Supplementary information II

Time-Independent Perturbation Theory & WKB Approximation

Part I

Time-Independent Perturbation Theory

Solving Problems Perturbatively

- For most realistic problems, the full Hamiltonian cannot be solved exactly.
- However, sometimes we can separate the full Hamiltonian into two parts

$$\hat{H} = \hat{H}_0 + \hat{H}'$$

where the unperturbed Hamiltonian has known solutions $E_n^{(0)}$ and $|\phi_n^{(0)}\rangle$

$$\hat{H}_0 \, |\phi_n^{(0)}\rangle = E_n^{(0)} \, |\phi_n^{(0)}\rangle$$

- If the "perturbation" Hamiltonian $\hat{H}'$ is small in some sense compared to $\hat{H}_0$, it only causes small corrections to $|\phi_n^{(0)}\rangle$ and $E_n^{(0)}$.
- In this section, we study the case when $\hat{H}'$ is time-**independent** and try to construct approximate solutions to $\hat{H} = \hat{H}_0 + \hat{H}'$.

Expressing the Problem in Powers of the Perturbation

- We rewrite $\hat{H}$ as $\hat{H} = \hat{H}_0 + \lambda \hat{H}'$, where λ is a dimensionless parameter by which we tune the magnitude of the perturbation and keep track of different perturbation terms
- In general the **exact** solutions to $\hat{H}$ can be written as

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$
$$|\phi_n\rangle = |\phi_n^{(0)}\rangle + \lambda |\phi_n^{(1)}\rangle + \lambda^2 |\phi_n^{(2)}\rangle + \dots$$

  where $E_n^{(i)}$ and $|\phi_n^i\rangle$ are the i^{th} order adjustments to the unperturbed energy and state due to the perturbation
- Substituting into the Schrödinger equation $E_n |\psi_n\rangle = \hat{H} |\psi_n\rangle$,

$$(\hat{H}_0 + \lambda \hat{H}')(|\phi_n^{(0)}\rangle + \lambda |\phi_n^{(1)}\rangle + \lambda^2 |\phi_n^{(2)}\rangle + \dots) =$$
$$(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots)(|\phi_n^{(0)}\rangle + \lambda |\phi_n^{(1)}\rangle + \lambda^2 |\phi_n^{(2)}\rangle + \dots)$$

Expressing the Solution in Powers of the Perturbation

- If we group the coefficients of each power of λ, we find

$$\begin{aligned} 0 =& [\hat{H}_0 \left|\phi_n^{(0)}\right\rangle - E_n^{(0)} \left|\phi_n^{(0)}\right\rangle] \\ &+ \lambda[\hat{H}_0 \left|\phi_n^{(1)}\right\rangle + \hat{H}' \left|\phi_n^{(0)}\right\rangle - E_n^{(0)} \left|\phi_n^{(1)}\right\rangle - E_n^{(1)} \left|\phi_n^{(0)}\right\rangle] \\ &+ \lambda^2[\ldots] + \lambda^3[\ldots] + \ldots \end{aligned}$$

- Since each term for a given power of λ must equal zero, we obtain the coupled equations

$$\begin{aligned} \hat{H}_0 \left|\phi_n^{(0)}\right\rangle &= E_n^{(0)} \left|\phi_n^{(0)}\right\rangle \\ \hat{H}_0 \left|\phi_n^{(1)}\right\rangle + \hat{H}' \left|\phi_n^{(0)}\right\rangle &= E_n^{(0)} \left|\phi_n^{(1)}\right\rangle + E_n^{(1)} \left|\phi_n^{(0)}\right\rangle \\ \hat{H}_0 \left|\phi_n^{(2)}\right\rangle + \hat{H}' \left|\phi_n^{(1)}\right\rangle &= E_n^{(0)} \left|\phi_n^{(2)}\right\rangle + E_n^{(1)} \left|\phi_n^{(1)}\right\rangle + E_n^{(2)} \left|\phi_n^{(0)}\right\rangle \\ &\vdots \end{aligned}$$

First-Order Perturbation Energy Correction

- To first order in the perturbation ($\sim \lambda^1$), we find $\hat{H}_0 \left|\phi_n^{(1)}\right\rangle + \hat{H}' \left|\phi_n^{(0)}\right\rangle = E_n^{(0)} \left|\phi_n^{(1)}\right\rangle + E_n^{(1)} \left|\phi_n^{(0)}\right\rangle$. We take its inner product with the unperturbed state $\left\langle\phi_n^{(0)}\right|$ to obtain

$$\left\langle\phi_n^{(0)}\right| \left(\hat{H}_0 \left|\phi_n^{(1)}\right\rangle + \hat{H}' \left|\phi_n^{(0)}\right\rangle\right) = E_n^{(0)} \left\langle\phi_n^{(0)}|\phi_n^{(1)}\right\rangle + E_n^{(1)} \left\langle\phi_n^{(0)}|\phi_n^{(0)}\right\rangle$$

$$E_n^{(0)} \left\langle\phi_n^{(0)}|\phi_n^{(1)}\right\rangle + \left\langle\phi_n^{(0)}|\hat{H}'|\phi_n^{(0)}\right\rangle = E_n^{(0)} \left\langle\phi_n^{(0)}|\phi_n^{(1)}\right\rangle + E_n^{(1)}$$

$$\therefore E_n^{(1)} = \left\langle\phi_n^{(0)}|\hat{H}'|\phi_n^{(0)}\right\rangle$$

- The first order correction to the energy of the n^{th} eigenstate due to the perturbation is simply the expectation value of $\hat{H}'$ in the unperturbed state $\left|\phi_n^{(0)}\right\rangle$

First-Order Wave Function Corrections

- Since the unperturbed eigenstates form a complete basis, the corrections generated by the perturbation can be written as a linear superposition of those states, e.g.,

$$\left|\phi_n^{(1)}\right\rangle = \sum_k \left|\phi_k^{(0)}\right\rangle \left\langle \phi_k^{(0)} \middle| \phi_n^{(1)} \right\rangle = \sum_{k\neq n} c_{nk} \left|\phi_k^{(0)}\right\rangle + c_{nn} \left|\phi_n^{(0)}\right\rangle$$

- To first order, $\hat{H}_0 \left|\phi_n^{(1)}\right\rangle + \hat{H}' \left|\phi_n^{(0)}\right\rangle = E_n^{(0)} \left|\phi_n^{(1)}\right\rangle + E_n^{(1)} \left|\phi_n^{(0)}\right\rangle$. We find c_{nk} by taking the inner product with $\left\langle \phi_k^{(0)} \right|$ for $k \neq n$:

$$\langle \phi_k^{(0)} | \hat{H}_0 | \phi_n^{(1)} \rangle + \langle \phi_k^{(0)} | \hat{H}' | \phi_n^{(0)} \rangle = E_n^{(0)} \langle \phi_k^{(0)} | \phi_n^{(1)} \rangle$$

$$E_k^{(0)} \langle \phi_k^{(0)} | \phi_n^{(1)} \rangle + \langle \phi_k^{(0)} | \hat{H}' | \phi_n^{(0)} \rangle = E_n^{(0)} \langle \phi_k^{(0)} | \phi_n^{(1)} \rangle$$

$$\therefore \langle \phi_k^{(0)} | \phi_n^{(1)} \rangle = \frac{\langle \phi_k^{(0)} | \hat{H}' | \phi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} = \frac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}}$$

First-Order Wave Function Correction Normalization

- For $n \neq k$, $c_{nk} = \dfrac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}}$. What about $n = k$?
- Return to $\hat{H}_0 \left|\phi_n^{(1)}\right\rangle + \hat{H}' \left|\phi_n^{(0)}\right\rangle = E_n^{(0)} \left|\phi_n^{(1)}\right\rangle + E_n^{(1)} \left|\phi_n^{(0)}\right\rangle$. Any solution $\phi_n^{(1)} + a\phi_n^{(0)}$ satisfies this equation for some scalar a. However, the final wave function should be normalized. We can ensure this to order λ by ensuring all corrections to $\left|\phi_n^{(0)}\right\rangle$ are normal to the original state:

$$1 = \langle \phi_n | \phi_n \rangle = \langle \phi_n^{(0)} | \phi_n^{(0)} \rangle + \lambda \left[\langle \phi_n^{(0)} | \phi_n^{(1)} \rangle + \langle \phi_n^{(1)} | \phi_n^{(0)} \rangle \right] + \mathcal{O}(\lambda^2)$$

- Therefore to order λ, $\left|\phi_n^{(1)}\right\rangle$ is orthogonal to $\left|\phi_n^{(0)}\right\rangle$, i.e., $c_{nn} = 0$. (This does not exactly normalize the state $|\phi_n\rangle$ yet, which still needs to be done separately after finishing the perturbation calculation.)

First-Order Perturbation Solution Summarized

- The exact solutions to the full Hamiltonian can therefore be approximated to first order in the perturbation as

$$|\phi_n\rangle \approx \left|\phi_n^{(0)}\right\rangle + \sum_{k\neq n} \frac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}} \left|\phi_k^{(0)}\right\rangle$$

$$E_n \approx E_n^{(0)} + H'_{nn}$$

  where $H'_{kn} = \langle \phi_k^{(0)} | \hat{H}' | \phi_n^{(0)} \rangle$, as long as the unperturbed energies are **nondegenerate**, i.e., $E_n^{(0)} \neq E_k^{(0)}$ in general.

- This suggests that perturbation theory is useful if $H'_{kn} \ll E_n^{(0)} - E_k^{(0)}$ (although this condition does not guarantee validity, or vice versa).

Second-Order Perturbation Correction

If we examine the next order ($\sim \lambda^2$) in the perturbation expansion

$$\hat{H}_0 \left|\phi_n^{(2)}\right\rangle + \hat{H}' \left|\phi_n^{(1)}\right\rangle = E_n^{(0)} \left|\phi_n^{(2)}\right\rangle + E_n^{(1)} \left|\phi_n^{(1)}\right\rangle + E_n^{(2)} \left|\phi_n^{(0)}\right\rangle$$

and follow the same procedure we will find

$$E_n^{(2)} = \left\langle \phi_n^{(0)} \middle| \hat{H}' \middle| \phi_n^{(1)} \right\rangle = \sum_{k \neq n} \frac{\left| \left\langle \phi_k^{(0)} \middle| \hat{H}' \middle| \phi_n^{(0)} \right\rangle \right|^2}{E_n^{(0)} - E_k^{(0)}}$$

and a similar expression for the 2^{nd} order wave function $\left|\phi_n^{(2)}\right\rangle$ in terms of $\left|\phi_n^{(0)}\right\rangle$.
In general we can determine the n^{th} order correction to the energy from the $(n-1)^{\text{th}}$ order correction to the eigenstate.

Example: 1-D Quantum Well

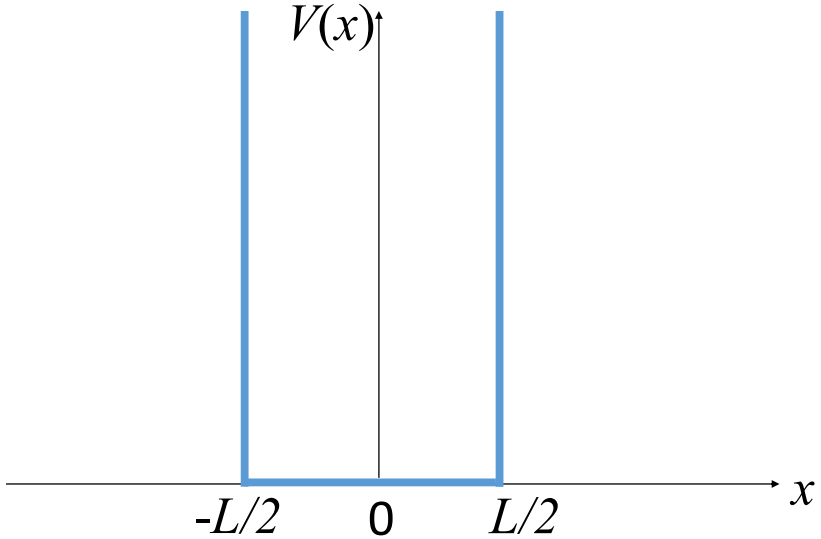
Consider an 1-D infinite potential well between $[-L/2, L/2]$. (We shift the well to make it symmetric around the origin). We rewrite the unperturbed eigenstates as

$$E_n^{(0)} = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

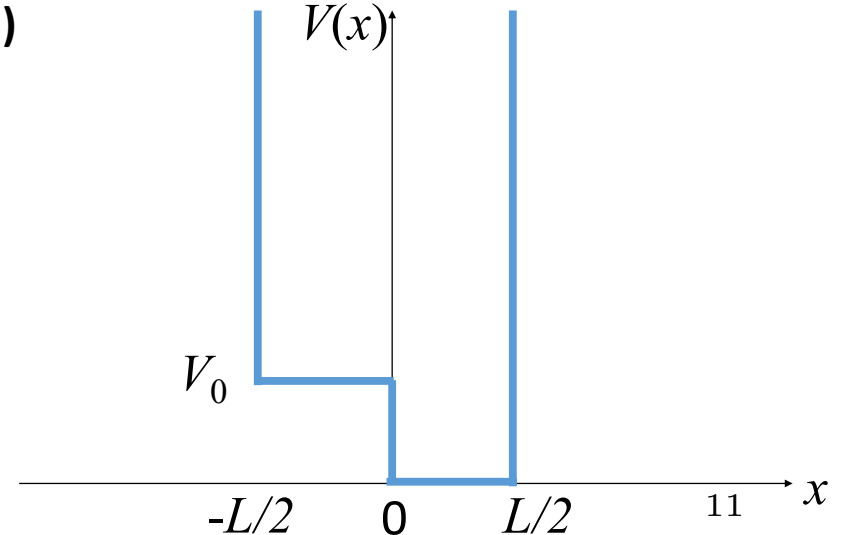
$$\phi_n^{(0)}(x) = \begin{cases} \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right) & \text{for odd } n \\ \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & \text{for even } n \end{cases}$$

($\phi_n^{(0)}(x) = 0$ outside the well.)
Suppose we add a perturbation $H' = V_0$ for $-L/2 \le x \le 0$ and $V = 0$ otherwise.

i)



ii)



1-D Quantum Well with Step Potential

The perturbative energy shift of the ground state $n = 1$ is

$$E_1^{(1)} = \langle \phi_1^{(0)} | \hat{H}' | \phi_1^{(0)} \rangle = \frac{2}{L} \int_{-L/2}^{0} V_0 \cos^2 \left(\frac{n\pi x}{L} \right) dx = \frac{V_0}{2}$$

The first order change in the wave function of the ground state is given by

$$|\phi_1^{(1)}\rangle = \sum_{k \neq 1} \frac{H'_{k1}}{E_1^{(0)} - E_k^{(0)}} \left| \phi_k^{(0)} \right\rangle$$

Let us compute the coefficients c_{1k} describing the admixture of the excited unperturbed states into the perturbed ground state.

1-D Quantum Well with Step Potential cont'ed

$$c_{1k} = \frac{\langle \phi_k^{(0)} | H' | \phi_1^{(0)} \rangle}{E_1^{(0)} - E_k^{(0)}}$$

For even $k = 2, 4, \ldots$

$$\begin{aligned} c_{1k} &= \frac{1}{E_1^{(0)}(1-k^2)} \int_{-L/2}^{0} \frac{2}{L} V_0 \cos\left(\frac{\pi x}{L}\right) \sin\left(\frac{k\pi x}{L}\right) dx \\ &= \frac{V_0}{E_1^{(0)}(1-k^2)} \frac{2k}{\pi(1-k)} \end{aligned}$$

For odd $k = 3, 5, \ldots$

$$c_{1k} = \frac{1}{E_1^{(0)}(1-k^2)} \int_{-L/2}^{0} \frac{2}{L} V_0 \cos\left(\frac{\pi x}{L}\right) \cos\left(\frac{k\pi x}{L}\right) dx = 0$$

First Order Solution to Step Potential Well

Therefore the shifted energy of the ground state, to first order, is

$$E_1 \approx \frac{\hbar^2 \pi^2}{2mL^2} + \frac{V_0}{2}$$

and the wave function for the new ground state to first order is

$$\phi_1(x) \approx \sqrt{\frac{2}{L}} \cos\left(\frac{\pi x}{L}\right) + \sqrt{\frac{2}{L}} \sum_{m=1}^{\infty} \frac{4mV_0}{E_1^{(0)}(1-(2m)^2)\pi(1-2m)} \sin\left(\frac{2m\pi x}{L}\right)$$

The Stark Effect: First Order Solution

- Consider an 1-D infinite potential well with an applied electric field $\hat{H} = \hat{H}_0 + \hat{H}'$ where $\hat{H}' = -eEx$.
- The electric field leads to a shift of the energy levels, which is known as the quantum confined Stark effect (and experimentally observable in semiconductor quantum wells, among other manifestations).
- However, the first order correction to the ground state (and all excited states with $n > 1$) vanishes:

$$\begin{aligned} E_1^{(1)} &= \langle \phi_1^{(0)} | \hat{H}' | \phi_1^{(0)} \rangle \\ &= \frac{2}{L} \int_{-L/2}^{L/2} \cos^2\left(\frac{\pi x}{L}\right) (-eEx) dx = 0 \end{aligned}$$

- Need to go to second order to get corrections to the energy levels...

Degenerate Perturbation Theory

- If we apply perturbation theory for a system where $\hat{H}_0$ has degeneracies, i.e., $E_n^{(0)} = E_k^{(0)}$ for some $n \neq k$, the 2^{nd} order energy shift diverges

$$c_{nk} = \frac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}} = \frac{H'_{kn}}{0}$$

- Degeneracies generally reflect a symmetry in the unperturbed Hamiltonian. If we break the symmetry with a perturbation $\hat{H}'$, the degeneracy should be broken as well.
- For degenerate states, we can construct linear combinations such that $H'_{kn} = 0$ for the new states. Using these states as a new basis for the perturbation expansion, the divergences in the coefficients c_{nk} vanish.

Curing Degeneracies in Perturbation Theory

- Suppose there is a q-fold degeneracy in the eigenstates of $\hat{H}_0$. We can construct q linear combinations of $|\phi_q^{(0)}\rangle$, which we denote as $|\bar{\phi}_q\rangle$, such that $H'_{kn} = \langle\bar{\phi}_k|\hat{H}'|\bar{\phi}_n\rangle = 0$ for $k, n \in \{q\}$.
- We can then replace our original basis set of eigenfunctions of $\hat{H}_0$ $\{\phi_1^{(0)}, \phi_2^{(0)}, \ldots, \phi_q^{(0)}, \phi_{q+1}^{(0)}, \phi_{q+2}^{(0)}, \ldots\}$ with a new basis set $\{\bar{\phi}_1, \bar{\phi}_2, \ldots, \bar{\phi}_q, \phi_{q+1}^{(0)}, \phi_{q+2}^{(0)}, \ldots\}$ that we can use for perturbation theory calculations.
- Note that the states $\{\bar{\phi}_1, \bar{\phi}_2, \ldots, \bar{\phi}_q\}$ are still eigenstates of $\hat{H}_0$ since they have the same eigenenergy in $\hat{H}_0$.

Curing Degeneracies - Matrix Notation

- Suppose the first three eigenstates of H_0 are degenerate. We work with the basis of eigenstates $\{\phi_1^{(0)}, \phi_2^{(0)}, \phi_3^{(0)}, \phi_4^{(0)}, \dots\}$.
- Then we diagonalize the 3×3 submatrix of H' to find new basis functions $\bar{\phi}_1, \bar{\phi}_2, \bar{\phi}_3$:

In $\{\phi_1^{(0)}, \phi_2^{(0)}, \phi_3^{(0)}, \phi_4^{(0)}, \dots\}$ basis:

$$H' = \begin{bmatrix} H'_{11} & H'_{12} & H'_{13} & H'_{14} & \dots \\ H'_{21} & H'_{22} & H'_{23} & H'_{24} & \dots \\ H'_{31} & H'_{32} & H'_{33} & H'_{34} & \dots \\ H'_{41} & H'_{42} & H'_{43} & H'_{44} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

where $H'_{ij} = \langle \phi_i^{(0)} | \hat{H}' | \phi_j^{(0)} \rangle$

In $\{\bar{\phi}_1, \bar{\phi}_2, \bar{\phi}_3, \phi_4^{(0)}, \dots\}$ basis:

$$\rightarrow \begin{bmatrix} E'_1 & 0 & 0 & H'_{\bar{1}4} & \dots \\ 0 & E'_2 & 0 & H'_{\bar{2}4} & \dots \\ 0 & 0 & E'_3 & H'_{\bar{3}4} & \dots \\ H'_{4\bar{1}} & H'_{4\bar{2}} & H'_{4\bar{3}} & H'_{44} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

where $H'_{\bar{i}j} = \langle \bar{\phi}_i | \hat{H}' | \phi_j^{(0)} \rangle$ and $E'_i = \langle \bar{\phi}_i | \hat{H}' | \bar{\phi}_i \rangle$ for $i = 1, 2, 3$ and $j > 3$.

Curing Degeneracies - Matrix Notation cont'ed

Specifically, for the example above we write down the submatrix (in the basis $|\phi_1^{(0)}\rangle, |\phi_2^{(0)}\rangle, |\phi_3^{(0)}\rangle$)

$$H'_{q=3} = \begin{bmatrix} H'_{11} & H'_{12} & H'_{13} \\ H'_{21} & H'_{22} & H'_{23} \\ H'_{31} & H'_{32} & H'_{33} \end{bmatrix}$$

and we search for the $q = 3$ eigenstates $|\bar{\phi}_i\rangle$ of this submatrix such that

$$H'_q |\bar{\phi}_i\rangle = E'_i |\bar{\phi}_i\rangle$$

The latter implies that $H'_{q=3}$ in the basis $|\bar{\phi}_1\rangle, |\bar{\phi}_2\rangle, |\bar{\phi}_3\rangle$ is

$$H'_{q=3} = \begin{bmatrix} E'_1 & 0 & 0 \\ 0 & E'_2 & 0 \\ 0 & 0 & E'_3 \end{bmatrix}$$

Degenerate Perturbation Theory Results

- The diagonal elements $E'_n = \langle \bar{\phi}_n | \hat{H}' | \bar{\phi}_n \rangle$ are the first-order perturbation corrections to $E_n^{(0)}$ for $n \leq q$.
- If $E'_m \neq E'_n$, the perturbation removes the degeneracy.
- For a q-fold degeneracy, the states $|\bar{\phi}_n\rangle = \sum_{m=1}^{q} c_{nm} \left| \phi_m^{(0)} \right\rangle$, where $c_{nm} = \langle \phi_m^{(0)} | \bar{\phi}_n \rangle$.
- In general, we obtain the energy shifts E'_n and the states $|\bar{\phi}_n\rangle$ by finding the eigenvalues and eigenfunctions of H'.
- Therefore we solve for E'_n by using the secular equation $\det |H' - E'_n I| = 0$ where I is the identity matrix. The corresponding eigenfunctions gives $|\bar{\phi}_n\rangle$.

Degenerate Perturbation Theory Recipe

- For q-fold degeneracy in $\hat{H}_0$, construct the $q \times q$ matrix of $\hat{H}'$, which we denote H'_q, in the set of $\{\phi_q^{(0)}\}$ degenerate eigenstates of $\hat{H}_0$.
- Diagonalize the perturbation matrix H'_q by solving the corresponding secular equation.
- The q roots of H'_q are the first-order energy shifts to the previously degenerate energies in $\hat{H}_0$.
- Replace the states $\{\phi_q^{(0)}\}$ with the states $\{\bar{\phi}_q\}$ which diagonalize H'_q and use the resulting basis $\{\bar{\phi}_1, \bar{\phi}_2, \ldots, \bar{\phi}_q, \phi_{q+1}^{(0)}, \phi_{q+2}^{(0)}, \ldots\}$ in the formulas for nondegenerate perturbation theory.

Part II

The Wentzel-Kramers-Brillouin(-Jeffreys) Approximation

WKB Approximation

WKB = Wentzel-Kramers-Brillouin (sometimes +J for Jeffreys) is a way to *semiclassically* approximate wave functions for slowly varying $V(x)$.
We write a general wave function $\psi(x) = Ae^{iS(x)/\hbar}$ where A is real and $S(x)$ is a complex function.
Substituting $\psi(x)$ in the Schrödinger equation we obtain

$$-i\hbar\frac{\partial^2 S(x)}{\partial x^2} + \left(\frac{\partial S(x)}{\partial x}\right)^2 = p^2(x)$$

$$p(x) = \sqrt{2m(E - V(x))} \equiv \hbar k(x)$$

Now expand $S(x)$ in powers of $\hbar$ such that

$$S(x) = S_0(x) + \hbar S_1(x) + \frac{\hbar^2}{2}S_2(x) + \cdots$$

WKB Approximation cont'ed

Using the series expansion of $S(x)$ we find

$$0 = \left[\left(\frac{\partial S_0(x)}{\partial x}\right)^2 - p^2(x)\right] + 2\hbar\left[\frac{\partial S_0}{\partial x}\frac{\partial S_1}{\partial x} - \frac{i}{2}\frac{\partial^2 S_0(x)}{\partial x^2}\right] +$$
$$\hbar^2\left[\frac{\partial S_0}{\partial x}\frac{\partial S_2}{\partial x} + \left(\frac{\partial S_1(x)}{\partial x}\right)^2 - i\frac{\partial^2 S_0(x)}{\partial x^2}\right] + \mathcal{O}(\hbar^3)$$

Every term of the series in $\hbar$ must vanish, i.e.,

$$\left(\frac{\partial S_0(x)}{\partial x}\right)^2 = p^2(x)$$
$$\frac{\partial S_0}{\partial x}\frac{\partial S_1}{\partial x} = \frac{i}{2}\frac{\partial^2 S_0(x)}{\partial x^2}$$
$$\frac{\partial S_0}{\partial x}\frac{\partial S_2}{\partial x} + \left(\frac{\partial S_1(x)}{\partial x}\right)^2 = i\frac{\partial^2 S_0(x)}{\partial x^2}$$
$$\vdots$$

WKB Approximation cont'ed

We can solve the equations sequentially:

$$S_0(x) = \pm \int_{x_0}^{x} p(x')dx' = \pm\hbar \int_{x_0}^{x} k(x')dx'$$

$$S_1(x) = \frac{i}{2} \ln\left(\frac{\partial S_0}{\partial x}\right) = \frac{i}{2} \ln(\hbar k(x))$$

Substituting $S_0 + \hbar S_1$ in ψ and absorbing integration constants in A

$$\psi(x) \approx Ak^{-1/2}(x) \exp\left(\pm i \int^{x} k(x')dx'\right) \text{ for } E>V(x)$$

$$\psi(x) \approx A\kappa^{-1/2}(x) \exp\left(\pm \int^{x} \kappa(x')dx'\right) \text{ for } E<V(x)$$

where $\kappa = \sqrt{2m(V(x) - E)/\hbar^2}$.

WKB Approximation - Range of Validity

Retaining lowest order terms is reasonable if $|\hbar S_1/S_0| \ll 1$. As long as k does not vanish (at classical turning points) and S_0 increases monotonically, this implies $|\hbar S_1'/S_0'| \ll 1$:

$$\left|\frac{\hbar S_1'(x)}{S_0(x)}\right| = \left|\frac{k'(x)}{2k^2(x)}\right| = \frac{\lambda(x)}{4\pi k(x)}\left|\frac{dk}{dx}\right| \ll 1$$

where $\lambda = 2\pi/k$ is the local de Broglie length.
In other words, the WKB approximation is valid when $V(x)$ changes so slowly that the local momentum is constant over a few wavelengths

$$\frac{\lambda(x)}{4\pi}\left|\frac{dk(x)}{dx}\right| \ll k(x)$$

WKB Approximation - Applications

- The WKB approximation breaks down near classical turning points because $k(x) \to 0$ and $\lambda \to \infty$. A boundary condition matching procedure can be performed to "patch" the wave functions in this region (refer to text for details).
- WKB is particularly useful for estimating tunneling rates and bound state energies. Since bound states imply standing waves, we require that

$$\int_{x_1}^{x_2} k(x)dx = \int_{x_1}^{x_2} \frac{\sqrt{2m(E - V(x))}}{\hbar} dx = n\pi + \delta\theta$$

  where x_1, x_2 are the classical turning points and n is an integer.
- $\delta\theta$ is an additional phase accounting for penetration of wave function into barrier. For each "soft" barrier, i.e., $V(x)$ changes smoothly around classical turning point, $\delta\theta$ contributes a phase of $-\pi/4$. For each "hard" barrier ($V(x) \to \infty$), $\delta\theta = 0$. If the potential is finite on both sides of the bound state, total $\delta\theta = -\pi/2$.

Tunneling in WKB Approximation

- In classically forbidden regions ($V(x) > E$), we can assume the form of the wave function
  $\psi(x) \approx \frac{A}{\sqrt{\kappa(x)}} \exp(\pm \int \kappa(x')dx')$ where where
  $\kappa(x) = \sqrt{\frac{2m(V(x) - E)}{\hbar^2}}$
- We can estimate the tunneling probability through a classically forbidden region bounded by $[x_1, x_2]$ using

$$T = \left| \frac{\Psi(x_2)}{\Psi(x_1)} \right|^2 \simeq \exp\left(-2 \int_{x_1}^{x_2} \kappa(x)dx \right)$$

- In practice this equation is very helpful for estimating tunneling in real physical systems, including semiconductor devices

Example: Computing Bound State Energy for SHO

Let $V(x) = m\omega x^2/2$ and define classical turning point $x_0 = \pm\sqrt{\frac{2E}{m\omega^2}}$

$$\begin{aligned}
\int_{x_1}^{x_2} k dx &= \int_{-x_0}^{x_0} \sqrt{\frac{2m(E - m\omega x^2/2)}{\hbar^2}} dx \\
&= \sqrt{\frac{2mE}{\hbar^2}} \int_{-x_0}^{x_0} \sqrt{1 - \frac{x^2}{x_0^2}} dx \\
&= \sqrt{\frac{2mE}{\hbar^2}} x_0 \int_0^{\pi} \sqrt{1 - \cos^2\theta} \sin\theta d\theta \\
&= \frac{2E}{\hbar\omega} \frac{\pi}{2} = (n - \frac{1}{2})\pi
\end{aligned}$$

for $n = 1, 2, 3, \ldots$. This implies $E = \hbar\omega(n + \frac{1}{2})$ for $n = 0, 1, 2 \ldots$ which coincides with the exact solution for the SHO.
Most of the time WKB is not so exact, but it is often a good estimate.

Example: Fowler-Nordheim Tunneling

- Consider the triangular potential barrier

$$V(x) = \begin{cases} V_0 - eFx & 0 \le x \le \dfrac{V_0}{eF} \\ 0 & \text{otherwise} \end{cases}$$

- The tunneling probability through the barrier can be estimated in the WKB approximation (where $x_0 = \frac{V_0 - E}{eF}$)

$$\begin{aligned} T(E) &= \exp\left(-2\int_0^{x_0} \sqrt{\frac{2m(V_0 - E - eFx)}{\hbar^2}}dx\right) \\ &= \exp\left(-2\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}\int_0^{x_0} \sqrt{1 - x/x_0}dx\right) \\ &= \exp\left(-\frac{4}{3}\sqrt{\frac{2m}{\hbar^2}}\frac{(V_0 - E)^{3/2}}{eF}\right) \end{aligned}$$