in phase space} = 2n\pi\hbar$$




Leads to a rough rule: "one quantum state per $(2\pi\hbar)$ area in phase space".

Now what if there is a classically disallowed region, but with finite energy?




Our real/imaginary part derivation doesn't work any more (because formally $p(x) = \sqrt{2m(E-V(x))}$ is imaginary for $x$, so we get imaginary $W(x)$.

However, we get the same equations if we don't impose any reality conditions, but rather solve order-by-order in $\hbar$. In other words:

$$\Psi = \exp\left(\frac{i}{\hbar}(S_0 + \hbar S_1 + \hbar^2 S_2 + \cdots)\right) \text{ and solve for } S_0, S_1 = -i\log(A) \text{ in perturbation series.}$$

Then we find:

$$W'(x) = \pm p(x) = \pm i q(x) \quad \text{where} \quad q(x) = \sqrt{2m(V(x)-E)} \qquad A(x) = \left(\frac{\tilde{K}}{p(x)}\right)^{1/2} = \frac{K}{q(x)^{1/2}}$$

These combine to give exponentially growing and falling WKB wave-functions appropriate to the classically forbidden region:

$$\Psi_{\pm}^{\text{forbidden}}(x) = \frac{1}{q(x)^{1/2}} \exp\left(\frac{\pm 1}{\hbar}\int q(x')dx'\right)$$

Now we can write a solution to our lumpy box problem:

$$\Psi_{WKB}(x) = \begin{cases} \frac{K_I}{q(x)^{1/2}} \exp\left(\frac{-1}{\hbar}\int_x^a q(x')dx'\right) & x < a \\ \frac{1}{p(x)^{1/2}}\left[K_{II}^{-}\exp\left(\frac{-i}{\hbar}\int_a^x p(x')dx'\right) + K_{II}^{+}\exp\left(\frac{i}{\hbar}\int_a^x p(x')dx'\right)\right] & a < x < b \\ \frac{K_{III}}{q(x)^{1/2}} \exp\left(\frac{-1}{\hbar}\int_b^x q(x')dx'\right) & x > b \end{cases}$$

Boundary conditions now give somewhat involved constraints. Won't solve them now, but note they are overdetermined. (set $K_I = 1$ as a normalization condition, then $K_{II}^{\pm}$ fixed by continuity of $\Psi$ & $\Psi'$ at $x=a$, so $\Psi_{III}$ must satisfy two equations. This gives the implicit equations that determine $E$.

A simpler, but still involved, case is when the boundaries of the classically allowed region are not vertical. Then there is a subtlety with the classical turning points. We'll pursue this in the next lecture.