5.E.2. The Spectral Density (Power Spectrum)

Consider a stochastic variable $\psi(t)$.

The experimental data on $\psi(t)$ is called a time series.

For time series of finite length T, we define

$$\psi(t\,;T) = \begin{cases} \psi(t) & -\frac{T}{2} \le t \le \frac{T}{2} \\ 0 & \text{otherwise} \end{cases}$$

with

$$\lim_{T\to\infty} \psi(t\,;T) = \psi(t)$$

The Fourier transform of $\psi(t\,;T)$ is

$$\begin{aligned} \tilde{\psi}(\omega\,;T) &= \int_{-\infty}^{\infty} d\,t\, e^{i\,\omega\,t}\, \psi(t\,;T) \\ &= \int_{-T/2}^{T/2} d\,t\, e^{i\,\omega\,t}\, \psi(t\,;T) \end{aligned} \tag{5.86}$$

Since $\psi(t\,;T)$ is real, we have

$$\tilde{\psi}^*(\omega\,;T) = \int_{-\infty}^{\infty} d\,t\, e^{-i\,\omega\,t}\, \psi(t\,;T) \;= \tilde{\psi}(-\omega\,;T)$$

The spectral density is defined as

$$S_{\psi,\,\psi}(\omega) = \lim_{T\to\infty} \frac{1}{T}\, \tilde{\psi}^*(\omega\,;T)\, \tilde{\psi}(\omega\,;T) \tag{5.87}$$

Using (5.86), we have

$$\begin{aligned} S_{\psi,\,\psi}(\omega) &= \lim_{T\to\infty} \frac{1}{T} \int_{-\infty}^{\infty} d\,t' \int_{-\infty}^{\infty} d\,t\; e^{-i\,\omega\,(t'-t)}\, \psi(t'\,;T)\, \psi(t\,;T) \\ &= \lim_{T\to\infty} \frac{1}{T} \int_{-\infty}^{\infty} d\,t \int_{-\infty}^{\infty} d\,\tau\, e^{-i\,\omega\,\tau}\, \psi(t+\tau\,;T)\, \psi(t\,;T) \qquad \tau = t' - t \\ &= \int_{-\infty}^{\infty} d\,\tau\, e^{-i\,\omega\,\tau} \langle\, \psi(t+\tau)\, \psi(t)\, \rangle_t \end{aligned} \tag{5.88}$$

where the time average is defined as

$$\langle\, f(t)\, \rangle_t = \lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{T/2} d\,t\; f(t) \tag{5.88a}$$

Hence,

$$\begin{aligned} \langle\, \psi(t+\tau)\, \psi(t)\, \rangle_t &= \lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{T/2} d\,t\, \psi(t+\tau\,;T)\, \psi(t\,;T) \\ &= \lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{T/2} d\,t\, \psi(t+\tau)\, \psi(t) \end{aligned} \tag{5.89}$$

where $\psi(t\,;T)$ are the measured values of ψ during one experiment.

For stationary (equilibrium) processes, we expect

$$\langle\, \psi(t+\tau)\, \psi(t)\, \rangle_t = \langle\, \psi(t+\tau)\, \psi(t)\, \rangle_\psi \equiv C_{\psi,\psi}(\tau) \tag{5.90}$$

where the ensemble average is defined as

$$\langle\, f(\psi)\, \rangle_\psi = \lim_{N\to\infty} \frac{1}{N} \sum_{i=1}^{N} f(\psi_i) \tag{5.90a}$$

with ψ_i being the measured value of ψ during the i^{th} experiment. Hence,

$$\langle \psi(t+\tau)\,\psi(t)\rangle_\psi = \lim_{N\to\infty}\frac{1}{N}\sum_{i=1}^{N}\psi_i(t+\tau)\,\psi_i(t) \tag{5.90b}$$

(5.88) thus becomes

$$\begin{aligned} S_{\psi,\psi}(\omega) &= \int_{-\infty}^{\infty} d\tau\, e^{-i\omega\tau}\langle \psi(t+\tau)\,\psi(t)\rangle_\psi \\ &= \int_{-\infty}^{\infty} d\tau\, e^{-i\omega\tau}\, C_{\psi,\psi}(\tau) \end{aligned} \tag{5.91}$$

The power spectrum is therefore simply the Fourier transform of the correlation function $C_{\psi,\psi}(\tau)$.

For the white noise described by (5.78) in §5.E.1,

$$\langle \xi(t+\tau)\,\xi(t)\rangle_\xi = g\,\delta(\tau)$$

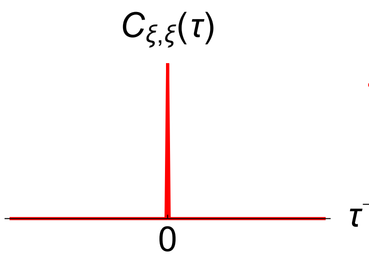
$$\to \qquad S_{\xi,\xi}(\omega) = g\; = 2\,\gamma\, k_B\, T \tag{5.92}$$

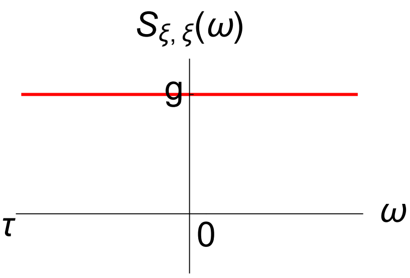
For the velocity correlation given by (5.84)

$$\Big\langle \langle v(t+\tau)\,v(t)\rangle_\xi \Big\rangle_T = \frac{k_B\,T}{m}\, e^{-(\gamma/m)\,|\tau|}$$

$$\begin{aligned} S_{v,v}(\omega) &= \frac{k_B\,T}{m}\left[\int_{-\infty}^{0} d\tau\, e^{-i\omega\tau}\, e^{(\gamma/m)\,\tau} + \int_{0}^{\infty} d\tau\, e^{-i\omega\tau}\, e^{-(\gamma/m)\,\tau}\right] \\ &= \frac{k_B\,T}{m}\left(\frac{1}{-i\,\omega+\frac{\gamma}{m}} + \frac{1}{i\,\omega+\frac{\gamma}{m}}\right) \\ &= \frac{k_B\,T}{m}\cdot\frac{2\,\gamma\,/m}{\omega^2+\frac{\gamma^2}{m^2}} \\ &= \frac{2\,\gamma\,k_B\,T}{m^2\,\omega^2+\gamma^2} \end{aligned} \tag{5.93}$$

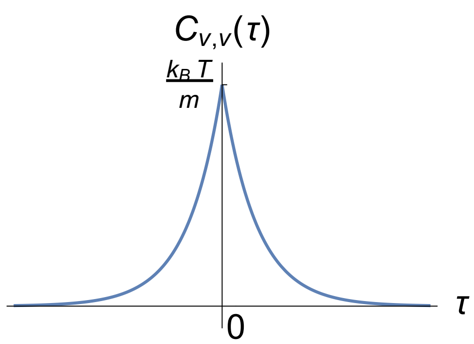
Plots of $C_{\xi,\xi}(\tau) = g\,\delta(\tau)$ and $S_{\xi,\xi}(\omega) = g$.





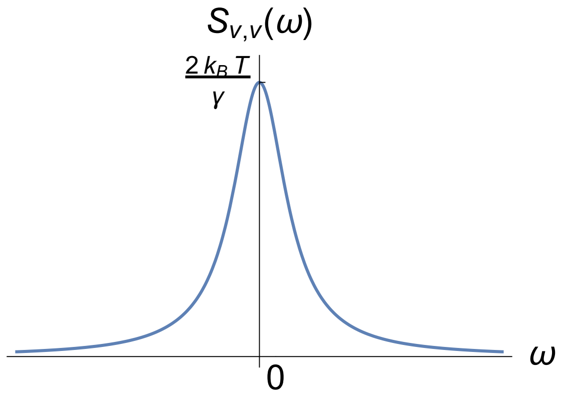
Plots of

$$C_{v,v}(\tau) = \frac{k_B\,T}{m}\, e^{-|\tau|\,\Gamma}\left\{\cosh\Delta\,|\tau| - \frac{\Gamma}{\Delta}\sinh\Delta\,|\tau|\right\}$$



and

$$S_{v,v}(\omega) = \frac{2\,\gamma\,k_B\,T}{m^2\,\omega^2 + \gamma^2}$$



Exercise 5.6

Compute the spectral density $S_{v,v}(\omega)$ for the harmonically bound Brownian particle considered in Exercise 5.5.

Plot the velocity correlation function $C_{v,v}(\tau)$ and spectral density $S_{v,v}(\omega)$ for the case $\omega_0 > \Gamma$, which corresponds an underdamped Brownian particle.

Answer

From Exercise 5.5,

$$\begin{aligned}
C_{v,v}(\tau) &= \left\langle \langle v(t+\tau)\,v(t)\rangle_\xi \right\rangle_T \\
&= \frac{k_B\,T}{m} e^{-|\tau|\Gamma}\left(\cosh\Delta\,|\tau| - \frac{\Gamma}{\Delta}\sinh\Delta\,|\tau|\right)
\end{aligned}$$

$$\begin{aligned}
\rightarrow \qquad S_{v,v}(\omega) &= \frac{k_B\,T}{m}\left[\int_{-\infty}^{0} d\tau\, e^{-i\,\omega\,\tau} e^{\tau\Gamma}\left(\cosh\Delta\,\tau + \frac{\Gamma}{\Delta}\sinh\Delta\,\tau\right)\right. \\
&\qquad \left. + \int_0^{\infty} d\tau\, e^{-i\,\omega\,\tau} e^{-\tau\Gamma}\left(\cosh\Delta\,\tau - \frac{\Gamma}{\Delta}\sinh\Delta\,\tau\right)\right] \\
&= \frac{k_B\,T}{m}\left[\int_0^{\infty} d\tau\, e^{i\,\omega\,\tau} e^{-\tau\Gamma}\left(\cosh\Delta\,\tau - \frac{\Gamma}{\Delta}\sinh\Delta\,\tau\right)\right. \\
&\qquad \left. + \int_0^{\infty} d\tau\, e^{-i\,\omega\,\tau} e^{-\tau\Gamma}\left(\cosh\Delta\,\tau - \frac{\Gamma}{\Delta}\sinh\Delta\,\tau\right)\right] \\
&= \frac{2\,k_B\,T}{m}\int_0^{\infty} d\tau\,\cos\omega\,\tau\; e^{-\tau\Gamma}\left(\cosh\Delta\,\tau - \frac{\Gamma}{\Delta}\sinh\Delta\,\tau\right)
\end{aligned}$$

For the underdamped case,

$$\Delta \equiv \sqrt{\Gamma^2 - \omega_0^2} = i\sqrt{\omega_0^2 - \Gamma^2} \equiv i\,\delta$$

$$\rightarrow \qquad S_{v,v}(\omega) = \frac{2\,k_B\,T}{m}\int_0^{\infty} d\tau\,\cos\omega\,\tau\; e^{-\tau\Gamma}\left(\cos\delta\,\tau - \frac{\Gamma}{\delta}\sin\delta\,\tau\right)$$

The integral can be evaluated using *Mathematica*, which gives

$$S_{v,v}(\omega) = \frac{4\,k_B\,T\,\Gamma\,\omega^2}{m\left(\Gamma^2 + (\delta-\omega)^2\right)\left(\Gamma^2 + (\delta+\omega)^2\right)}$$

$$= \frac{4 k_B T \gamma \omega^2}{m^2 (\omega^2 - 2 \omega \delta + \omega_0^2)(\omega^2 + 2 \omega \delta + \omega_0^2)}$$

Code

```
A = Assuming[Γ > 0 && δ > 0 && ω > 0, ∫_0^∞ Cos[ω τ] ⅇ^(-Γ τ) (Cos[δ τ] - Γ/δ Sin[δ τ]) ⅆτ]
```

$$\frac{2 \Gamma \omega^2}{(\Gamma^2 + (\delta - \omega)^2)(\Gamma^2 + (\delta + \omega)^2)}$$

```
A /. Γ → Sqrt[ω0^2 - δ^2] // Simplify
```

$$\frac{2 \omega^2 \sqrt{-\delta^2 + \omega_0^2}}{(\omega (-2 \delta + \omega) + \omega_0^2)(\omega (2 \delta + \omega) + \omega_0^2)}$$

Plots

```
(* C_{ξ,ξ}(τ) *)
delta[x_] := { 0   x ≠ 0
             { 1   x == 0
data = Table[{τ, delta[τ]}, {τ, -1, 1, .01}];
ListPlot[data,
      Axes → {True, False},
      AxesLabel → {"τ", "C_{ξ,ξ}(τ)"},
      AxesOrigin → {0, 0},
      Ticks → {{{0, "0"}}, {0}},
      Joined → True,
      PlotStyle → Red,
      PlotRange → {-.2, 1.1},
 PlotLabel → "C_{ξ,ξ}(τ)"]

(* S_{ξ,ξ}(ω) *)
Plot[1, {ω, -1, 1},
      AxesLabel → {"ω", "S_{ξ,ξ}(ω)"},
      AxesOrigin → {0, 0},
      Ticks → {{{0.1, "0", .001}}, {{1, "g"}}},
      PlotStyle → Red,
      PlotRange → {-.5, 1.3}]

(* C_{v,v}(τ) *)
Cvv[τ_] := ⅇ^(-Abs[τ]) (Cosh[τ] - Sinh[Abs[τ]]);
Plot[Cvv[τ], {τ, -3, 3},
      PlotRange → {-.1, 1.1},
      AxesLabel → {"τ", "C_{v,v}(τ)"},
      Ticks → {{{.2, "0", .001}}, {{1, "k_B T/m"}}}]
```

```
(* S_{v,v}(ω) *)
Svv[ω_, γ_] := γ/(ω^2 + γ^2);
γ = .4;
Plot[Svv[ω, γ], {ω, -3, 3},
     PlotRange → {- .1, 1.1 Svv[0, γ]},
     AxesLabel → {"ω", "S_{v,v}(ω)"},
     Ticks → {{{.2, "0", .001}}, {{Svv[0, γ], "(2 k_B T)/γ"}}}]
```