Brownian dynamics and power spectra

It is useful to analyze diffusion and motion on the micro-scale through the power-spectral-density (PSD `http://en.wikipedia.org/wiki/Power_spectral_density`) of the motion.

The PSD $P_{xx}(x(t))$ of a time-series $x(t)$ is defined as the norm-squared $|\tilde{x}|^2$ of the Fourier transform $\tilde{x}$:

$$P_{xx}(x(t)) = |\tilde{x}(\omega)|^2$$

We may define the Fourier transform of x and its time-derivative $\dot{x}$ as

$$x(t) \leftrightarrow \tilde{x}(\omega)$$

$$\dot{x}(t) \leftrightarrow i\omega\tilde{x}(\omega)$$

For Brownian dynamics we know from the fluctuation-dissipation theorem (`http://en.wikipedia.org/wiki/Fluctuation-dissipation_theorem`) that the PSD of a random thermal force, the driving term in the equation of motion, is

$$P_{xx}(F_R) = \left|\widetilde{F_R}\right|^2 = 4k_B T\gamma$$

where γ is the drag-coefficient of the particle.

Example: Diffusion

A massless particle undergoing free diffusion. The equation of motion is
$\gamma\dot{x} = F_R$ which Fourier transformed is $\gamma i\omega\tilde{x} = \widetilde{F_R}$ and leads to the PSD

$$P_{xx}(x) = |\tilde{x}|^2 = \frac{\left|\widetilde{F_R}\right|^2}{|i\gamma\omega|^2} = \frac{4k_B T\gamma}{\gamma^2\omega^2}$$

Example: Trapped massless particle

A massless particle undergoing diffusion and trapped by a harmonic spring has the equation of motion

$$\gamma\dot{x} + kx = F_R$$

which leads to

$$\gamma i\omega\tilde{x} + k\tilde{x} = \widetilde{F_R}$$

and for the PSD

$$|\tilde{x}|^2 = \frac{4k_B T\gamma}{k^2 + \gamma^2\omega^2}$$