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

$$\tilde{\psi}(\omega\,;T) = \int_{-\infty}^{\infty} d\,t\, e^{i\,\omega\,t}\,\psi(t\,;T) \tag{5.86}$$

$$= \int_{-T/2}^{T/2} d\,t\, e^{i\,\omega\,t}\,\psi(t\,;T)$$

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

$$S_{\psi,\,\psi}(\omega) = \lim_{T\to\infty} \frac{1}{T}\int_{-\infty}^{\infty} d\,t'\int_{-\infty}^{\infty} d\,t\; e^{-i\,\omega\,(t'-t)}\,\psi(t'\,;T)\,\psi(t\,;T)$$

$$= \lim_{T\to\infty} \frac{1}{T}\int_{-\infty}^{\infty} d\,t\int_{-\infty}^{\infty} d\,\tau\, e^{-i\,\omega\,\tau}\,\psi(t+\tau\,;T)\,\psi(t\,;T) \qquad \tau = t' - t$$

$$= \int_{-\infty}^{\infty} d\,\tau\, e^{-i\,\omega\,\tau}\langle\,\psi(t+\tau)\,\psi(t)\,\rangle_t \tag{5.88}$$

where

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

$$= \lim_{T\to\infty} \frac{1}{T}\int_{-T/2}^{T/2} d\,t\,\psi(t+\tau)\,\psi(t)$$

For stationary (equilibrium) processes,

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

(5.88) thus becomes

$$S_{\psi,\,\psi}(\omega) = \int_{-\infty}^{\infty} d\,\tau\, e^{-i\,\omega\,\tau}\langle\,\psi(t+\tau)\,\psi(t)\,\rangle_\psi$$

$$= \int_{-\infty}^{\infty} d\,\tau\, e^{-i\,\omega\,\tau}\,C_{\psi,\psi}(\tau) \tag{5.91}$$

The power spectrum is therefore simply the Fourier transform of the correlation function.

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

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

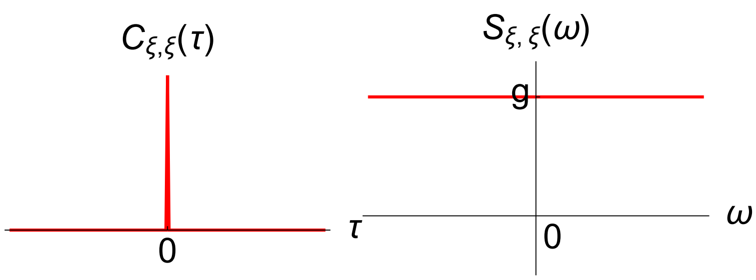
$$\to \qquad S_{\xi,\,\xi}(\omega) = g \;= 2\,\gamma\,k_B\,T \tag{5.92}$$

For the velocity correlation given by (5.84)

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

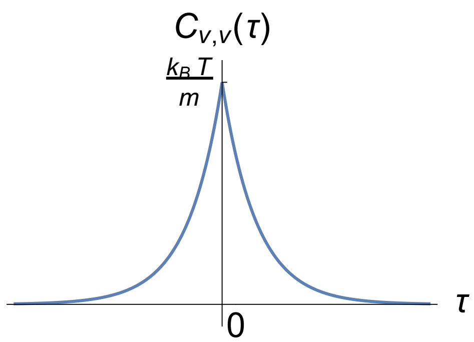
$$\begin{aligned}
S_{v,v}(\omega) &= \frac{k_B T}{m}\left[\int_{-\infty}^{0} d\tau\, e^{-i\omega\tau} e^{(\gamma/m)\tau} + \int_{0}^{\infty} d\tau\, e^{-i\omega\tau} e^{-(\gamma/m)\tau}\right] \\
&= \frac{k_B T}{m}\left(\frac{1}{-i\omega + \frac{\gamma}{m}} + \frac{1}{i\omega + \frac{\gamma}{m}}\right)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

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



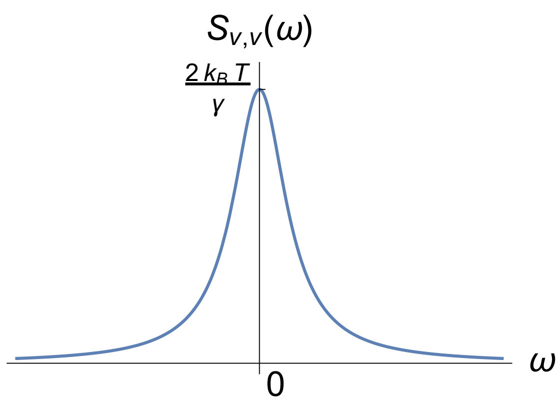
Plots of

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



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,

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

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

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

$$
\begin{aligned}
S_{v,v}(\omega) &= \frac{4 k_B T\, \Gamma\, \omega^2}{m \left(\Gamma^2 + (\delta - \omega)^2 \right) \left(\Gamma^2 + (\delta + \omega)^2 \right)} \\
&= \frac{4 k_B T\, \gamma\, \omega^2}{m^2 \left(\omega^2 - 2\,\omega\,\delta + \omega_0^2 \right) \left(\omega^2 + 2\,\omega\,\delta + \omega_0^2 \right)}
\end{aligned}
$$

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]
```

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

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

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

Plots

```
(* Cξ,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", "Cξ,ξ(τ)"},
      AxesOrigin → {0, 0},
      Ticks → {{{0, "0"}}, {0}},
      Joined → True,
      PlotStyle → Red,
      PlotRange → {-.2, 1.1},
 PlotLabel → "Cξ,ξ(τ)"]

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

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

(* Sv,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", "Sv,v(ω)"},
      Ticks → {{{.2, "0", .001}}, {{Svv[0, γ], "2 kB T/γ"}}}]
```