Linear-Response Theory, Kubo Formula, Kramers-Kronig Relations, and Fluctuation-Dissipation Theorem

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Abstract

In an informal way a somewhat lengthy presentation and proof of Linear-Response theory, Kubo Formula, Kramers-Kronig relations, and of the Fluctuation-Dissipation theorem is given.

1 Introduction

This is an informal paper, not intended for publication. The topics, linear-response theory, Kubo formula, Kramers-Kronig relations and fluctuation-dissipation theorem, are closely connected and belong to the most important and at the same time most complicated issues of quantum statistics. On the other hand, they belong partially to the set of canonical topics of any advanced lecture on statistical physics; i.e., any graduate student of physics should know them, since they are even contained in good dictionaries, although often in an insufficient way.

This gives reason enough for a short presentation by some kind of internal report, as short as possible and as long as necessary.

2 Basic definitions: Cause and Effect

Let us consider the Hamiltonian $\mathcal{H}$ of a system in thermal equilibrium, slightly perturbed at times $t' > t_0$ by a dynamical field (see below). Thus

$$\mathcal{H} = \mathcal{H}_0 - h(t) \cdot \hat{B}$$

Here $\mathcal{H}_0$ corresponds to thermodynamic equilibrium and the self-adjoint operator $\hat{B}$, together with the time-dependent real function $h(t)$, describes the perturbation, which is assumed to vanish for $t \leq t_0$.

As a consequence, for any self-adjoint operator $\hat{A}$ the expectation value is slightly perturbed out of thermodynamic equilibrium, and

$$\langle \hat{A} \rangle(t) = \langle \hat{A} \rangle_{\hat{\rho}_0} + \langle \delta \hat{A} \rangle(t)$$

where $\hat{\rho}_0$ is the statistical operator corresponding to thermodynamic equilibrium, e.g. $\hat{\rho}_0 = e^{-\beta \mathcal{H}_0}/Z(T)$. $T$ is the Kelvin temperature, $Z(T)$ the well-known partition function and $\beta = 1/(k_B T)$, with the Boltzmann constant $k_B$. 

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Now the last term in (2) depends linearly on the perturbation. Thus one can write
\[ \langle \hat{\delta} \hat{A} \rangle(t) = \int_{t_0}^{\infty} dt' X_{\hat{A},\hat{B}}(t - t') h(t') \] (3)

(Actually, because of causality, the upper integration limit, \( \infty \), can be replaced by \( t \), and the lower one, \( t_0 \), by \(-\infty \), if the perturbation is switched on adiabatically.)

The function \( X_{\hat{A},\hat{B}}(t - t') \) is (apart from a minus sign) identical with the retarded Green’s function \( G_{\hat{A},\hat{B}}(t - t') \), and, which is important, its Fourier transform is the generalized thermodynamic susceptibility \( \chi_{\hat{A},\hat{B}}(\omega) \), which plays a most-important role in the following.

All this is linear response theory, i.e. we have \( t > t' \), such that one can deliberately introduce a Heaviside function \( \Theta(t - t') \), where it is necessary. This fact is a simple expression of causality and means simply that cause, \( t' \), and effect, \( t \), are simply ordered as \( t' < t \).

3 The Kubo Formula

In fact, by perturbation, one gets easily by modification of the statistical operator (this is a typical exercise) the Kubo formula

\[ X_{\hat{A},\hat{B}}(\tau) = \frac{i}{\hbar} \Theta(\tau) \langle [\hat{A}(\tau), \hat{B}(0)] \rangle_{\hat{\rho}_0}. \] (4)

Here the time dependence of the operators is defined as in the interaction representation, i.e. with \( \mathcal{H}_0 \).

As above one defines the Fourier transformation of a function \( f(\tau) \) precisely as follows:

\[ f(\tau) = \int_{-\infty}^{\infty} d\omega \tilde{f}(\omega)e^{-i\omega \tau}, \] (5)

with

\[ \tilde{f}(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\tau f(\tau)e^{i\omega \tau} \] (6)

The shift of the factor \( 1/(2\pi) \) to the second term is useful for the form of the convolution theorem used below.

Namely the fact that in (4) the result can be written as a product of a function \( \Theta(\tau) \) times a function \( \langle [\hat{A}(\tau), ...] \rangle \) transfers to the following result, where the r.h.s. is a convolution in the \( \omega \)-space

\[ \chi_{\hat{A},\hat{B}}(\omega) = \frac{1}{2\pi \hbar} \int_{-\infty}^{\infty} d\omega' \frac{\langle ... \rangle(\omega')}{\omega' - \omega + i\epsilon} \] (7)

Here the terms in the denominator arises from the convoluted Fourier transform of the function \( \Theta(x) \).
4 Kramers-Kronig Relations

Now the Kramers-Kronig relations arise from the well-known dispersion relation

$$\frac{1}{x + i\epsilon} = CP \frac{1}{x} - i\pi \delta(x),$$

(8)

where $CP$ means the Cauchy principal part, $CP \int_{-\infty}^{\infty} \frac{dx}{x} f(x) := \left[ \int_{-\infty}^{-\epsilon} + \int_{\epsilon}^{\infty} \right] \frac{dx}{x} f(x)$. From this one gets the Kramers-Kronig relations, for example

$$\operatorname{Re} \chi_{\hat{A}, \hat{B}}(\omega) = -\frac{1}{\pi} CP \int_{-\infty}^{\infty} d\omega' \frac{\operatorname{Im} \chi_{\hat{A}, \hat{B}}(\omega')}{\omega' - \omega},$$

(9)

i.e. the real part is determined by the imaginary part and vice versa.

All this is well-known, but complicated. However, the most complicated part is still in front of us:

5 Fluctuation-Dissipation Theorem

Finally the fluctuations come into play. We define a Fluctuation Function

$$\phi_{\hat{A}, \hat{B}}(\tau) := \frac{1}{2} \cdot \langle \hat{A}(\tau)\hat{B}(0) + \hat{B}(0)\hat{A}(\tau) \rangle,$$

(10)

i.e., the non-commutivity of the operators is taken into account. The Fourier transform of this function is called as usual $\tilde{\phi}_{\hat{A}, \hat{B}}(\omega)$ Now, in a matrix representation, one has the following decomposition of the operator products $\hat{A}(\tau)\hat{B}(0)$:

$$\hat{A}(\tau)\hat{B}(0) = \sum_{m,n} A_{m,n}B_{n,m}e^{i\omega_{m,n}\tau},$$

(11)

(This so-called Lehmann-Szymanzik-Zimmermann decomposition arose 1955 from a famous paper in high energy physics). The indices $m$ and $n$ correspond to an arbitrary matrix representation of the operators $\hat{A}$ and $\hat{B}$, respectively, and again the interaction representation has been used. The quantity $\omega_{m,n}$ is of course defined as $(E_m - E_n)/\hbar$.

Applying the same decomposition systematically, and using the Fourier transform of the function $e^{i\omega_{m,n}\tau}$, which is $2\pi\delta(\omega_{m,n} + \omega)$, one finally gets the following relation between the dissipative part (i.e., usually the imaginary part, more precisely the even part of the frequency spectrum) of the susceptibility:

$$\tilde{\phi}_{\hat{A}, \hat{B}}(\omega) \equiv \hbar \cdot \cotanh\left(\frac{\beta\hbar\omega}{2}\right) \chi''_{\hat{A}, \hat{B}}(\omega),$$

(12)

where $\beta$ and $\hbar$ have their usual meaning, while the function $\cotanh(x)$ is the hyperbolic cotan. At low temperatures, the prefactor in front of $\chi''$ simplifies to $2k_B T/\omega$, with the Boltzmann constant $k_B$, i.e., the fluctuation spectrum is equal to the dissipation spectrum times $2k_B T/\omega$.

Here one implicitly assumes ergodicity; i.e., the theorem is not valid for glassy systems.
6 Applications

Applications of the equations are manifold. I only mention the *Einstein relation* between the diffusivity $D$ of a Brownian particle, the Kelvin temperature $T$ and the mobility $\mu$,

$$D = k_B T \mu . \quad (13)$$

Also Langevin equations, *white noise* and the noise spectrum of a resistor (Nyquist theory) are mentioned.

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Literature