Position Autocorrelation Function for a Harmonic Oscillator

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

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

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

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

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,

$$\Omega = \frac{E_o}{h}\int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dx\ \delta(H(x,p) - E) = \frac{E_o}{h}\int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dx\ \delta\left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - E\right) \tag{3}$$

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

$$\begin{aligned} \bar{p} &= \frac{p}{\sqrt{2m}} \quad ; \quad \sqrt{2m}d\bar{p} = dp \\ \bar{x} &= \sqrt{\frac{m\omega^2}{2}}x \quad ; \quad \sqrt{\frac{2}{m\omega^2}}d\bar{x} = dx \end{aligned} \tag{4}$$

and substituting them into the partition function.

$$\Omega = \frac{E_o}{h}\sqrt{2m}\sqrt{\frac{2}{m\omega^2}}\int_{-\infty}^{\infty} d\bar{p}\int_{-\infty}^{\infty} d\bar{x}\ \delta\left(\bar{p}^2 + \bar{x}^2 - E\right) = \frac{2E_o}{h\omega}\int_{-\infty}^{\infty} d\bar{p}\int_{-\infty}^{\infty} d\bar{x}\ \delta\left(\bar{p}^2 + \bar{x}^2 - E\right) \tag{5}$$

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.

$$\begin{aligned} \bar{p} &= \sqrt{r\omega}\cos(\theta) \\ \bar{x} &= \sqrt{r\omega}\sin(\theta) \end{aligned} \tag{6}$$

We define the coordinates this way so that the jacobian is simply a factor of ω.

$$|J| = \begin{vmatrix} \frac{\partial\bar{p}}{\partial r} & \frac{\partial\bar{p}}{\partial\theta} \\ \frac{\partial\bar{x}}{\partial r} & \frac{\partial\bar{x}}{\partial\theta} \end{vmatrix} = \begin{vmatrix} \sqrt{\omega}\cos(\theta)/2\sqrt{r} & -\sqrt{r\omega}\sin(\theta) \\ \sqrt{\omega}\sin(\theta)/2\sqrt{r} & \sqrt{r\omega}\cos(\theta) \end{vmatrix} = \frac{\omega}{2}\cos^2(\theta) + \frac{\omega}{2}\sin^2(\theta) = \frac{\omega}{2} \tag{7}$$

The integrals become redefined as,

$$\int_{-\infty}^{\infty} d\bar{p}\int_{-\infty}^{\infty} d\bar{x} = \int_0^{2\pi} d\theta \int_0^{\infty} dr|J| = \frac{\omega}{2}\int_0^{2\pi} d\theta\int_0^{\infty} dr \tag{8}$$

Equation (5) becomes,

$$\Omega = \frac{E_o}{h}\int_0^{2\pi} d\theta\int_0^{\infty} dr\ \delta\left(r\omega - E\right) \tag{9}$$

The integral over θ is trivial,

$$\Omega = \frac{2\pi E_o}{h} \int_0^\infty dr\ \delta\left(r\omega - E\right) \tag{10}$$

and we can set $r' = r\omega$,

$$\Omega = \frac{2\pi E_o}{h\omega} \int_0^\infty dr'\ \delta\left(r' - E\right) \tag{11}$$

to get an integral of a dirac delta function over all space which is equal to 1. So we are left with,

$$\Omega = \frac{2\pi E_o}{h\omega} = \frac{E_o}{\hbar\omega}. \tag{12}$$

Now we can begin deriving a form for the correlation function. We start with the definition of $C_{xx}(t)$ in the microcanonical ensemble (we take $t = 0$ to be our initial time) as a phase space average,

$$C_{xx}(t) = \langle x(0)x(t)\rangle = \frac{E_o}{h\Omega} \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dx\ x(0)\ x(t)\delta(H(x,p) - E) \tag{13}$$

where E_o/h is a constant from the partition function Ω. Integrating Hamilton's equations for a Harmonic Oscillator yields the equation of motion

$$x(t) = x(0)\cos(\omega t) + \frac{p(0)}{m\omega}\sin(\omega t) \tag{14}$$

where $p(0)$ is the initial momentum. We can drop the 0 in the initial x and p since we need to consider each point in phase space as an initial condition in order to compute the integral. Plugging $x(t)$ and equation (12) into our defintion leaves us with,

$$C_{xx}(t) = \frac{\omega}{2\pi} \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dx\ x\left[x\cos(\omega t) + \frac{p}{m\omega}\sin(\omega t)\right]\delta\left(\frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - E\right) \tag{15}$$

We will now make the same transformation as in equation (4) to make $(x,p) \to (\bar{x},\bar{p})$.

$$\begin{aligned}
C_{xx}(t) &= \frac{\omega}{2\pi}\sqrt{2m}\sqrt{\frac{2}{m\omega^2}} \int_{-\infty}^{\infty} d\bar{p} \int_{-\infty}^{\infty} d\bar{x}\ \sqrt{\frac{2}{m\omega^2}}\bar{x}\left[\sqrt{\frac{2}{m\omega^2}}\bar{x}\cos(\omega t) + \frac{\sqrt{2m}}{m\omega}\bar{p}\sin(\omega t)\right]\delta\left(\bar{p}^2 + \bar{x}^2 - E\right) \\
&= \frac{\omega}{2\pi}\frac{2}{\omega} \int_{-\infty}^{\infty} d\bar{p} \int_{-\infty}^{\infty} d\bar{x}\ \sqrt{\frac{2}{m\omega^2}}\bar{x}\left[\sqrt{\frac{2}{m\omega^2}}\bar{x}\cos(\omega t) + \sqrt{\frac{2}{m\omega^2}}\bar{p}\sin(\omega t)\right]\delta\left(\bar{p}^2 + \bar{x}^2 - E\right) \\
&= \frac{1}{\pi} \int_{-\infty}^{\infty} d\bar{p} \int_{-\infty}^{\infty} d\bar{x}\ \frac{2}{m\omega^2}\bar{x}\left[\bar{x}\cos(\omega t) + \bar{p}\sin(\omega t)\right]\delta\left(\bar{p}^2 + \bar{x}^2 - E\right) \\
&= \frac{2}{\pi m\omega^2} \int_{-\infty}^{\infty} d\bar{p} \int_{-\infty}^{\infty} d\bar{x}\ \bar{x}\left[\bar{x}\cos(\omega t) + \bar{p}\sin(\omega t)\right]\delta\left(\bar{p}^2 + \bar{x}^2 - E\right)
\end{aligned} \tag{16}$$

And then make the second transformation to polar coordinates as in equation (6).

$$\begin{aligned}
C_{xx}(t) &= \frac{2}{\pi m\omega^2}\frac{\omega}{2} \int_0^{2\pi} d\theta \int_0^\infty dr\ \sqrt{r\omega}\sin(\theta)\left[\sqrt{r\omega}\sin(\theta)\cos(\omega t) + \sqrt{r\omega}\cos(\theta)\sin(\omega t)\right]\delta\left(r\omega - E\right) \\
&= \frac{1}{\pi m\omega} \int_0^{2\pi} d\theta \int_0^\infty dr\ r\omega\sin(\theta)\left[\sin(\theta)\cos(\omega t) + \cos(\theta)\sin(\omega t)\right]\delta\left(r\omega - E\right)
\end{aligned} \tag{17}$$

The following trig identity, $\sin(x)\cos(y) + \sin(y)\cos(x) = \sin(x+y)$, yields,

$$\begin{aligned}
C_{xx}(t) &= \frac{1}{\pi m} \int_0^{2\pi} d\theta \int_0^\infty dr\ r\sin(\theta)\left[\sin(\theta + \omega t)\right]\delta\left(r\omega - E\right) \\
&= \frac{1}{\pi m} \int_0^\infty dr\ r\ \delta\left(r\omega - E\right) \int_0^{2\pi} d\theta \sin(\theta)\sin(\theta + \omega t)
\end{aligned} \tag{18}$$

The theta integral is trivial.

$$\begin{aligned}
\int_0^{2\pi} d\theta \sin(\theta)\sin(\theta+\omega t) &= \int_0^{2\pi} d\theta \sin(\theta)\left[\sin(\theta)\cos(\omega t)+\cos(\theta)\sin(\omega t)\right] \\
&= \cos(\omega t)\int_0^{2\pi} d\theta \sin^2(\theta) + \sin(\omega t)\int_0^{2\pi} d\theta \sin(\theta)\cos(\theta) \\
&= \cos(\omega t)\int_0^{2\pi} d\theta \frac{1}{2}\left[1-\cos(2\theta)\right] + \sin(\omega t)\int_0^{2\pi} d\theta \sin(\theta)\cos(\theta) \\
&= \frac{\cos(\omega t)}{2}\int_0^{2\pi} d\theta \left[1-\cos(2\theta)\right] + \sin(\omega t)\int_0^{0} du\, u \\
&= \frac{\cos(\omega t)}{2}\left(\theta - \frac{\sin(2\theta)}{2}\right)\Bigg|_0^{2\pi} + 0 \\
&= \frac{\cos(\omega t)}{2}(2\pi) \\
&= \pi\cos(\omega t)
\end{aligned} \tag{19}$$

So we are left with,

$$C_{xx}(t) = \frac{1}{m}\int_0^{\infty} dr\; r\cos(\omega t)\delta\left(r\omega - E\right) \tag{20}$$

If we set $r' = r\omega$ we are left with another delta function that is simple to evaluate with the following identity, $\int_{-\infty}^{\infty} f(x)\delta(x-a) = f(a)$, (remembering that $r \in [0,\infty)$)

$$\begin{aligned}
C_{xx}(t) &= \frac{1}{m}\int_0^{\infty} \frac{dr'}{\omega}\;\frac{r'}{\omega}\cos(\omega t)\delta\left(r' - E\right) \\
&= \frac{1}{m\omega^2}\cos(\omega t)\int_0^{\infty} dr'\; r'\delta\left(r' - E\right) \\
&= \frac{1}{m\omega^2}\cos(\omega t)E
\end{aligned} \tag{21}$$

And we finally derive the position autocorrelation function in the microcanonical ensemble,

$$C_{xx}(t) = \frac{E}{m\omega^2}\cos(\omega t) \tag{22}$$

where E is the constant total energy of the system.