# HW #10 (221A), due Nov 17, 4pm

1. Any Hamiltonian can be recast to the form

$$H = U \begin{pmatrix} E_1 & 0 & \cdots & 0 \\ 0 & E_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & E_n \end{pmatrix} U^\dagger \tag{1}$$

where $U$ is a general $n$-by-$n$ unitarity matrix.

   (a) Show that the time evolution operator is given by

$$e^{-iHt/\hbar} = U \begin{pmatrix} e^{-iE_1t/\hbar} & 0 & \cdots & 0 \\ 0 & e^{-iE_2t/\hbar} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e^{-iE_nt/\hbar} \end{pmatrix} U^\dagger. \tag{2}$$

   (b) For a two-state problem, the most general unitarity matrix is

$$U = e^{i\theta} \begin{pmatrix} \cos\theta e^{i\phi} & -\sin\theta e^{i\eta} \\ \sin\theta e^{-i\eta} & \cos\theta e^{-i\phi} \end{pmatrix}. \tag{3}$$

   Work out the probabilities $P(1 \to 2)$ and $P(2 \to 1)$ over time interval $t$, and verify that they are the same despite the apparent $T$-violation due to complex phases. (NB: This is the same problem as the neutrino oscillation in the midterm if you set $E_i = \sqrt{\vec{p}^2c^2 + m_i^2c^4} \approx |\vec{p}|c + \frac{m_i^2c^3}{2|\vec{p}|}$ and set all phases to zero.)

   (c) For a three-state problem, however, the time-reversal invariance can be broken. Calculate the difference $P(1 \to 2) - P(2 \to 1)$ for the following form of the unitary matrix

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{23} & s_{23} \\ 0 & -s_{23} & c_{23} \end{pmatrix} \begin{pmatrix} c_{13} & 0 & s_{13}e^{-i\delta} \\ 0 & 1 & 0 \\ -s_{13}e^{i\delta} & 0 & c_{13} \end{pmatrix} \begin{pmatrix} c_{12} & s_{12} & 0 \\ -s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{4}$$

   where other five unimportant phases are already dropped. The notation is $s_{12} = \sin\theta_{12}$, $c_{23} = \cos\theta_{23}$, etc.

(d) (optional) For CP-conjugate states (*e.g.*., anti-neutrinos vs neutrinos), the Hamiltonian is given by substituting $U^*$ in place of $U$. Show that the probabilities $P(1 \to 2)$ and $P(\bar{1} \to \bar{2})$ can differ (CP violation) yet CPT is respected, *i.e.*, $P(1 \to 2) = P(\bar{2} \to \bar{1})$.

2. Consider a periodic replusive potential of the form

$$V = \sum_{n=-\infty}^{\infty} \lambda \delta(x - na) \tag{5}$$

with $\lambda > 0$. The general solution for $-a < x < 0$ is given by

$$\psi(x) = Ae^{i\kappa x} + Be^{-i\kappa x}, \tag{6}$$

with $\kappa = \sqrt{2mE}/\hbar$. Using the Bloch's theorem, wave function for the next period $0 < x < a$ is given by

$$\psi(x) = e^{ika}(Ae^{i\kappa(x-a)} + Be^{-i\kappa(x-a)}) \tag{7}$$

for $|k| \leq \pi/a$. Answer the following questions.

(a) Write down the continuity condition for the wave function and the required gap for its derivative at $x = 0$ (see the notes on the second page). Show that the phase $e^{ika}$ under the discrete translation $x \to x + a$ is given by $\kappa$ as

$$e^{ika} = \cos \kappa a + \frac{1}{\kappa d} \sin \kappa a \pm i \sqrt{1 - \left( \cos \kappa a + \frac{1}{\kappa d} \sin \kappa a \right)^2}\ . \tag{8}$$

Here and below, $d \equiv \hbar^2/m\lambda$.

(b) Take the limit of zero potential $d \to \infty$ and show that there are no gaps between bands as expected for a free particle.

(c) When the potential is weak but finite (large $d$), show analytically that there appear gaps between bands at $k = \pm\pi/a$.

(d) Plot the relationship between $\kappa$ and $k$ for a weak potential ($d = 3a$) and a strong potential ($d = \frac{1}{3}a$) (both solutions together).

(e) You always find two values of $k$ at the same energy (or $\kappa$). What discrete symmetry guarantees this degeneracy?

# How to deal with a delta-function potential

Suppose you have a Hamiltonian $H = \frac{p^2}{2m} + \lambda\delta(x)$. The time-dependent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\psi''(x) + \lambda\delta(x)\psi(x) = E\psi(x). \tag{9}$$

Let us integrate both sides of the equation for a small interval $x \in [-\epsilon, \epsilon]$, and we will send $\epsilon \to 0$ in the end. For the right-hand side of the equation,

$$\int_{-\epsilon}^{\epsilon} dx E\psi(x) \to 0. \tag{10}$$

The left-hand side of the equation is more complicated. The first term is

$$\int_{-\epsilon}^{\epsilon} dx \frac{-\hbar^2}{2m}\psi''(x) = \left[-\frac{\hbar^2}{2m}\psi'(x)\right]_{-\epsilon}^{\epsilon} = -\frac{\hbar^2}{2m}(\psi'(+\epsilon) - \psi'(-\epsilon)). \tag{11}$$

On the other hand, the second term is

$$\int_{-\epsilon}^{\epsilon} dx \lambda\delta(x)\psi(x) = \lambda\psi(0). \tag{12}$$

Putting everything together,

$$-\frac{\hbar^2}{2m}(\psi'(+\epsilon) - \psi'(-\epsilon)) + \lambda\psi(0) = 0, \tag{13}$$

or

$$\psi'(+\epsilon) - \psi'(-\epsilon) = \frac{2m\lambda}{\hbar^2}\psi(0). \tag{14}$$

Therefore, the wave function must be continuous across the delta function, while the derivative is discontinuous.

You can work on problem 22, Chapter 2 of Sakurai, and find that there is one bound state with a negative delta function potential, and a continuum of positive energy eigenstates.