Position Autocorrelation Function for a Harmonic Oscillator

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As always we define the Hamiltonian for the 1D system.

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$$

In the canonical ensemble, $C_{xx}(t)$ for a 1D HO has a simple form,

$$C_{xx}(t) = \frac{kT}{m\omega^2}\cos(\omega t)$$

where k is Boltzmann's constant and T is temperature. Computing this value numerically with a Molecular Dynamics trajectory poses an issue because the correlation function requires that the dynamics be realistic - something that cannot be generated for a system coupled to a thermal bath. We can overcome this issue by defining the correlation function in the microcanonical ensemble.

The first thing we need to do is compute the partition function for a Harmonic Oscillator in the microcanonical ensemble, i.e. we need to compute,

$$\Omega = \frac{E_o}{h}\int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dx\ \delta(H(x,p) - E) = \frac{E_o}{h}\int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dx\ \delta\left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 - E\right)$$

which is non-trivial but doable. We begin by defining some new coordinates,

$$\bar{p} = \frac{p}{\sqrt{2m}} \qquad \sqrt{2m}d\bar{p} = dp$$
$$\bar{x} = \sqrt{\frac{m\omega^2}{2}}x \qquad \sqrt{\frac{2}{m\omega^2}}d\bar{x} = dx$$

and substitute into the partition function.

$$\Omega = \frac{E_o}{h}\sqrt{2m}\sqrt{\frac{2}{m\omega^2}}\int_{-\infty}^{\infty} d\bar{p} \int_{-\infty}^{\infty} d\bar{x}\ \delta\left(\bar{p}^2 + \bar{x}^2 - E\right) = \frac{2E_o}{h\omega}\int_{-\infty}^{\infty} d\bar{p} \int_{-\infty}^{\infty} d\bar{x}\ \delta\left(\bar{p}^2 + \bar{x}^2 - E\right)$$

The delta function requires that we consider points where $p^2 + x^2 = E$ which resembles the equation for a circle so we can consider a conversion to polar coordinates.

$$\bar{p} = \sqrt{r\omega}\cos(\theta)$$
$$\bar{x} = \sqrt{r\omega}\sin(\theta)$$

We define the coordinates this way so that the jacobian equals ω when redefining the integrals.

$$|J| = \begin{vmatrix} \frac{\partial\bar{p}}{\partial r} & \frac{\partial\bar{p}}{\partial\theta} \\ \frac{\partial\bar{x}}{\partial r} & \frac{\partial\bar{x}}{\partial\theta} \end{vmatrix} = \begin{vmatrix} \sqrt{\omega}\cos(\theta)/2\sqrt{r} & -\sqrt{r\omega}\sin(\theta) \\ \sqrt{\omega}\sin(\theta)/2\sqrt{r} & \sqrt{r\omega}\cos(\theta) \end{vmatrix} =$$

$$\int_{-\infty}^{\infty} d\bar{p} \int_{-\infty}^{\infty} d\bar{x} = \int_{-0}^{2\pi} d\theta \int_{0}^{\infty} dr|J|$$