Lovesay

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Relation (B.38) is the so-called fluctuation dissipation theorem, for $S(\omega)$ is the spectrum of spontaneous fluctuation in the variable B, and the right-hand side is the response, or dissipation, of the target sample. We will explicitly verify that the right-hand side is the energy dissipation in a later development. More general forms of the theorem are given in § B.7.

If $\phi(t)$ is an odd function of t, the fluctuation dissipation theorem reduces to

$$S(\omega)=\{1+n(\omega)\}\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}t\,\sin(\omega t)\phi(t)$$
$$=\{1+n(\omega)\}\frac{1}{\pi}\chi''[\omega]. \tag{B.40}$$

The last form follows from the definition of the generalized susceptibility (B.5), and it is the form that is most useful in the interpretation of neutron scattering data. We now verify that $\phi(t)$ is an odd function of the time. Consider, for example, the coherent scattering in terms of the particle density fluctuations. In this instance

$$\hat{B}\equiv\hat{\rho}_{\boldsymbol{\kappa}}=\sum_j \exp(-\mathrm{i}\boldsymbol{\kappa}\cdot\hat{\mathbf{R}}_j), \tag{B.41}$$

where $\hat{\mathbf{R}}_j$ is the position operator of the jth particle. The correlation function of interest is

$$\langle\hat{\rho}_{\boldsymbol{\kappa}}\hat{\rho}^{+}_{\boldsymbol{\kappa}}(t)\rangle\equiv\langle\hat{\rho}_{\boldsymbol{\kappa}}\hat{\rho}_{-\boldsymbol{\kappa}}(t)\rangle.$$

For target samples that possess inversion symmetry, the correlation function depends on the magnitude of $\boldsymbol{\kappa}$ and not its direction, so that

$$\langle\hat{\rho}_{\boldsymbol{\kappa}}\hat{\rho}_{-\boldsymbol{\kappa}}(t)\rangle=\langle\hat{\rho}_{-\boldsymbol{\kappa}}\hat{\rho}_{\boldsymbol{\kappa}}(t)\rangle.$$

These results are sufficient to prove that the corresponding response function is an odd function of time.

The fluctuation dissipation theorem can be used to obtain $S(\omega)$ for a given model of $\chi''[\omega]$. For the damped harmonic oscillator model discussed in § B.3,

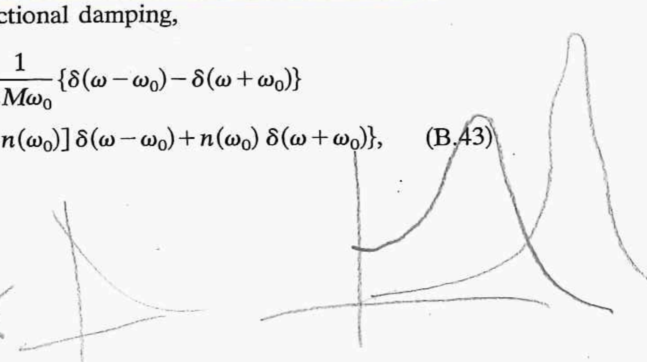
$$S(\omega)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\mathrm{d}t\,\exp(-\mathrm{i}\omega t)\langle\hat{x}\hat{x}(t)\rangle$$
$$=\{1+n(\omega)\}\frac{1}{\pi M}\frac{\gamma\omega}{\{(\omega^2-\omega_0^2)^2+(\gamma\omega)^2\}}. \tag{B.42}$$

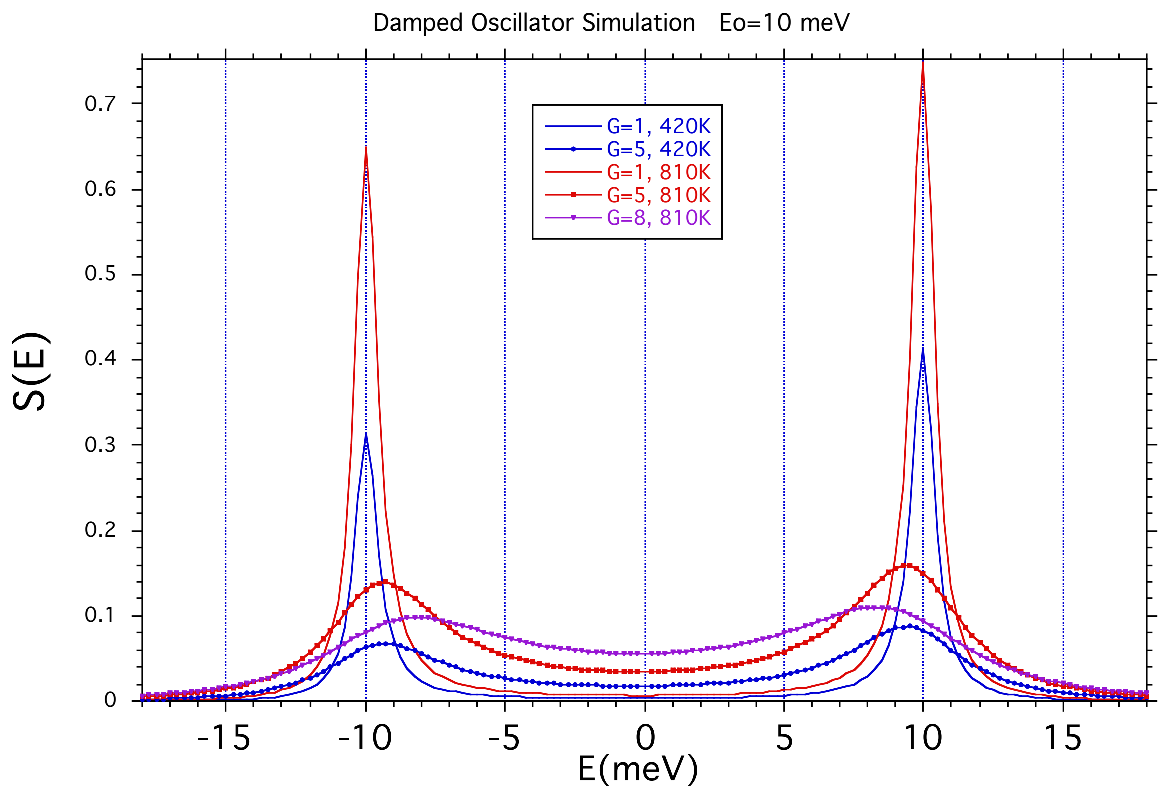
In the limit of vanishing frictional damping,

$$S(\omega)=\{1+n(\omega)\}\frac{1}{2M\omega_0}\{\delta(\omega-\omega_0)-\delta(\omega+\omega_0)\}$$
$$=\frac{1}{2M\omega_0}\{[1+n(\omega_0)]\,\delta(\omega-\omega_0)+n(\omega_0)\,\delta(\omega+\omega_0)\}, \tag{B.43}$$

$$\left(1+\frac{1}{e^{E/k_BT}-1}\right)$$

$k_B = 0.08617\ \mathrm{meV/K}$




Damped Oscillator Simulation Eo=10 meV
G=1, 420K
G=5, 420K
G=1, 810K
G=5, 810K
G=8, 810K
S(E)
E(meV)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
-15
-10
-5
0
5
10
15

Damped Harmonic Oscillator

$$S(\omega) = \{1 + n(\omega)\} \frac{1}{\pi M} \frac{\gamma\omega}{\{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2\}}$$

Bose population

$$\{1 + n(\omega)\} = \left| 1 + \frac{1}{\left(e^{\hbar\omega/k_B T} - 1\right)} \right|$$

where $k_B = 8.6173324 \times 10^{-5}$ eV/K

$= 0.086173324$ meV/K

Fit $I(E)$ as

Amplitude

Damping

$$\mathrm{ABS}\left[1 + \frac{1}{\exp(E/k_B T) - 1}\right] \frac{A\gamma E}{\left[(E^2 - E_p^2)^2 + \gamma^2 E^2\right]} \quad \left(+ \text{ offset of HERIX } E_0\right)$$

known temperature

phonon energy

Input: known temperature, Data

Fit: 4 parameters:

HERIX E_0 — $E=0$ position shifts at HERIX

E_p = phonon energy

A Amplitude $\doteq 1/\pi M$

γ = Damping coefficient