Quantum Theory
lecture 5: approximation methods

- variational principle — S-5.4
- semiclassics (Bohr-Sommerfeld quantization) — S-2.5
- WKB approximation — S-2.5
- resonant tunneling
- Landau levels

S = Sakurai (2nd edition)

Variational principle

the lowest eigenvalue E_0 of H (the ground state energy) is bounded from above by

$$\begin{aligned}\langle\psi|H|\psi\rangle &= \sum_{n,m}\langle\psi|\psi_n\rangle\langle\psi_n|H|\psi_m\rangle\langle\psi_m|\psi\rangle \\ &= \sum_n E_n|\langle\psi_n|\psi\rangle|^2 \geqslant E_0\sum_n|\langle\psi_n|\psi\rangle|^2 = E_0.\end{aligned}$$

for a normalized state ψ; more generally, for any ψ,

$$E_0 \leqslant \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}.$$

Bohr-Sommerfeld quantization

before the arrival of the Schrödinger equation, Bohr and Sommerfeld had found a way to quantize periodic motion by demanding that the phase accumulated in one period should be an integer multiple of 2π:

$$\frac{1}{\hbar}\oint p\,dx + \gamma = 2\pi n, \quad n = 0, 1, 2, \ldots$$

- $p = mv + qA$ is the canonical momentum (sum of mechanical momentum mv and electromagnetic momentum qA)
- γ is a phase shift picked up at the two turning points

  $\gamma = \pm\pi$ at a hard wall, $\gamma = -\pi/2$ at a smooth turning point
- particle in a box: $2pL/\hbar - 2\pi = 2\pi n \Rightarrow p = \pi n\hbar/L, \;\; E = \frac{1}{2m}(\pi n\hbar/L)^2$ *(exact)*

triangular potential well: *approximate* (see exercise 5.1)
- more and more accurate in the large-n limit (“semiclassical”)

WKB approximation

Wenzel-Kramers-Brillouin (Schrödinger eq.) + Jeffreys (more general diff.eq.)
probability amplitude ψ that a particle from $\vec{r}_i$ reaches $\vec{r}_f$ is the sum of the amplitudes along all *classical* paths connecting $\vec{r}_i$ to $\vec{r}_f$

$$\psi = \sum_{\text{paths}} \frac{1}{\sqrt{v(\vec{r}_f)}} \exp\left(\frac{i}{\hbar} \int_{\vec{r}_i}^{\vec{r}_f} \vec{p} \cdot d\vec{l} + i\gamma \right)$$

- factor $1/\sqrt{v} \Rightarrow$ current density $j = v|\psi|^2$ constant along path
- phase shift γ (a.k.a. Maslov index) is π at a hard wall (infinite potential) where $\psi = 0$, so that incident and reflected waves cancel
- at a smooth turning point, v changes sign
$\Rightarrow e^{i\gamma} = 1/\sqrt{-1} = -i \Rightarrow \gamma = -\pi/2$
- sum over paths would be *exact* if we would include also nonclassical paths (Feynman's path integral)

resonant tunneling

see exercise 5.3

Landau levels

see exercise 5.2

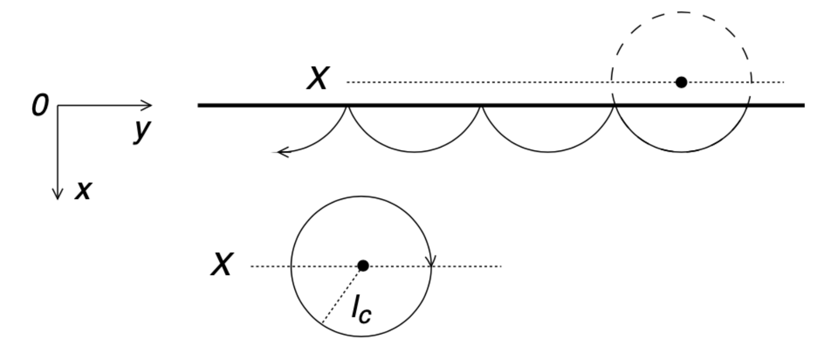
cyclotron orbit: radius $l_c = mv/eB$, frequency $\omega_c = eB/m$

$\oint \vec{p} \cdot d\vec{l} = \oint (m\vec{v} + e\vec{A}) \cdot d\vec{l} = 2\pi l_c m v - e\pi l_c^2 B = \pi (mv)^2/eB = 2\pi E/\omega_c$

BS quantization (two soft turning points): $2\pi E/\hbar\omega_c = 2\pi n - \gamma \Rightarrow E = (n + \frac{1}{2})\hbar\omega_c$ — *exact*

flux through orbit is quantized: $\Phi = \pi l_c^2 B = 2\pi E/e\omega_c = (n + \frac{1}{2})h/e$

Edge state



to include the effect of a boundary along the y-axis, choose a gauge $A = Bx\hat{y}$;
projection of motion on x-axis is periodic, apply BS rule:
$\oint mv_x dx = \oint eBy(x)dx = e\Phi = h(n + \frac{3}{4})$ (one hard and one soft turning point)
translational invariance along $y \Rightarrow p_y$ is conserved — corresponds to x-coordinate of center of cyclotron orbit: $p_y = mv_y + eBx = -eB(x - X) + eBx = eBX$
Hellmann-Feynman: $\langle v_y \rangle = dE(p_y)/dp_y = (eB)^{-1} dE(X)/dX$