EE201/MSE207 Lecture 15

Perturbation theory (Ch. 6)
(time-independent, nondegenerate, Sec. 6.1)

Usually solving TISE $\hat{H}\psi = E\psi$ is too complicated; need approximations.
Perturbation theory is one of approximate methods to solve TISE.

Idea: separate Hamiltonian into simple and small parts (if possible)

$\hat{H} = \hat{H}_0 + \hat{H}_1$ where $\hat{H}_0\psi = E\psi$ is simple (can be solved), $\hat{H}_1$ is small

Trick: $\hat{H} = \hat{H}_0 + \lambda\,\hat{H}_1$ then power series in $\lambda \ll 1$, and then $\lambda = 1$

$$\begin{cases} \psi_n = \psi_n^{(0)} + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \dots \\ E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots \end{cases}$$

notation $\psi = |\psi\rangle$

$$\left(\hat{H}_0 + \lambda\hat{H}_1\right)\left(\psi_n^{(0)} + \lambda\psi_n^{(1)} + \dots\right) = \left(E_n^{(0)} + \lambda E_n^{(1)} + \dots\right)\left(\psi_n^{(0)} + \lambda\psi_n^{(1)} + \dots\right)$$

order λ^0: $\hat{H}_0\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)}$ (solvable exactly)

order λ^1: $\hat{H}_0\psi_n^{(1)} + \hat{H}_1\psi_n^{(0)} = E_n^{(0)}\psi_n^{(1)} + E_n^{(1)}\psi_n^{(0)}$

order λ^2: . . .

order λ^3: . . .

. . .

First-order perturbation theory (λ^1)

$$\hat{H}_0\psi_n^{(1)} + \hat{H}_1\psi_n^{(0)} = E_n^{(0)}\psi_n^{(1)} + E_n^{(1)}\psi_n^{(0)}$$

Multiply by $\left[\psi_n^{(0)}(x)\right]^*$ and integrate, $\int_{-\infty}^{\infty} dx$, or (the same) $\langle\psi_n^{(0)}|\ldots$

$$\underbrace{\langle\psi_n^{(0)}|\hat{H}_0|\psi_n^{(1)}\rangle} + \langle\psi_n^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle = \underbrace{E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle} + E_n^{(1)}$$

equal

notation

$$\langle\psi_1|\hat{H}|\psi_2\rangle = \langle\psi_1|\hat{H}\,\psi_2\rangle$$

$$\boxed{E_n^{(1)} = \langle\psi_n^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle}$$

First-order correction to energy is just the average (expectation) value of $\hat{H}_1$ in the unperturbed state (very natural)

First-order perturbation theory (cont.)

$$\hat{H}_0\psi_n^{(1)} + \hat{H}_1\psi_n^{(0)} = E_n^{(0)}\psi_n^{(1)} + E_n^{(1)}\psi_n^{(0)}$$

Now find correction $\psi_n^{(1)}$ to wavefunction

Rewrite $\quad (\hat{H}_0 - E_n^{(0)})\ \psi_n^{(1)} = -(\hat{H}_1 - E_n^{(1)})\ \psi_n^{(0)}$

Expand in zero-order eigenstates $\quad \psi_n^{(1)} = \sum_{m\neq n} c_m^{(n)}\ \psi_m^{(0)} \qquad c_n^{(n)} = 0$

from normalization

$$\sum_{m\neq n}(E_m^{(0)} - E_n^{(0)})\ c_m^{(n)}\ \psi_m^{(0)} = -(\hat{H}_1 - E_n^{(1)})\ \psi_n^{(0)}$$

Multiply by $\langle\psi_l^{(0)}|$: $\quad (E_l^{(0)} - E_n^{(0)})\ c_l^{(n)} = -\langle\psi_l^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle + E_n^{(1)}\delta_{ln}$

For $n = l$ we obtain the previous formula for $E_n^{(1)}$ (another way of derivation)

For $n \neq l$: $\quad c_l^{(n)} = \dfrac{\langle\psi_l^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_l^{(0)}}$

Rename $l \to m$

$$\psi_n^{(1)} = \sum_{m\neq n} \frac{\langle\psi_m^{(0)}|\hat{H}_1|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}\ \psi_m^{(0)}$$

First-order perturbation theory: summary

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

$$\hat{H}_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$$

$$\begin{cases} \psi_n = \psi_n^{(0)} + \psi_n^{(1)} + \ \dots \\ E_n = E_n^{(0)} + E_n^{(1)} + \ \dots \end{cases}$$

$$E_n^{(1)} = \langle \psi_n^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle$$

$$\psi_n^{(1)} = \sum_{m \neq n} \frac{\langle \psi_m^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} \psi_m^{(0)}$$

Remark. Correction to ψ_n is not good if $E_m^{(0)} = E_n^{(0)}$ (i.e. when degeneracy). Then the formalism is a little different. Usually degeneracy is lifted (disappears) due to perturbation. For example, in hydrogen atom there is fine structure (due to relativistic correction and spin-orbit) and hyperfine structure (due to magnetic interaction of electron and proton).

Second-order perturbation: similar but lengthier

Result for second-order correction to energy of *n*th level:

$$E_n^{(2)} = \sum_{m \neq n} \frac{\left| \langle \psi_m^{(0)} | \hat{H}_1 | \psi_n^{(0)} \rangle \right|^2}{E_n^{(0)} - E_m^{(0)}}$$

WKB approximation (Ch. 8)

(Wentzel, Kramers, Brillouin, 1926)

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

E can be discrete or continuous

If $V(x)=\text{const}$, then easy to solve

Idea: If $V(x)$ varies slowly, then modify solution for $V(x)=\text{const}$.

Two cases: $E>V(x)$ (classical region)

$E<V(x)$ (tunneling)

WKB approximation, classical region, $E > V(x)$

If $V(x) = \text{const} = V$, then $\psi(x) = A\, e^{\pm ikx}$, $\quad k = \dfrac{\sqrt{2m(E-V)}}{\hbar}$

Then for $V(x)$ we expect $\quad \psi(x) \approx A(x) \exp\left[\pm i \int^x k(x')\, dx'\right]$

From conservation of the probability current $\quad J = \dfrac{i\hbar}{2m}\left(\psi \dfrac{d\psi^*}{dx} - \psi^* \dfrac{d\psi}{dx}\right)$

we obtain $\quad A(x) \propto \dfrac{1}{\sqrt{k(x)}}$ $\quad$ Therefore

$$\psi(x) \approx \frac{\text{const}}{\sqrt{k(x)}} \exp\left[\pm i \int^x k(x')\, dx'\right]$$

$$k(x) = \frac{\sqrt{2m[E - V(x)]}}{\hbar}$$

slightly different in the textbook, $\pm \frac{i}{\hbar} \int p(x)\, dx$

Remark 1. $1/\sqrt{k(x)} \propto 1/\sqrt{v(x)}$, so $|\psi|^2 \propto 1/v(x)$, as it should be.

Remark 2. If $m(x)$ (as in SiGe technology), then $A(x) \propto \sqrt{m(x)/k(x)}$.

Remark 3. WKB approximation works well only for slowly changing $V(x)$.

WKB approximation, tunneling, $E < V(x)$

If $V(x) = \text{const} = V$, then $\psi(x) = A\, e^{\pm \lambda x}$, $\qquad \lambda = \dfrac{\sqrt{2m(V-E)}}{\hbar}$

Similarly

$$\psi(x) \approx \frac{\text{const}}{\sqrt{\lambda(x)}} \exp\left[\pm \int^{x} \lambda(x')\, dx'\right]$$

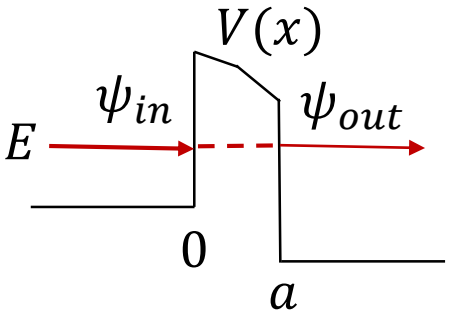
$$\lambda(x) = \frac{\sqrt{2m[V(x)-E]}}{\hbar}$$

WKB approximation is often used to estimate probability of tunneling (coefficient of transmission) through a strong (almost "opaque") tunnel barrier

Tunneling probability

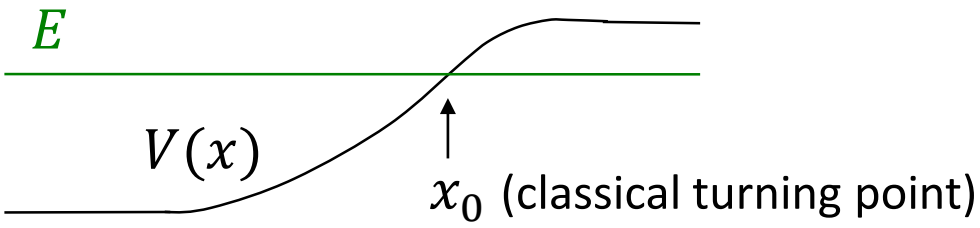
$T \simeq |\psi_{\text{out}}|^2 / |\psi_{\text{in}}|^2 \qquad T \ll 1$

$$T \simeq \exp(-2 \int_0^a \lambda(x)\, dx)$$



(very crudely; we neglect all pre-exponential factors, which usually are within one order of magnitude, while exponential factor can typically be $10^{-3} - 10^{-10}$)

WKB, connection between the two regions



assume smooth $V(x)$
(different result for
an abrupt potential)

WKB approximation does not work well in the vicinity of x_0, we need a better approximation near x_0 (linear potential, Airy functions).

Result:

$$\psi(x) \approx \begin{cases} \dfrac{C}{\sqrt{\lambda(x)}} \exp\left[-\displaystyle\int_{x_0}^{x} \lambda(x')dx'\right], & x > x_0 \\ \dfrac{2\,C}{\sqrt{k(x)}} \sin\left[\dfrac{\pi}{4} + \displaystyle\int_{x}^{x_0} k(x')dx'\right], & x < x_0 \end{cases}$$

Variational principle (Ch. 7)

Only Sec. 7.1

Theorem: For an arbitrary $|\psi\rangle$, the ground state energy E_g satisfies inequality

$$E_g \leq \langle\psi|\hat{H}|\psi\rangle = \langle\hat{H}\rangle$$

Proof is simple. Let us expand $|\psi\rangle = \sum_n c_n|\psi_n\rangle$. Then since $E_n \geq E_g$, we get

$$\langle\hat{H}\rangle = \sum_n |c_n|^2 E_n \geq E_g \sum_n |c_n|^2 = E_g$$

This theorem can be useful to estimate E_g (or at least to find an upper bound)

Idea: Use trial wavefunctions $|\psi\rangle$ with many adjustable parameters and minimize $\langle\hat{H}\rangle$. Hopefully $\min\langle\hat{H}\rangle$ is close to E_g.

Extensions of this method can also be used to find $|\psi_g\rangle$,
first-excited state energy and wavefunction (using subspace orthogonal to $|\psi_g\rangle$),
second-excited state, etc.