Physics 137B MT2 Review

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March 20, 2024

Contents

1 Time-independent Perturbation Theory

1.1 Non-degenerate case

-Do later

1.2 Degenerate case

- Many important systems have degenerate states, meaning the corrections to the eigenstates $|n^{(1)}\rangle$ are ill-defined due to the $1/(E_n^{(0)} - E_k^{(0)})$ factor diverging for degenerate states.
- But there is still hope. The degenerate states $\{|k\rangle_1^{(0)}, \cdots, |k\rangle_N^{(0)}\}$ span a degenerate subspace $\mathbb{V}_{\text{degen}}$ of the original hilbert space $\mathcal{H}$. So, the eigenvectors of $\hat{H}^{(0)}$ are ambiguous: *Any* linear combination $a_1|k\rangle_1^{(0)} + \cdots + a_N|k\rangle_1^{(0)}$ is an eigenvector of the hamiltonian $\hat{H}^{(0)}$.
- If we can find a different basis of $\mathbb{V}_{\text{degen}}$ whose basis vectors are

Come back to this.

2 Variational Principle

Often, we only need the energies of a state (especially the ground state). If we are fine with just an estimate (actually an upper bound), then we can get away with using the *Variational Principle* rather than solving the full eigenvalue problem.

Theorem: Consider a system described by Hamiltonian $\hat{H}$. For *any* normalized wavefunction ψ, we have

$$\langle\psi|\hat{H}|\psi\rangle \geq E_{\text{g.s.}}$$

Proof: Write later. It's not long.

The above theorem tells us that the expected value of the hamiltonian will always be greater than the ground state, for any normalized state ψ. So if guess a good *trial wavefunction*, perhaps using known properties of the eigenstates like parity, we can pretty often get a good estimate for the ground state energy.

More specifically, what we can do is

Procedure

- Define a trial wavefunction that depends on a (number of) parameter(s) $\psi(\alpha)$, calculate the corresponding expected energy $E(\alpha) = \langle\psi(\alpha)|\hat{H}|\psi(\alpha)\rangle$.
- Find where the minimum occurs by solving for α^* in

$$\frac{\partial E(\alpha^*)}{\partial \alpha} = 0$$

- Then, $E(\alpha^*)$ is an estimate for $E_{\text{g.s.}}$

Example: Quantum Harmonic Oscillator with a Guassian Trial Function.

2.1 Excited States

We can guess the first excited state's energy if we are able to able to guess a trial wavefunction which is orthogonal to the ground state $\langle\psi|0\rangle = 0$.

- In general we don't know $|0\rangle$ so this is difficult, but sometimes we can guarantee $\langle\psi|0\rangle = 0$ using parity or some quantum number (ex. angular momentum) i.e. using symmetry considerations.

This works becauese

Theorem: $\langle\psi|0\rangle = 0 \implies \langle\psi|\hat{H}|\psi\rangle \geq E_1$.

Proof:

$$\begin{aligned}
\langle\psi|\hat{H}|\psi\rangle &= \sum_n \underbrace{\langle\psi|n\rangle}_{=0 \text{ if } n=0} \langle n|\hat{H}|\psi\rangle \\
&= \sum_{n\neq 0} \langle\psi|n\rangle E_n \langle n|\psi\rangle \\
&= E_n \sum_{n\neq 0} \langle\psi|n\rangle\langle n|\psi\rangle \\
&= E_n \langle\psi|\psi\rangle \\
&= E_n \geq E_{E_1} \text{ (Since } n \neq 0)
\end{aligned}$$

2.2 Excited state using ground state guess

If this is not possible, we can construct a trial for the 1st excited state which is orthogonal to our trial function for the ground state

$$|\psi_1\rangle = \frac{|\phi\rangle - \langle\psi_0|\phi\rangle}{\sqrt{N}}$$

where the ψ's represent trial wavefunctions and ϕ represents the true ground state.

And $\langle\phi|\phi\rangle = \langle\psi_0|\psi_0\rangle = 1$ [Expand on this section after watching recording again.]

3 WKB Approximation

The WKB (a.k.a. Semiclassical) approximation is useful for potentials that change slowly in space.

3.1 Basic Idea

If we straight up have a constant potential $V(x) = V_0$, then the solutions to the TISE can be of two types depending on the energy in the region.

In regions where $E > V$, the wavefunction is of the form

$$\psi(x) = Ae^{\pm ikx}, \qquad k = \frac{\sqrt{2m(E - V_0)} \in \mathbb{R}}{\hbar}$$

These solutions are oscillatory, with wavelength $\lambda = 2\pi/k$. Now, if instead of being completely constant, suppose our potential $V(x)$ is *almost constant* i.e. it changes very slowly in comparison λ. It would be reasonable to think the solutions are probably still *alomst sinusoidal*, just with amplitude and phase that possibly change (slowly) along space.

Similary, in regions where $E < V_0$, the wavefunction is of the form

$$\psi(x) = Ae^{\pm \kappa x}, \qquad \kappa = \frac{\sqrt{2m(V_0 - E)} \in \mathbb{R}}{\hbar}$$

These solutions are exponential. So, if our potential is *almost constant*, it seems reasonable that our solution should be *almost exponential*, just decaying/growing at a different rate.

The approximation, however, breaks down at the turning points $E \approx V_0$. In small neighborhoods around these turning points, we solve Schroedinger's Equations using other methods and use the obtained solutions to *connect* the solutions in the other regions.

3.2 Classically Allowed and Forbidden Regions

If we have constant potential $V(x) = V$, then the solutions are of the form

$$\psi(x) = A \exp\left[\pm i \frac{p_0 x}{\hbar}\right]$$

where

$$p_0 = \sqrt{2m(E - V)}$$

Motivated by the constant potential case, we define the *local momentum* in a slowly varying $V(x)$ by

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

and the *local de Broglie Wavelength*

$$\lambda(x) = \frac{h}{p(x)} = \frac{2\pi\hbar}{p(x)}$$

Okay, now consider the 1-D Schroedinger Equation:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x)$$

Or, equivalently,

$$\boxed{\frac{d^2}{dx^2}\psi(x) = -\frac{p(x)}{\hbar^2}\psi(x)}$$

where $\psi(x)$ is the local momentum defined earlier.

Now, in general, we can assume that our wavefunction is of the form

$$\psi(x) \sim \exp\left[-\frac{i}{\hbar}S(x)\right]$$

(I think this works in general because we can imagine $S(x)$ is of the form $F(x) - i\hbar\ln(A(x))$, which makes $\psi(x) = A(x)\exp\left[-\frac{i}{\hbar}F(x)\right]$ so $\psi(x)$ has a phases $F(x)$ and amplitude $A(x)$).

Anyway, plugging this into the dfferential equation above and re-expressing, the differential equation becomes

$$\boxed{\left(S'(x)\right)^2 - i\hbar S''(x) = p^2(x)}$$

Now the useful bit. We claim that when $V(x)$ varies slowly, $ih S''(x) \approx 0$. There are two ways to think about this

- When $V(x) = V_0$ is constant, $p(x) = p_0$ is constant and obtain a solution $S(x)$ linear in x, so $S''(x) = 0$. Thus, for slowly varying potentials, $S''(x) \approx 0$ so $i\hbar S''(x) \approx 0$.
- In the $\hbar \to 0$ limit (as weird as this is), the term $i\hbar S''(x) \approx 0$. Physically, this is like tweaking the parameters of the universe to make the local de Broglie wavelenth smaller, making the potential look constant to the quantum particle.

This motivates us to take $\hbar$ as our small parameter for $S(x)$

$$S(x) = \sum_{n=0}^{\infty} \hbar^n S_n(x)$$

Plugging this in, we have

$$\left(S_0' + \hbar S_1' + \hbar^2 S_2' + \cdots\right)^2 - i\hbar\left(S_0'' + \hbar S_1'' + \hbar^2 S_2'' + \cdots\right) - p^2(x) = 0$$

In the $\hbar \approx 0$, all second order (and higher) terms are treated as negligible, so we have

$$\left(S_0'\right)^2 - p^2(x) + \hbar\left(2S_0'S_1' - iS_0''\right) + \mathcal{O}(\hbar^2) = 0$$

Separating out the $\hbar^0$ and $\hbar^1$ terms, we get two equations:

$$\begin{aligned}\left(S_0'\right)^2 - p^2(x) &= 0\\ 2S_0'S_1' - iS_0'' &= 0\end{aligned}$$

Solving these, we obtain

$$\begin{aligned}S_0(x) &= \pm\int_{x_0}^{x} p(x')dx'\\ S_1(x) &= -\frac{1}{2i}\ln\left[p(x)\right] + C\end{aligned}$$

So, reconstructing the wavefunction,

$$\begin{aligned}\psi(x) = \exp\left[-\frac{i}{\hbar}S(x)\right] &\approx \exp\left[-\frac{i}{\hbar}\left(S_0(x) + \hbar S_1(x)\right)\right]\\ &= \exp\left[\pm\int_{x_0}^{x} p(x')dx'\right]\exp\left[-\frac{1}{2i}\ln\left[p(x)\right] + C\right]\\ &= \frac{A}{\sqrt{p(x)}}\exp\left[\pm\int_{x_0}^{x} p(x')dx'\right]\end{aligned}$$

Thus, the general solution to the WKB Approximation Scheme is

$$\boxed{\psi(x) = \frac{A}{\sqrt{p(x)}} \exp\left[+\int_{x_0}^{x} p(x')dx'\right] + \frac{B}{\sqrt{p(x)}} \exp\left[-\int_{x_0}^{x} p(x')dx'\right]}$$

in the classically allowed region ($E > V(x)$) and

$$\boxed{\psi(x) = \frac{A}{\sqrt{|p(x)|}} \exp\left[+\int_{x_0}^{x} |p(x')|dx'\right] + \frac{B}{\sqrt{|p(x)|}} \exp\left[-\int_{x_0}^{x} |p(x')|dx'\right]}$$

in the classically forbidden ($E < V(x)$) region.

3.3 Connection Formulae

Write soon

Why is it called 'Semiclassical Approximation'?

The *de Broglie wavelength* of a particle tells us when classical mechanics is an accurate description.

$$\lambda_{\text{de Broglie}} = \frac{h}{p} = \frac{2\pi\hbar}{p}$$

When our problem is on length-scales much greater than $\lambda_{\text{de Broglie}}$, classical mechanics gives us physically insightful results.

Now, if we forcefully take the limit $\hbar \to 0$, then $\lambda_{\text{de Broglie}} \to 0$ so classical mechanics becomes a good description of reality (in a super handwavey way). In the WKB Approximation, we treat $\hbar$ as our tiny parameter for the eigenstates, and the region in which the approximation holds if roughly when the local de Broglie wavelength varies slowly.

3.4 Arbitrary Potential between Walls

3.5 Tunneling

Write soon

4 Time-dependent Perturbation Theory