Approximation Methods

PHY 852 Chapter 6 Review

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WKB approximation

Classical region:

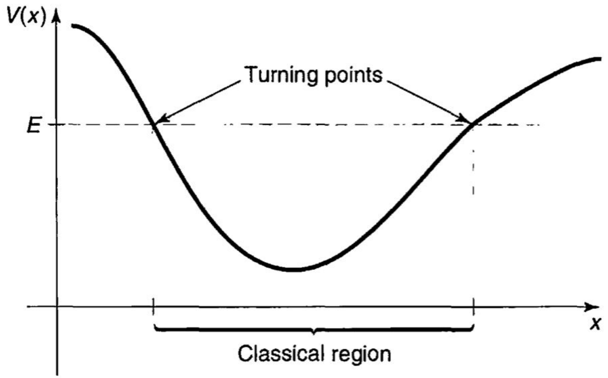
- Define $p(x) = \sqrt{2m(E - V(x)}$
- We have a wavefunction of the form:

$$\psi_{WKB}(x) = A_+ e^{i\phi(x)} + A_- e^{-i\phi(x)}$$

$$\phi(x) = \frac{1}{\hbar}\int_0^x dx' p(x')$$

- Between two turning points we should have

$$\phi(a) = \pi/2$$



WKB approximation

Tunnelling region:

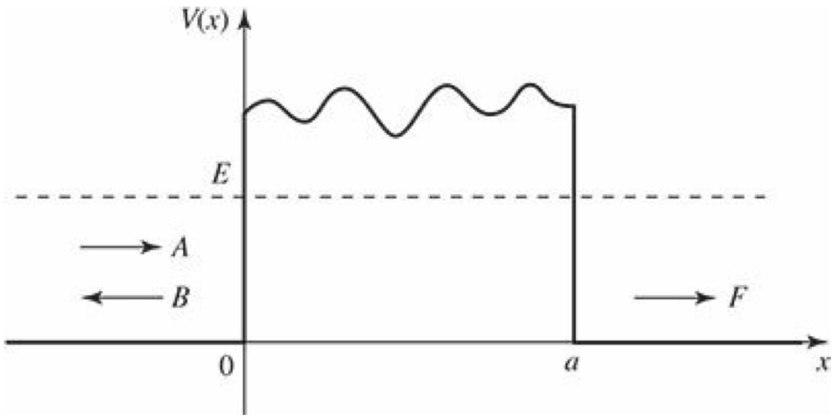
- Define $q(x) = \sqrt{2m(V(x) - E)}$
- We have a wavefunction of the form:

$$\psi_{WKB}(x) = A_+ e^{\phi(x)} + A_- e^{-\phi(x)}$$

$$\phi(x) = \frac{1}{\hbar}\int_0^x dx' q(x')$$

- Calculate tunneling probability:

$$P_{a\to b} \approx \exp\left\{-\frac{2}{\hbar}\int_a^b dx\sqrt{2m(V(x) - E)}\right\}$$



Variational Theory

- If you have some Hamiltonian, chose a (normalized) trial wave function that has a parameter you can vary, ex: $\psi(r) = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$
- Calculate the expectation value of the Hamiltonian and minimize with respect to the variable parameter: $\frac{\partial}{\partial a} \langle\psi| H |\psi\rangle = 0$
- Use this value of your variable parameter (here it is a) to get an estimate of the energy
- This method always leads to an overestimation of the energy

Sudden approximation

- If a system changes very rapidly from one Hamiltonian to another, at t=0 in the new potential landscape it will be in the same state as it was previously
- This is different than a slow/adiabatic transition from one Hamiltonian to another, where you allow for a system to relax to its ground state with every infinitesimal step
- In the adiabatic case, a system will stay in the ground state

Time-independent perturbation theory

- Consider a Hamiltoniar H_0 with known eigenstates $|n\rangle$ with energy ϵ_n
- Add a small perturbation $H = H_0 + V$
- The first order correction to the energy can be solved for using the eigenstates of H_0:

$$E_n^1 = \langle \psi_n^0 | H | \psi_n^0 \rangle$$

- First order corrections to wavefunction:

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

- Second order corrections:

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

Fermi’s Golden Rule

- We have utilized the interaction picture to formulate time-dependant perturbation theory.
- If we have a time-independent potential that is either is slowly turned on or off, considering only up to first order perturbation theory, we get the Fermi’s Golden Rule:

$$R_{i \to n}(t) = \frac{2\pi}{\hbar} |V_{ni}|^2 \delta(\epsilon_n - \epsilon_i)$$

Quick Reminders

- In order to transform summations to integrals we need to multiply by the density of states:

$$\sum_k \to \frac{L}{2\pi}\int_{-\infty}^{\infty} dk, \quad \text{one dimension,}$$

$$\sum_k \to \frac{A}{(2\pi)^2}\int_{-\infty}^{\infty} d^2k, \quad \text{two dimensions,}$$

$$\sum_k \to \frac{\Omega}{(2\pi)^3}\int d^3k, \quad \text{three dimensions.}$$

- Also, to be able to integrate the delta function, the integration variable needs to be converted from momentum to energy:

$$\begin{aligned} dk &= \frac{dE}{dE/dk} = \frac{dE}{\hbar v_k}, \\ &= dE\frac{m}{\hbar^2 k}, \quad \text{non}-\text{relativistic,} \\ &= dE\frac{E}{\hbar^2 k}, \quad \text{relativistic,} \\ &= \frac{dE}{\hbar c}, \quad \text{massless.} \end{aligned}$$

Harmonic Perturbations

- If we have instead a harmonically time-dependant potential, we can write it as:

$$\langle n|V_S(t)|m\rangle = V_{nm}e^{\eta t}\cos(\omega t) = \frac{1}{2}V_{nm}e^{\eta t}\left(e^{i\omega t} + e^{-i\omega t}\right).$$

- Thus, it is basically the same situation we had in the derivation of the Fermi's golden rule, but now the phases can be absorbed inside the time evolution phase, leading to:

$$\frac{d}{dt}P_{i\to n}(t) = \frac{2\pi}{\hbar}\frac{|V_{ni}|^2}{4}\left[\delta(\epsilon_n - \epsilon_i + \hbar\omega) + \delta(\epsilon_n - \epsilon_i - \hbar\omega)\right]$$

- The cosine is no longer part of V!
- Don't forget the factor of 1/4 since it is not in the formula sheet.
- Consider only the delta function of the allowed transition.

Example 6.7 from the lecture notes:

Consider a particle of mass m in the ground state of a δ function potential,

$$V_0(x) = -\beta\delta(x)$$

The particle feels a harmonic potential

$$V(t) = eEx\cos(\omega t), \quad \hbar\omega > |\text{G.S. energy}|$$

Estimate the ionization rate using first-order perturbation theory. To simplify the problem, assume the outgoing momentum is high enough that the outgoing wave can be treated as a plane wave, i.e. the corrections due to the delta function potential are small. This is a one-dimensional example that has much in common with radiative excitation.

- First, we write down the initial state (the bound state of the delta function potential) and the final state (here, free electrons), and their energies:

$$\psi_0(x) = \sqrt{\frac{q}{2}} e^{-q|x|}, q = \frac{m\beta}{\hbar^2}$$

$$\psi_k(x) = \frac{e^{ikx}}{\sqrt{L}}, k = \sqrt{\frac{2m(\hbar\omega - B)}{\hbar^2}} \qquad \text{where } B = \frac{\hbar^2 q^2}{2m}$$

- We should have used the scattering state of the delta function as a final state, but we are making the approximation that the final state does not feel the interaction.

- Second, we calculate the interaction matrix elements:

$$
\begin{aligned}
V_{k0} &= \sqrt{\frac{q}{2L}} \int dx\, eExe^{-ikx} e^{-q|x|} \\
&= -ieE\sqrt{\frac{q}{2L}} \int dx\, x \sin(kx) e^{-q|x|} \\
&= ieE\sqrt{\frac{q}{2L}} \frac{d}{dk} \int dx\ \cos(kx) e^{-q|x|} \\
&= ieE\sqrt{\frac{q}{2L}} \frac{d}{dk} \left\{ \frac{1}{q+ik} + \frac{1}{q-ik} \right\} \\
&= ieE\sqrt{\frac{2}{L}} \frac{2kq^{3/2}}{(q^2+k^2)^2}.
\end{aligned}
$$

- Note that the cosine was not included!

- Finally, apply the Fermi's golden rule and summing over all possible final states:

$$
\begin{aligned}
\mathcal{R} &= \frac{\pi}{2\hbar}\int \frac{L dk}{2\pi}\,|V_{k0}|^2\delta(\epsilon_k - \hbar\omega - B) \\
&= \frac{1}{\hbar}\frac{e^2E^2k^2q^3}{(q^2+k^2)^4}\frac{4}{|d\epsilon_k/dk|} \\
&= \frac{4m}{\hbar^3}\frac{e^2E^2kq^3}{(q^2+k^2)^4}.
\end{aligned}
$$

- We picked a factor of 1/4 due to the Harmonic perturbation.
- Only one delta function contributed to the transition which corresponds to final energies larger than the initial bound energy.
- We also picked a factor of 2 since we have two final states with opposite momentum.