Interaction representation.

In cases in which the Hamiltonian can be decomposed as $H(t) = H_0 + H_1(t)$ it is useful, especially when $H_1(t)$ is a small perturbation on H_0 to introduce:

$$|\psi_I(t)\rangle = e^{itH_0/\hbar} |\psi(t)\rangle$$

$$A_I(t) = e^{itH_0/\hbar} A \, e^{-itH_0/\hbar}$$

where $|\psi(t)\rangle$ and A are the Schrodinger representations of a state and an operator.

Under these conditions, the evolution equation for the state in the interaction representation is

$$i\hbar \frac{\partial |\psi_I(t)\rangle}{\partial t} = \underset{\substack{\uparrow \\ \text{the perturbation Hamiltonian in the} \\ \text{interaction representation}}}{H_{1I}(t)} |\psi_I(t)\rangle$$

The equation of motion can be formally integrated:

$$|\psi_I(t)\rangle = |\psi_I(t_0)\rangle - \frac{i}{\hbar}\int_{t_0}^{t} dt' \, H_{1I}(t') \, |\psi_I(t')\rangle$$

which then admits a formal solution by iteration, leading to

$$|\psi_I(t)\rangle = \underset{\substack{\uparrow \\ \text{time ordering operator when the exponential is} \\ \text{expanded in Taylor series.}}}{T} \exp\left\{ -\frac{i}{\hbar}\int_{t_0}^{t} dt' \, H_{1I}(t') \right\} |\psi_I(t_0)\rangle$$

The operator $U_I(t, t_0) = T \, e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt' H_{1I}(t')}$ is the evolution operator.

- The equation of motion for operators also follows, as is standard, from the commutator with the Hamiltonian. In the interaction representation:

$$i\hbar \frac{\partial}{\partial t} \rho_I = [H_{1I}, \rho_I]$$

We have written it for the density matrix in the interaction representation.

We define the non-equilibrium average of a quantity $m(\vec{r},t)$ ~~in the~~ as the quantum mechanical expectation value taken over the density matrix. In order to do so it is convenient to use the Heisenberg representation in which the density matrix is constant in time, and the operators are the quantities that evolve.

$$\langle m(\hat{r},t) \rangle_{NE} = \mathrm{Tr}\{\rho \, m_H(\hat{r},t)\} \quad \text{and} \quad \rho = \rho_{eq}$$

Interpret classically: average over distribution of initial conditions.

if, for example, the system was in equilibrium at the time the perturbation $H_1(t)$ was turned on.

This can be rewritten as:

Need to check this equation transforming interaction and Heisenberg rep's.

~~ES~~ I?

U is U_I as defined.

$$\langle m(\vec{r},t) \rangle_{NE} = \mathrm{Tr}\left\{\rho_{eq} \, U^{+}(t) \, m_I(\vec{r},t) \, U(t)\right\}$$

Linear response theory involves expanding the evolution operator only to first order in the interaction Hamiltonian:

$$\langle m(\vec{r},t) \rangle_{NE} = \mathrm{Tr}\, \rho_{eq}\left\{\left(1 + \frac{i}{\hbar}\int_{0}^{t} dt' \, H_{1I}(t')\right) m_I(\vec{r},t) \cdot \left(1 - \frac{i}{\hbar}\int_{0}^{t} dt' \, H_{1I}(t')\right)\right\}$$

(or $-\infty$)

Keeping only first order terms in H_1 we have:

$$\boxed{\langle m(\vec{r},t)\rangle_{NE} = \langle m\rangle_{eq} + \frac{i}{\hbar}\int_0^t dt' \left\langle \left[H_{1I}(t'), m_I(\vec{r},t)\right]\right\rangle_{eq}}$$

How to compute a non equilibrium average to first order in the perturbation

Often the interaction Hamiltonian linearly couples the order parameter (or operator here) and an externally imposed field that leads to the deviation from equilibrium. The hamiltonian of such a system is:

$$H = H_0 - \int d\vec{r}\; m(\vec{r},t)\, h(\vec{r},t) \qquad \Big(\text{"}m(r,t)\text{"} = -\frac{\delta H}{\delta h(r,t)}$$

the conjugate to the field.

and as described $\langle m(\vec{r},t)\rangle = Tr\left[\rho_{eq}\, m_H(\vec{r},t)\right]$

with $\rho_{eq} = \frac{1}{Z} e^{-\beta H_0}$

In this particular case we ~~have~~ can write: ((-) from $\frac{\delta H}{}$ $-mh$, (-) from reordering commutator)

$$\langle m(\vec{r},t)\rangle_{NE} = \langle m\rangle_{eq} + \frac{i}{\hbar}\int_0^t dt' \int d\vec{r}' \left\langle \left[m_I(\vec{r},t), m_I(\vec{r}',t')\, h(\vec{r}',t')\right]\right\rangle_{eq}$$

h is imposed externally

$$= \langle m\rangle_{eq} + \frac{i}{\hbar}\int_0^t dt' \int d\vec{r}' \left\langle \left[m_I(\vec{r},t), m_I(\vec{r}',t')\right]\right\rangle_{eq} \cdot h(\vec{r}',t')$$

This is conventionally written:

[illegible]

$$\underset{\langle m\rangle_{NE} - \langle m\rangle_{eq}}{\underset{\shortparallel}{\delta\langle m(\vec{r},t)\rangle}} = 2i\int_0^t dt' \int d\vec{r}'\; \chi''(\vec{r}-\vec{r}', t-t')\, h(\vec{r}',t')$$

$$\chi'' = \frac{1}{2\hbar} \left\langle \left[m_I(\vec{r},t), m_I(\vec{r}',t') \right] \right\rangle_{eq.}$$ the so called linear response function, or dynamic susceptibility.

More generally, in the case of a list of order parameters m_α and a list of external fields, one writes:

$$\delta \langle m_\alpha(\vec{r},t) \rangle = 2i \int_0^t dt' \int dr' \sum_{\beta} \chi''_{\alpha\beta}(\vec{r}-\vec{r}', t-t')\, h_\beta(\vec{r}',t')$$

with $$\chi''_{\alpha\beta}(\vec{r}-\vec{r}', t-t') = \frac{1}{2\hbar} \left\langle \left[m_{\alpha I}(\vec{r},t), m_{\beta I}(\vec{r}',t') \right] \right\rangle_{eq}$$

(*:) The important observation is that the non-equilibrium average can be written in terms of equilibrium averages.

(*:) The averages are over the equilibrium ensemble so that $\langle m_I \rangle_{eq} = \langle m \rangle_{eq}$, the second being the average with H_0.

→ the operators in $\langle [\ ,\ ] \rangle_{eq}$ evolve only with the evolution operator U_0 → they are fluctuations in equilibrium in the absence of external perturbations.

It is customary to introduce $\chi_{\alpha\beta}(\vec{r}-\vec{r}', t-t') = 2i\, \theta(t-t')\, \chi''_{\alpha\beta}(r-r',t$

and write $$\delta \langle m_\alpha(\vec{r},t) \rangle = \int_{-\infty}^{\infty} dt' \int d\vec{r}' \sum_\beta \chi_{\alpha\beta}(\vec{r}-\vec{r}', t-t') \cdot h_\beta(\vec{r}',t')$$

instead of zero. → $-\infty$

which can be Fourier transformed into:

$$\boxed{\langle \delta \hat{m}_\alpha \rangle(\vec{k},\omega) = \sum_\beta \hat{\chi}_{\alpha\beta}(\vec{k},\omega)\, \hat{h}_\beta(\vec{k},\omega)}$$

general expression for deviations from equilibrium linear in the applied field. The coefficient is the wavevector, frequency dependent susceptibility.

General notation: assume a Hamiltonian:

$$H_T(t) = H(t) - B(t)\,h(t)$$

We have in linear response:

$$\langle \delta A(t)\rangle = 2i\int_0^t dt'\,\chi''_{AB}(t,t')\,h(t')$$

with $\chi''_{AB}(tt') = \frac{1}{2\hbar}\langle [A(t), B(t')]\rangle_{eq}$.

$$\downarrow$$

$$\frac{\delta H}{\delta h(t)}$$

the derivative vs. the conjugate variable to the field.

(ROTON Homework)

Fluctuation-dissipation relation.-

Let us define the following equilibrium correlation function:

$$\bar{S}_{AB}(t-t') = \langle A(t)B(t')\rangle_{eq} =$$

$$= \frac{1}{Z}\,\mathrm{Tr}\left(e^{-\beta H} A(t)B(t')\right) = \frac{1}{Z}\,\mathrm{Tr}\left(e^{-\beta H} A(t)\, e^{\beta H} e^{-\beta H} B(t')\right)$$

[H is H_0, the time independent or equilibrium Hamiltonian]

~~By definition of the Heisenberg representation:~~ The time evolution of an operator:

$$A(t) = e^{itH/\hbar} A\, e^{-itH/\hbar}$$

so that $$e^{-\beta H} A(t)\, e^{\beta H} = e^{-\beta H} e^{itH/\hbar} A\, e^{-itH/\hbar} e^{\beta H}$$

$$= e^{i(t+i\beta\hbar)H/\hbar} A\, e^{-i(t+i\beta\hbar)H/\hbar} = A(t+i\beta\hbar)$$

Therefore:

$$\bar{S}_{AB}(t-t') = \frac{1}{Z}\,\mathrm{Tr}\left(A(t+i\beta\hbar)\, e^{-\beta H} B(t')\right)$$

Since $\mathrm{Tr}(ABC) = \mathrm{Tr}(CAB)$, we have.-

$$\bar{S}_{AB}(t-t') = \frac{1}{Z}\,\mathrm{Tr}\left(e^{-\beta H} B(t')\, A(t+i\beta\hbar)\right) = \bar{S}_{BA}(t'-t-i\beta\hbar$$

This leads to the following symmetry property.

$$\bar{S}_{AB}(\omega) = \int d(t-t')\, e^{i\omega(t-t')}\, \bar{S}_{AB}(t-t') =$$

$$= \int d(t-t')\, e^{i\omega(t-t')} \int \frac{d\omega}{2\pi}\, \bar{S}_{BA}(t'-t-i\beta\hbar) =$$

$$= \int d(t-t')\, e^{i\omega(t-t')} \int \frac{d\omega}{2\pi}\, \bar{S}_{BA}(\omega')\, e^{-i\omega'(t'-t-i\beta\hbar)} =$$

$$= \int \frac{d\omega}{2\pi}\, \bar{S}_{BA}(\omega') \int d(t-t')\, e^{i\omega(t-t')}\, e^{-i\omega'(t'-t)}\, e^{-\beta\hbar\omega'}$$

$$= \int \frac{d\omega}{2\pi}\, \bar{S}_{BA}(\omega')\, e^{-\beta\hbar\omega'} \underbrace{\int d(t-t')\, e^{i(t-t')(\omega+\omega')}}_{2\pi\,\delta(\omega+\omega')}$$

$$= \bar{S}_{BA}(-\omega)\, e^{+\beta\hbar\omega}$$

$$\rightarrow \quad \bar{S}_{AB}(\omega) = e^{+\beta\hbar\omega}\, \bar{S}_{BA}(-\omega)$$

excitation at frequency ω between A and B

energy difference in the excitation.

reverse excitation.

This is reminiscent of detailed balance.

By definition of response function (do not write the spectral integrals).

$$\chi''_{AB}(t-t') = \frac{1}{2\hbar}\langle [A(t), B(t')] \rangle = \frac{1}{2\hbar}\langle A(t)B(t') - B(t')A(t) \rangle$$

$$= \frac{1}{2\hbar}\left[\bar{S}_{AB}(t-t') - \bar{S}_{BA}(t'-t) \right]$$

If we Fourier transform:

$$\chi''_{AB}(\omega) = \frac{1}{2\hbar}\left[\bar{S}_{AB}(\omega) - \bar{S}_{BA}(-\omega) \right]$$

$$= \frac{1}{2\hbar}\left[\bar{S}_{AB}(\omega) - \bar{S}_{AB}(\omega)\, e^{-\beta\hbar\omega} \right] = \boxed{\frac{1-e^{-\beta\hbar\omega}}{2\hbar}\, \bar{S}_{AB}(\omega) = \chi''_{AB}(\omega}$$

→ the linear response function χ''_{AB} is proportional to the equilibrium correlation of fluctuations : fluctuation - dissipation relation.

At this point, one conventionally introduces a "symmetrized" correlation function:

$$S_{AB}(t-t') = \frac{1}{2}\left[\bar{S}_{AB}(t-t') + \bar{S}_{BA}(t'-t)\right]$$

$$\Rightarrow \quad S_{AB}(\omega) = \frac{1}{2}\left[\bar{S}_{AB}(\omega) + \bar{S}_{BA}(-\omega)\right] =$$

$$= \frac{1}{2}\bar{S}_{AB}(\omega)\left(1 + e^{-\beta\hbar\omega}\right)$$

$$\rightarrow \quad \chi''_{AB}(\omega) = \frac{1 - e^{-\beta\hbar\omega}}{\cancel{2}\hbar}\,\cancel{2}\,S_{AB}(\omega)\,\frac{1}{1+e^{-\beta\hbar\omega}} =$$

$\Rightarrow$ [illegible]

$$= \frac{1}{\hbar}\,\frac{e^{\beta\hbar\omega/2} - e^{-\beta\hbar\omega/2}}{e^{\beta\hbar\omega/2} + e^{-\beta\hbar\omega/2}}\cdot S_{AB}(\omega) \Rightarrow \frac{1}{\hbar}\tanh\left(\frac{\beta\hbar\omega}{2}\right)S_{AB}$$

~~Which the~~
~~imaginary part~~
~~of $\hat{X}$ earlier.~~
yes

or : $\boxed{S_{AB}(\omega) = \hbar\coth\left(\frac{\beta\hbar\omega}{2}\right)\chi''_{AB}(\omega)}$ a different version of the fluctuation–dissipation relation.

Classical limit $\rightarrow$ $S_{AB}(\omega) = \frac{2}{\beta\omega}\chi''_{AB}(\omega)$

Example: electric conductivity. –

Apply a slowly varying electric field $\vec{E}(t)$ to a set of charges. The ~~addition~~ energy is:

$$H_I = \sum_{i=1}^{N} q_i\,\phi(\vec{r}_i)$$ where $\phi(\vec{r})$ is the electrostatic potential.

$$= \int d^dx \sum_i q_i\,\delta(\vec{x}-\vec{r}_i)\,\phi(\vec{x}) =$$

$$= \int d^dx\,\rho(x)\,\phi(x)$$ where the density $\rho(x) = \sum_{i=1}^{N} q_i\,\delta(\vec{x}-\vec{r}_i)$

The imposed field and electrostatic potential are related through:

$$\vec{E}(\vec{x},t) = -\nabla\phi(\vec{x},t)$$