HW #9 (221A), due Nov 12, 4pm

1. Consider a symmetric rectangular double-well potential
$$V = \begin{cases} \infty & \text{for } |x| > a+b \\ 0 & \text{for } a < |x| < a+b \\ V_0 > 0 & \text{for } |x| < a. \end{cases} \tag{1}$$
Assuming that V_0 is very high, obtain the energies of the two low-lying states and plot their wave functions.

2. Consider a periodic replusive potential of the form
$$V = \sum_{n=-\infty}^{\infty} \lambda \delta(x - na) \tag{2}$$
with $\lambda > 0$. The general solution for $-a < x < 0$ is given by
$$\psi(x) = Ae^{i\kappa x} + Be^{-i\kappa x}, \tag{3}$$
with $\kappa = \sqrt{2mE}/\hbar$. Using the Bloch's theorem, wave function for the next period $0 < x < a$ is given by
$$\psi(x) = e^{ika}(Ae^{i\kappa(x-a)} + Be^{-i\kappa(x-a)}) \tag{4}$$
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 κ as
   $$e^{ika} = \cos\kappa a + \frac{1}{\kappa d}\sin\kappa a \pm i\sqrt{1 - \left(\cos\kappa a + \frac{1}{\kappa d}\sin\kappa a\right)^2}. \tag{5}$$
   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 κ 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 κ). 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

$$-\frac{\hbar^2}{2m}\psi''(x) + \lambda\delta(x)\psi(x) = E\psi(x). \tag{6}$$

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,

$$\int_{-\epsilon}^{\epsilon} dx E\psi(x) \to 0. \tag{7}$$

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

$$\int_{-\epsilon}^{\epsilon} dx \frac{-\hbar^2}{2m}\psi''(x) = \left[-\frac{\hbar^2}{2m}\psi'(x)\right]_{-\epsilon}^{\epsilon} = -\frac{\hbar^2}{2m}(\psi'(+\epsilon) - \psi'(-\epsilon)). \tag{8}$$

On the other hand, the second term is

$$\int_{-\epsilon}^{\epsilon} dx \lambda\delta(x)\psi(x) = \lambda\psi(0). \tag{9}$$

Putting everything together,

$$-\frac{\hbar^2}{2m}(\psi'(+\epsilon) - \psi'(-\epsilon)) + \lambda\psi(0) = 0, \tag{10}$$

or

$$\psi'(+\epsilon) - \psi'(-\epsilon) = \frac{2m\lambda}{\hbar^2}\psi(0). \tag{11}$$

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.