Home Work 4

1. (Ch. 6, EOC ex. 3) Verify the formula that the Franck–Condon spectrum is equal to the Fourier transform of a wavepacket autocorrelation function,
$$\sigma(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} <\psi(0)|\psi(t)> e^{iEt/\hbar}\, dt, \tag{1.1}$$
by working out the formula analytically for the harmonic oscillator potential.
   a. First construct the wavepacket autocorrelation function,
   $$C(t) = <\psi(0)|\psi(t)> = \int_{-\infty}^{\infty} \psi(x,0)^*\psi(x,t)\, dx, \tag{1.2}$$
   using the analytic formula for the coherent state wavepacket. After some rearrangement, the correlation function should be
   $$C(t) = e^{-\frac{\Delta^2}{2}\left(1-e^{-i\omega t}\right)-\frac{i}{2}\omega t}, \tag{1.3}$$
   where $\Delta = \sqrt{m\omega/\hbar}x_0$ is the so-called dimensionless displacement and x_0 is the initial displacement of the center of the coherent state from the minimum of the harmonic potential (assume $p_0 = 0$).
   b. Calculate the spectrum by performing the Fourier transform of the above result analytically. *Hint: Consider the expression $e^{\frac{\Delta^2}{2}e^{-i\omega t}}$ to be of the form e^x. Expand in a Taylor's series and integrate term by term.* Your answer should agree with the standard expression for the spectrum, which is a set of δ-functions with a Poisson distribution of amplitudes:
   $$\sigma(E) = \sum_{n=0}^{\infty} e^{-\frac{\Delta^2}{2}}\frac{\Delta^{2n}}{2^n n!}\delta(E-(n+\frac{1}{2})\hbar\omega) \tag{1.4}$$

2. (Ch. 6, EOC ex. 4) In this exercise we will analyze the origin of the short time decay of the autocorrelation function in the previous exercise, by deriving the functional form of the decay two different ways.
   a. First, expand the exponential in the exponent of eq. **??** in a Taylor series, up to second order in t. This gives a Gaussian fit to the short time behavior of $C(t)$.
   b. Now, start from eq. **??**, substitute the analytic expression for the coherent state, $\Psi(x,t)$, expand x_t and p_t up to first order in t (take $p_0 = 0$), and finally do the integral over x. The answer should agree with the result from the previous part. Does the decay of $C(t)$ come from motion in x_t or p_t? Interpret this result using the Wigner phase space picture for the evolution of a coherent state shown in the previous chapter?

3. (Ch. 6, EOC ex. 5) Verify the formula for an eigenstate in terms of an integral over wavepackets having the appropriate phases,
$$\frac{1}{2\pi\hbar}\psi(x,t)e^{\frac{i}{\hbar}Et}\, dt = N_n\psi_n(x)\delta(E-E_n) \tag{3.1}$$
by working out the formula analytically for the harmonic oscillator potential. For this potential, $E_n = (n+\frac{1}{2})\hbar\omega$; for $\psi(x,t)$ use the formula for the coherent state wavepacket.
   a. First rearrange the coherent state wavepacket into the form
   $$\Psi(X,t) = (\frac{\pi\hbar}{m\omega})^{1/4}\exp\left(-\frac{X^2}{2}-\frac{\Delta^2}{4}+X\Delta e^{-i\omega t}-\frac{(\Delta e^{-i\omega t})^2}{4}-i\omega t2\right), \tag{3.2}$$
   where we have introduced the dimensionless coordinate $X = \sqrt{\frac{m\omega}{\hbar}}x$ and $\Delta = \sqrt{\frac{m\omega}{\hbar}}x_0$.

b. Do the integral over t. *Hint: Identify part of your expression for* $\Psi(x,t)$ *with the generating function for the Hermite polynomials,* $e^{2xz-z^2} = \sum_{n=0}^{\infty} \mathrm{H}_n(x)\frac{z^n}{n!}$. At energies $E \neq E_n$ you should obtain 0, while for $E = E_n$ you should obtain the well–known expression for the harmonic oscillator wavefunctions,

$$\psi_n(X) = \frac{1}{\sqrt{2^n n!}} \mathrm{H}_n(X) e^{-\frac{X^2}{2}}, \tag{3.3}$$

times a Dirac δ-function, multiplied by a proportionality constant N_n. Compare the expression for N_n with the spectral intensity in Exercise 3b., and comment on its physical interpretation.