

[nex65] Spectral representation of dynamical quantities.

Consider a quantum Hamiltonian system with known eigenvalues and eigenvectors,

$$H|n\rangle = E_n|n\rangle, \quad n = 0, 1, \dots,$$

in thermal equilibrium at temperature T . Express (a) the structure function $S_{AA}(\omega)$, (b) the spectral density $\Phi_{AA}(\omega)$, (c) the dissipation function $\chi''_{AA}(\omega)$, and (d) the generalized susceptibility $\chi_{AA}(\omega + i\epsilon)$, all defined in [nln39], in terms of the temperature parameter $\beta = 1/k_B T$, the energy levels E_n , and the matrix elements $\langle n|A|m\rangle$. For simplicity assume that $\langle A \rangle \doteq Z^{-1} \text{Tr}[e^{-\beta H} A] = 0$. The last part uses the result of [nex63] and yields the result,

$$\chi_{AA}(\omega + i\epsilon) = \frac{1}{Z} \sum_{m,n} (e^{-\beta E_m} - e^{-\beta E_n}) \frac{|\langle n|A|m\rangle|^2}{\hbar\omega - (E_m - E_n) + i\hbar\epsilon}.$$

Solution: