"Many particle systems out of equilibrium" Problems, Series 9, 2006-07.

Problem 20. Fluctuation dissipation theorem

Consider a system described by the time dependent Hamiltonian $H = H_0 - A\phi(t)\theta(t - t_0)$, with A a Hermitean operator and ϕ a real function of time. For $t < t_0$ the system is in thermal equilibrium at temperature $1/(k_B\beta)$.

a) Show that, in linear response approximation, the time derivative of the average energy satisfies the equation

$$\langle \frac{dH}{dt} \rangle = -2i\dot{\phi}(t) \int_{t_0}^{t} d\tau \, M_{AA}(\tau)\phi(t - \tau). \tag{1}$$

b) Determine the response of the expectation values of A to driving fields $\phi(t) = \phi_0 \exp i\omega t$ and $\phi(t) = \phi_0 \exp -i\omega t$ respectively. From the fact that the response to the real field $\phi(t) = \phi_0 \cos \omega t$ has to be real, show that the following two identities hold:

$$Im[(\omega)] = Im[M_{AA}(-\omega)], \tag{2}$$

$$Re[M_{AA}(\omega)] = -Re[M_{AA}(-\omega)]. \tag{3}$$

c) Show that the average energy dissipated per unit time into the system in response to the field $\phi(t) = \phi_0 \cos \omega t$ is given by

$$Q(\omega) = \frac{\omega}{2\hbar}[1 - \exp(-\beta\hbar\omega)]S_{AA}(\omega)\phi_0^2. \tag{4}$$

Since this equation relates the dissipation in response to an oscillating field of frequency ω to the average strength of the Fourier components of the fluctuations in A, this relationship is called the *fluctuation dissipation theorem.* There are slight variations in the way this theorem is formulated. Extensions to relationships between S_{BA} and M_{BA} are also called fluctuation dissipation theorems.

How does the theorem generalize to the case of an arbitrary driving field, which is a superposition of fields at various frequencies?

Problem 21. Quantum mechanical dielectric response

We consider again a dilute gas consisting of diatomic molecules. We approximate these molecules as rigid rotors with a fixed moment of inertia $I = \mu_{rel}a^2$ with respect to the axis of rotation and a fixed electric dipole moment μ_0. Here $m_{rel} = m_1m_2/(m_1 + m_2)$ and a is the fixed distance between the atoms. The Hamiltonian of one such molecule is given by

$$H = H_{tr} + H_{rot}, \tag{5}$$

with the translational part given by

$$H_{tr} = -\frac{\hbar^2}{2M}\nabla^2_{\boldsymbol{R}} \tag{6}$$

and the rotational part by

$$H_{rot} = \frac{\boldsymbol{L}^2}{2I}, \tag{7}$$

with $M = m_1 + m_2$ the total mass of the molecule, $\boldsymbol{R} = (m_1\boldsymbol{r}_1 + m_2\boldsymbol{r}_2)/M$ the center of mass position operator and $\boldsymbol{L}$ the angular momentum operator.

a) What are the eigenvalues and eigenfunctions of H_{rot}?

b) Show that the dissipation function for a single molecule subject to a canonical distribution satisfies

$$\langle \dot{\mu}_z(0)|\mu_z(t)\rangle = \sum_l \frac{\mu_0^2(l+1)\omega_{l+1}}{3Z_{rot}}\cos(\omega_{l+1}t)\exp -\frac{\beta\hbar^2 l(l+1)}{2I}][1-\exp(-\beta\hbar\omega_{l+1})], \tag{8}$$

with $\omega_l = \hbar l/I$ and

$$Z_{rot} = \sum_l (2l+1)\exp -\frac{\beta\hbar^2 l(l+1)}{2I}. \tag{9}$$

(Hint: evaluate the trace involved by summing over the eigenfunctions of H_{rot}.)

c) Now assume again that the molecules collide with other molecules with a small collision frequency ν and express the frequency dependent dielectric constant in terms of a sum over the rotational quantum numbers l and m through a calculation analogous to that of problem 18c.

d) Determine the low temperature behavior of the dielectric constant (how does ν depend on temperature?) and show that for high temperatures the classical result found in problem 18c is recovered.

A useful relationship satisfied by spherical harmonics is

$$\cos\theta Y_l^m(\theta,\phi) = \left[\frac{(l+1)^2 - m^2}{(2l+1)(2l+3)}\right]^{\frac{1}{2}} Y_{l+1}^m(\theta,\phi) + \left[\frac{l^2 - m^2}{(2l-1)(2l+1)}\right]^{\frac{1}{2}} Y_{l-1}^m(\theta,\phi). \tag{10}$$

Another useful relationship is

$$\sum_{-l}^{l} m^2 = \frac{1}{3}(2l+1)(l+1)l.$$