Problem Set #3

Solutions

$\boxed{1}$ a) $\psi(x,t) = c_1 \varphi_1(x) e^{-i\omega_1 t}$, where $\varphi_1(x)$ is an eigenfunction of H

$$\langle \Theta(t) \rangle = \int \varphi_1(x) e^{+i\omega_1 t} \Theta \varphi_1(x) e^{-i\omega_1 t} dx$$

$$= \int \varphi_1(x) \Theta \varphi_1(x) = \langle \Theta(t=0) \rangle$$

b) $\psi(x,t) = c_n \varphi_n(x) e^{-i\omega_n t} + c_m \varphi_m(x) e^{-i\omega_m t}$, where $\omega_n = n\omega$, $\omega_m = m\omega$ (integer) & $\omega = \sqrt{\frac{k}{m}}$ the H.O. fundamental

$$\rightarrow c_n \varphi_n(x) e^{-i\frac{\Omega}{2}t} + c_m \varphi_m e^{+i\frac{\Omega}{2}t}, \quad \text{where } \Omega = \omega_n - \omega_m$$

There I absorbed a global time-dependent phase into the coefficients. Only relative phases matter, so this is always OK.

$$\langle \Theta(t) \rangle = \int (c_n^* \varphi_n(x) e^{+i\frac{\Omega}{2}t} + c_m^* \varphi_m(x) e^{-i\frac{\Omega}{2}t}) \Theta (c_n \varphi_n(x) e^{-i\frac{\Omega}{2}t} + c_m \varphi_m(x) e^{+i\frac{\Omega}{2}t})$$

$$= |c_n|^2 + |c_m|^2 + \int c_n^* c_m \varphi_n(x) \Theta \varphi_m(x) e^{i\Omega t} + \int c_m^* c_n \varphi_m(x) \Theta \varphi_n(x) e^{-i\Omega t}$$

Since Θ is observable, the operator is self-adjoint, a.k.a. Hermitian

$$\Rightarrow \int \varphi_n(x) \Theta \varphi_m(x) = \int (\Theta \varphi_n(x))^* \varphi_m(x) = \int \varphi_m(x) (\Theta \varphi_n(x))^*$$

$$= \left[\int \varphi_m(x) \Theta \varphi_n(x) \right]^*$$

$\Rightarrow$ The two integrals are complex conjugates of one another

$$\Rightarrow \langle \Theta(t) \rangle = |c_n|^2 + |c_m|^2 + 2\,\mathrm{Re}\left[c_n^* c_m \int \varphi_n(x)\, \Theta\, \varphi_m(x)\right] \cos \Omega t$$

where $\Omega = n\omega - m\omega = \underbrace{(n-m)}_{\text{integer}}\omega$

Period is $T = \dfrac{2\pi}{(n-m)\omega}$, which is an integral fraction of the H.O. fundamental period $\dfrac{2\pi}{\omega}$

$\Rightarrow$ Our oscillations can have a shorter period if $|n-m| > 1$, but it is also periodic at $\dfrac{2\pi}{\omega}$. In other words, this periodicity always shows up in the H.O., regardless of how you prepare the states.

c) The same math as above applies, except $\Omega = \omega_2 - \omega_1$ is no longer an integer multiple of a fundamental frequency. So, for most potentials, there is no guaranteed periodicity, the oscillations depend entirely on the state preparation.

2. (a) Make use of the orthogonality of the eigenfunctions to get the c_n's:

$$\int_0^\pi dx\, \sin(mx)\sin(nx) = \frac{\pi}{2}\delta_{nm}, \tag{8}$$

therefore:

$$\begin{aligned}\sqrt{\frac{2}{\pi}}\int_0^\pi dx\, \sin(mx)f(x) &= \frac{2}{\pi}\int_0^\pi dx\, \sin(mx)\sum_{n=1}^{\infty} c_n \sin(nx) \\ &= \frac{2}{\pi}\sum_{n=1}^{\infty} c_n \int_0^\pi dx\, \sin(mx)\sin(nx) \\ &= \sum_{n=1}^{\infty} c_n \delta_{mn} = c_m \end{aligned} \tag{9}$$

With $f(x)$ at hand, we get:

$$c_n = \sqrt{\frac{2}{\pi}}\int_{\pi/6}^{\pi/3} dx\, \sin(nx)\sqrt{\frac{6}{\pi}}. \tag{10}$$

The integral should be straightforward and yields:

$$c_n = \frac{2\sqrt{3}}{n\pi}\left[\cos\left(\frac{n\pi}{6}\right) - \cos\left(\frac{n\pi}{3}\right)\right]. \tag{11}$$

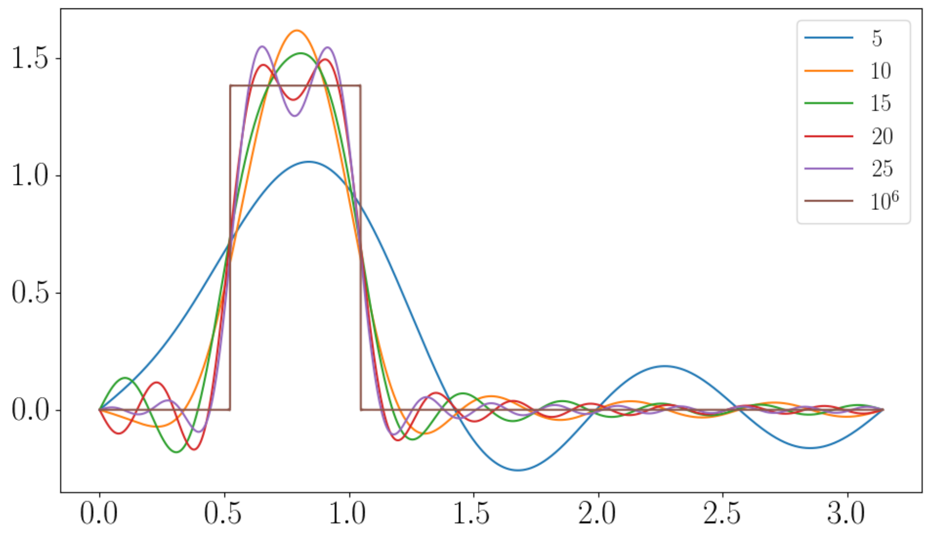

Figure 1: Fourier approximation of a step function for increasing number of terms.

Plugging the c_n's into eq. (1) of the problem set leads us to the Fourier series for $f(x)$:

$$f(x) = \sqrt{3}\left(\frac{2}{\pi}\right)^{3/2} \sum_{n=1}^{\infty} \frac{1}{n}\left[\cos\left(\frac{n\pi}{6}\right) - \cos\left(\frac{n\pi}{3}\right)\right]\sin(nx) \tag{12}$$

(b) Your plots should show how adding more and more terms according to the Fourier series expansion of $f(x)$, it will approach the $\sqrt{6/\pi}$ step with increasing accuracy, according to Fig. 1.

(c) The eigenvalues are

$$E_n = \frac{1}{2m}\left(\frac{\hbar\pi n}{a}\right)^2 \propto n^2 \tag{13}$$

such that the solution to the time dependent Schrödinger equation is in the form

$$\psi(x,t) \propto \sum_{n=1}^{\infty} \frac{1}{n}\left[\cos\left(\frac{n\pi}{6}\right) - \cos\left(\frac{n\pi}{3}\right)\right]\sin(nx)e^{-in^2t}. \tag{14}$$

As showns in Figs. 2 and 3, for a sufficient number of terms ($\sim 10^3$) in the series, your plots for $|\psi(x,t)|^2$ should show a clear step function at $t = 0$, and for times

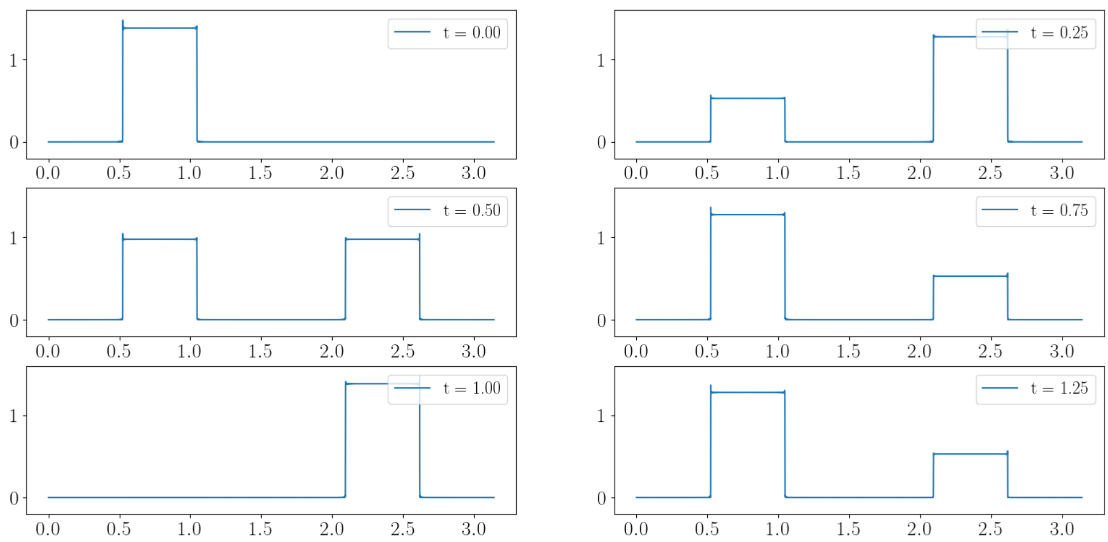

Figure 2: Behavior of a prepared step wave function inside an infinite square well for time as a multiple of the natural period. Time is labelled in the upper right of each plot. Evaluated with 10^5 Fourier terms.

which are a multiple of π, the wave functions reappears at differents places, almost as bouncing between the walls (Fig 2). For t different of a multiple of π, the wave function is more delocalized (Fig. 3).

(d) In that case:

$$\psi(x,t) = \sqrt{\frac{2}{\pi}} \sum_{n=1}^{\infty} c_n \sin(nx) e^{-nt/8} e^{-in^2 t}, \tag{15}$$

with c_n given by (11). The probability density will be, given the prescription:

$$|\psi(x,t)|^2 = a(t)|\phi_1(x)|^2 + \frac{2}{\pi} \left| \sum_{n=1}^{\infty} c_n \sin(nx) e^{-nt/8} e^{-in^2 t} \right|^2 . \tag{16}$$

Normalization will impose the integral over the well length of the above equation to be unity. The $\phi_n(x)$ eigenfunctions are supposed to be normalized, and are

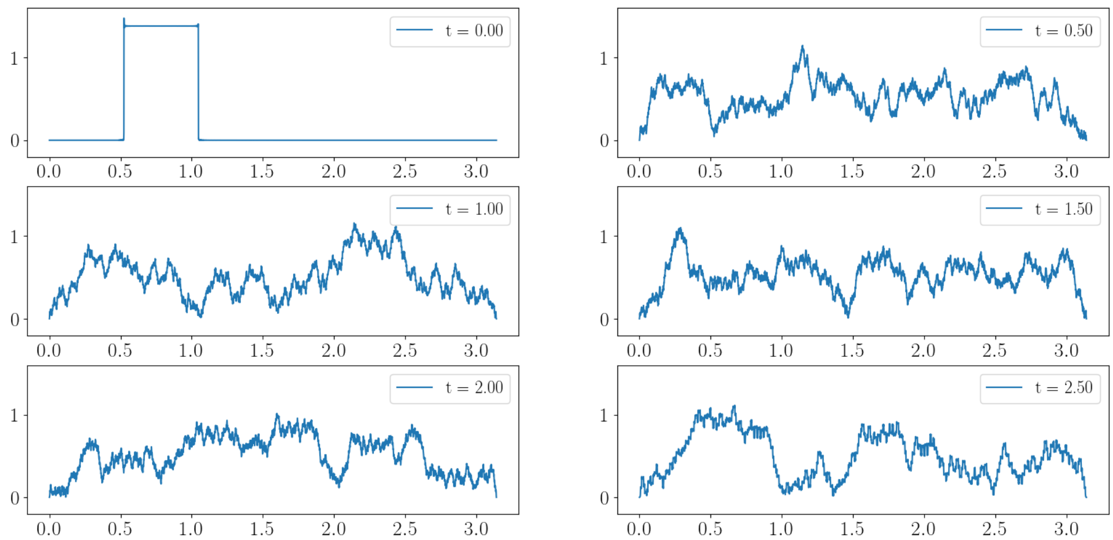

Figure 3: Behavior of a prepared step wave function inside an infinite square well for time as a multiple of 0.5 (arbitrary units). Time is labelled in the upper right of each plot. Evaluated with 10^5 Fourier terms.

orthogonal over the period, according to (9). Therefore:

$$
\begin{aligned}
1 &= a(t) + \frac{2}{\pi} \sum_{n,n'} c_n c^{\star}_{n'} \sin(nx) \sin(n'x) e^{-(n+n')t/8} e^{-i(n^2-n'^2)t} \delta_{n,n'} \\
&= a(t) + \frac{2}{\pi} \sum_{n=1}^{\infty} |c_n|^2 e^{-nt/4}.
\end{aligned} \tag{17}
$$

Hence, using (11):

$$
a(t) = 1 - \frac{12}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \left[\cos\left(\frac{n\pi}{6}\right) - \cos\left(\frac{n\pi}{3}\right) \right]^2 e^{-nt/4}. \tag{18}
$$

The probability density with this prescription is evaluated numerically and plotted below. The state initially prepared as a step function decays to the ground state after a certain time.

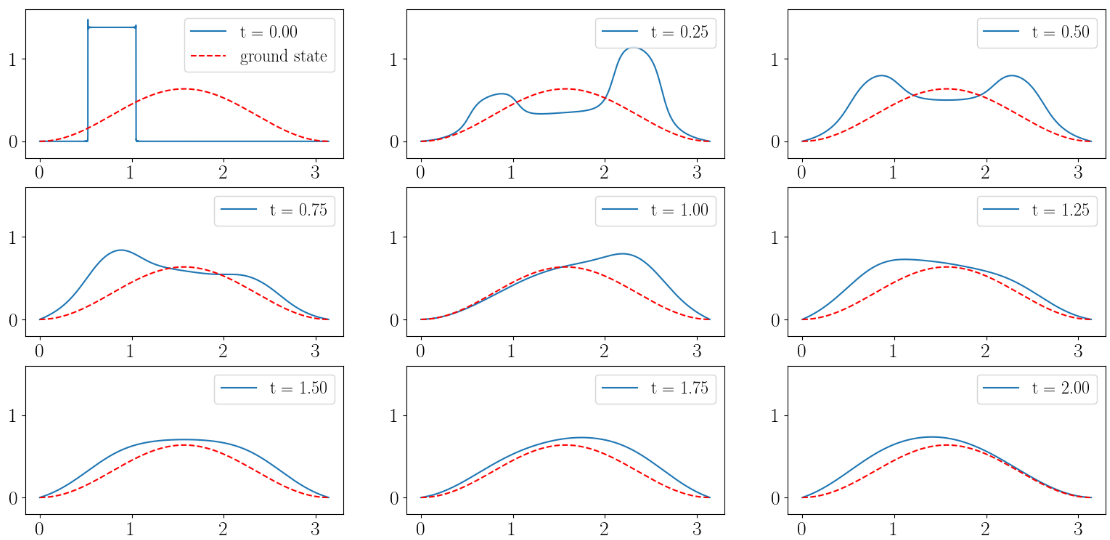

Figure 4: Wave function prepared as a step slowly decaying to the ground state inside an infinite square well. Evaluated with 10^5 Fourier terms.