Quantum fluctuation-dissipation theorem: a time domain formulation

Noëlle POTTIER
Groupe de Physique des Solides\textsuperscript{1}, Université Paris 7,
Tour 23, 2 place Jussieu, 75251 Paris Cedex 05, France,

and

Alain MAUGER
Laboratoire des Milieux Désordonnés et Hétérogènes\textsuperscript{2},
Université Paris 6, Tour 22, Case 86,
4 place Jussieu, 75252 Paris Cedex 05, France.

Abstract
A time-domain formulation of the equilibrium quantum fluctuation-dissipation theorem (FDT) in the whole range of temperatures is presented. In the classical limit, the FDT establishes a proportionality relation between the dissipative part of the linear response function and the derivative of the corresponding equilibrium correlation function. At zero temperature, the FDT takes the form of Hilbert transform relations between the dissipative part of the response function and the corresponding symmetrized equilibrium correlation function, which allows to establish a connection with analytic signal theory. The time-domain formulation of the FDT is especially valuable when out-of-equilibrium dynamics is concerned, as it is for instance the case in the discussion of aging phenomena.

PACS numbers:
05.30.-d Quantum statistical mechanics.

KEYWORDS:
Corresponding author:
Noëlle POTTIER
Groupe de Physique des Solides, Université Paris 7,
Tour 23, 2 place Jussieu, 75251 Paris Cedex 05, France
Fax number: +33 1 43 54 28 78. E-mail: pottier@gps.jussieu.fr

\textsuperscript{1} Laboratoire associé au C.N.R.S. (U.M.R. n° 7588) et aux Universités Paris 7 et Paris 6.
\textsuperscript{2} Laboratoire associé au C.N.R.S. (U.M.R. n° 7603) et à l’Université Paris 6.
1. Introduction

The fluctuation-dissipation theorem (FDT), valid for dynamic variables in equilibrium, is usually written in a form which involves generalized susceptibilities and spectral densities, which are frequency-dependent quantities [1]-[4]. However, in order to discuss certain time-dependent properties, it may be more convenient to have at hand a formulation of the theorem in the time domain. This need is for instance well illustrated in the discussion of aging effects in response and/or correlation functions of out-of-equilibrium dynamic variables. Then, the equilibrium FDT is a priori not applicable and has to be modified by the introduction of a violation factor or of an effective temperature, which can conveniently be defined in terms of time-dependent quantities [5]-[8].

Following arguments outlined in [3], we develop below in a direct and simple manner different ways in which the equilibrium quantum FDT can be formulated in the time domain. The corresponding expressions of the theorem, which are established in the whole range of temperatures, allow in particular for a discussion of both the classical limit [3] and the zero-temperature case. In this latter situation, an interesting connection, which does not seem to have been put forward previously, is shown to exist with analytic signal theory [9]-[10].

2. Time domain formulation of the equilibrium FDT

Let us consider here a system in equilibrium described in the absence of external perturbations by a time-independent hamiltonian $H_0$. In the following we will be concerned with equilibrium average values which we will denote as $\langle \ldots \rangle$, the symbol $\langle \ldots \rangle$ standing for $\text{Tr} \rho_0 \ldots$, with $\rho_0 = e^{-\beta H_0} / \text{Tr} e^{-\beta H_0}$.

Since we intend to discuss about linear response functions and symmetrized equilibrium correlation functions generically denoted as $\tilde{\chi}_{BA}(t,t')$ and $\tilde{C}_{BA}(t,t')$, we shall assume that the observables of interest $A$ and $B$ do not commute with $H_0$ (were it the case, the response function $\tilde{\chi}_{BA}(t,t')$ would indeed be zero). This hypothesis implies in particular that $A$ and $B$ are centered : $\langle A \rangle = 0$, $\langle B \rangle = 0$.

Generally speaking, the time domain formulations of the equilibrium FDT establish the link between the linear response function $\tilde{\chi}_{BA}(t,t')$ and the symmetrized equilibrium correlation function $\tilde{C}_{BA}(t,t') = \frac{1}{2} [\langle A(t')B(t) \rangle + \langle B(t)A(t') \rangle]$ (or the derivative $\partial \tilde{C}_{BA}(t,t')/\partial t'$).

2.1. The response function in terms of the correlation function

Consider two quantum-mechanical observables $A$ and $B$ with thermal equilibrium correlation functions verifying the property

$$\langle A(t' - i\hbar \beta)B(t) \rangle = \langle B(t)A(t') \rangle, \quad \beta = 1/kT, \quad (2.1)$$

and compute the contour integral

$$I = \oint_{\Gamma} \langle A(\tau)B(t) \rangle \frac{\pi}{\beta \hbar} \frac{1}{\sinh \frac{\pi(\tau - t')}{\beta \hbar}} d\tau \quad (2.2)$$
where \( t \) is a real time and \( \Gamma \) the closed contour in the complex \( \tau \)-plane represented on Fig. 1. One checks easily that the integrand in \( I \) does not present any singularities inside \( \Gamma \). Actually, denoting by \( |\lambda\rangle \) and \( E_\lambda \) the eigenstates and eigenenergies of the system hamiltonian \( H_0 \), one has

\[
\langle A(\tau)B(t) \rangle = \frac{1}{Z} \sum_{\lambda,\lambda'} A_{\lambda\lambda'} B_{\lambda'\lambda} e^{-\beta E_\lambda + i(\tau-t)(E_\lambda-E_{\lambda'})}, \quad Z = \text{Tr} e^{-\beta H_0},
\]

(2.3)

which displays the fact that the continuation to the region \(-\beta \leq \Im \tau \leq 0\) of the complex \( \tau \)-plane of the correlation function \( \langle A(\tau)B(t) \rangle \) is analytic [3], [11].

According to the Cauchy theorem, the integral \( I \) is thus equal to zero. In the limit \( R \to \infty \), one obtains, by gathering the various contributions to \( I \), the relation

\[
i\pi \left[ \langle B(t)A(t') \rangle - \langle A(t')B(t) \rangle \right] = \text{vp} \int_{-\infty}^{\infty} dt'' \left[ \langle A(t'')B(t) \rangle + \langle B(t)A(t'') \rangle \right] \frac{\pi}{\beta\hbar} \frac{1}{\sinh \pi(t''-t')} \frac{1}{\beta\hbar},
\]

(2.4)

where the symbol \( \text{vp} \) denotes the Cauchy principal value. Taking into account the Kubo formula for the response function, one gets from Eq. (2.4) the expression

\[
\tilde{\chi}_{BA}(t, t') = \frac{2}{\pi\hbar} \Theta(t-t') \text{vp} \int_{-\infty}^{\infty} dt'' \tilde{C}_{BA}(t, t'') \frac{\pi}{\beta\hbar} \frac{1}{\sinh \pi(t''-t')} \frac{1}{\beta\hbar},
\]

(2.5)

where \( \Theta(t) \) denotes the unit step-function.

Eq. (2.5) allows to compute the response function \( \tilde{\chi}_{BA} \) in terms of the symmetrized correlation function \( \tilde{C}_{BA} \). Then, introducing the dissipative part \( \tilde{\xi}_{BA} \) of \( \tilde{\chi}_{BA} \), as defined by

\[
\tilde{\chi}_{BA}(t, t') = 2i \Theta(t-t') \tilde{\xi}_{BA}(t, t'),
\]

(2.6)

one gets from Eq. (2.5):

\[
i\hbar \tilde{\xi}_{BA}(t, t') = \frac{1}{\pi} \text{vp} \int_{-\infty}^{\infty} dt'' \tilde{C}_{BA}(t, t'') \frac{\pi}{\beta\hbar} \frac{1}{\sinh \pi(t''-t')} \frac{1}{\beta\hbar}.
\]

(2.7)

Since the two-time equilibrium averages involved in \( \tilde{\xi}_{BA} \) and \( \tilde{C}_{BA} \) only depend on the time differences involved, Eq. (2.7) can be rewritten as a convolution product, that is

\[
i\hbar \tilde{\xi}_{BA}(t) = \frac{1}{\pi} \tilde{C}_{BA}(t) * \text{vp} \frac{\pi}{\beta\hbar} \frac{1}{\sinh \pi t} \frac{1}{\beta\hbar},
\]

(2.8)

the convolution in the r.h.s. being taken with respect to \( t \).
2.2. The correlation function in terms of the response function

The expression of the correlation function in terms of the response function can be derived, either in the same way as above (i.e. by using contour integration), or by inverting the convolution product (2.8).

Compute on the contour $\Gamma$ (Fig. 1) the integral

$$J = \oint_{\Gamma} \langle A(\tau)B(t) \rangle \frac{\pi}{\beta \hbar} \coth \frac{\pi(\tau - t)}{\beta \hbar} d\tau.$$ \hspace{1cm} (2.9)

Using similar arguments as above (i.e. noticing that $J = 0$ since there are no singularities of the integrand of $J$ inside $\Gamma$), one obtains the relation

$$\frac{1}{2} [\langle A(t')B(t) \rangle + \langle B(t)A(t') \rangle] =$$

$$-\frac{i}{2\pi} \text{vp} \int_{-\infty}^{\infty} dt'' \left[ \langle B(t)A(t'') \rangle - \langle A(t'')B(t) \rangle \right] \frac{\pi}{\beta \hbar} \coth \frac{\pi(t'' - t)}{\beta \hbar},$$ \hspace{1cm} (2.10)

that is

$$\tilde{C}_{BA}(t, t') = -\frac{\hbar}{2\pi} \text{vp} \int_{-\infty}^{\infty} dt'' \left[ \tilde{\chi}_{BA}(t, t'') - \tilde{\chi}_{AB}(t'', t) \right] \frac{\pi}{\beta \hbar} \coth \frac{\pi(t'' - t)}{\beta \hbar},$$ \hspace{1cm} (2.11)

or

$$\tilde{C}_{BA}(t, t') = -\frac{1}{\pi} \text{vp} \int_{-\infty}^{\infty} dt'' i\hbar \tilde{\xi}_{BA}(t, t'') \frac{\pi}{\beta \hbar} \coth \frac{\pi(t'' - t)}{\beta \hbar}.$$ \hspace{1cm} (2.12)

Before going further, let us add a comment. The arguments which have previously been used in the computation of the integral $I$ must be refined in order to show, first, that the integrals in the r.h.s. of Eqs. (2.10)-(2.12) are properly defined, and, second, that the contributions to the integral $J$ (Eq. (2.9)) of the two vertical segments of abscissas $R$ and $-R$ of the contour $\Gamma$ (Fig. 1) do vanish in the limit $R \to \infty$. The question stems from the fact that the function $\coth(\pi t/\beta \hbar)$ tends towards a finite limit for large values of its argument, contrary to the function $1/\sinh(\pi t/\beta \hbar)$ involved in the computation of $I$, which tends towards zero (this latter property insuring that the integrals in the r.h.s. of Eqs. (2.4), (2.5) and (2.7) are properly defined and that the contribution to $I$ of the above-mentioned segments is actually zero in the limit $R \to \infty$).

A sufficient condition is $\lim_{R \to \infty} \langle A(\pm R - i\hbar y)B(t) \rangle = \langle A \rangle \langle B \rangle$ ($= 0$ since $A$ and $B$ are centered)$^{1}$. Thus, when treating systems with a finite number of degrees of freedom, and oscillating response and correlation functions, in which case this limit does not even exist, it will be convenient to introduce a small damping which will be eventually let equal to zero, or, which amounts to the same, to treat the response and correlation functions as distributions. Further details will be provided when treating the harmonic oscillator example (Section 2.4).

$^{1}$ Note that for $y = 0$ this condition amounts to $\lim_{R \to \infty} \langle A(\pm R)B(t) \rangle = 0$ while for $y = \beta$ it amounts to $\lim_{R \to \infty} \langle B(t)A(\pm R) \rangle = 0$. 
Eq. (2.12) can be viewed as the reciprocal of Eq. (2.7), since it allows to compute the symmetrized correlation function $\tilde{C}_{BA}$ in terms of the dissipative part $\tilde{\xi}_{BA}$ of $\tilde{\chi}_{BA}$. It can be rewritten, using convolution product notations, as

$$\tilde{C}_{BA}(t) = -\frac{1}{\pi} i\hbar \tilde{\xi}_{BA}(t) * \frac{\pi}{\beta\hbar} \text{vp} \coth \frac{\pi t}{\beta\hbar}. \tag{2.13}$$

Note that this latter expression can also be obtained directly by inverting the convolution product (2.8), which is easily done by using the relation

$$\frac{\pi}{\beta\hbar} \text{vp} \frac{1}{\sinh \frac{\pi t}{\beta\hbar}} * \frac{\pi}{\beta\hbar} \text{vp} \coth \frac{\pi t}{\beta\hbar} = -\pi^2 \delta(t), \tag{2.14}$$
demonstrated in Appendix A.

Eq. (2.8) together with the inverse relation (2.13) constitute a formulation of the equilibrium FDT in the time domain.

2.3. Relation with the usual frequency domain formulation

Eqs. (2.8) and (2.13) just correspond by Fourier transformation to the usual fluctuation-dissipation relations between the dissipative part $\xi_{BA}(\omega)$ of the susceptibility and the Fourier transform $C_{BA}(\omega)$ of the symmetrized correlation function [1]-[4]:

$$\xi_{BA}(\omega) = \frac{1}{\hbar} \tanh \frac{\beta\hbar\omega}{2} C_{BA}(\omega), \quad C_{BA}(\omega) = \hbar \coth \frac{\beta\hbar\omega}{2} \xi_{BA}(\omega). \tag{2.15}$$

Indeed, taking the Fourier transform of formulas (2.15), with the following definition of the Fourier transformation $F(\omega) = \int_{-\infty}^{\infty} dt \tilde{F}(t) e^{i\omega t}$, $\tilde{F}(t) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega C_{BA}(\omega) e^{-i\omega t}$, and making use of the Fourier formulas (A.3) and (A.6), one obtains Eqs. (2.8) and (2.13), rewritten below for clarity:

$$i\hbar \tilde{\xi}_{BA}(t) = \frac{1}{\pi} \tilde{C}_{BA}(t) * \frac{\pi}{\beta\hbar} \text{vp} \frac{1}{\sinh \frac{\pi t}{\beta\hbar}}, \quad \tilde{C}_{BA}(t) = -\frac{1}{\pi} i\hbar \tilde{\xi}_{BA}(t) * \frac{\pi}{\beta\hbar} \text{vp} \coth \frac{\pi t}{\beta\hbar}. \tag{2.16}$$

2.4. A basic example: the harmonic oscillator

Let us consider as a basic example a harmonic oscillator of mass $m$ and angular frequency $\omega_0$, in thermal equilibrium at temperature $T$. The oscillator displacement being denoted by $x$, one has

$$\langle x(t)x \rangle = \frac{\hbar}{2m\omega_0} \left[ (1 + n) e^{-i\omega_0 t} + n e^{i\omega_0 t} \right] \tag{2.17}$$

and

$$\langle xx(t) \rangle = \frac{\hbar}{2m\omega_0} \left[ n e^{-i\omega_0 t} + (1 + n) e^{i\omega_0 t} \right], \tag{2.18}$$
where $n = 1/(e^{\beta \hbar \omega} - 1)$ is the Bose-Einstein function at temperature $T$. One deduces from Eqs. (2.17) and (2.18) the expressions of $\tilde{\xi}_{xx}(t)$ and $\tilde{C}_{xx}(t)$:

$$i\hbar \tilde{\xi}_{xx}(t) = \frac{\hbar}{2m\omega_0} \sin \omega_0 t$$

and

$$\tilde{C}_{xx}(t) = \frac{\hbar}{2m\omega_0} \coth \frac{\beta \hbar \omega_0}{2} \cos \omega_0 t.$$  \hspace{1cm} (2.19)

The fluctuation-dissipation relations (2.8) and (2.13) respectively read:

$$\sin \omega_0 t = \frac{1}{\pi} \coth \frac{\beta \hbar \omega_0}{2} \cos \omega_0 t * \frac{\pi}{\beta \hbar} \text{vp} \frac{1}{\sinh \frac{\pi t}{\beta \hbar}}$$

and

$$\coth \frac{\beta \hbar \omega_0}{2} \cos \omega_0 t = -\frac{1}{\pi} \sin \omega_0 t * \frac{\pi}{\beta \hbar} \text{vp} \coth \frac{\pi t}{\beta \hbar}.$$ \hspace{1cm} (2.21)

Both formulas can be easily checked by a direct calculation, which we report in Appendix B, together with supplementary details\(^2\) on the contour integration needed to compute the integral $J$ (Eq. (2.9)).

Now, coming back to the general case, let us discuss, first the classical limit, then the zero-temperature case.

### 3. The classical limit

Before entering the discussion of this limit, we shall propose another form of the first FDT relation (Eqs. (2.7) or (2.8)) in the time domain. It gives the expression of the linear response function in terms of the derivative of the equilibrium correlation function [3], and reveals to be especially useful when studying the classical limit.

#### 3.1. Expression of the response function in terms of the derivative of the correlation function

Integrating by parts, one can recast Eq. (2.7) into the equivalent form

$$i\hbar \tilde{\xi}_{BA}(t, t') = \frac{1}{\pi} \int_{-\infty}^{\infty} dt'' \frac{\partial \tilde{C}_{BA}(t, t'')}{\partial t'} \log \left| \coth \frac{\pi (t'' - t')}{2\beta \hbar} \right|,$$ \hspace{1cm} (3.1)

or, making use of convolution product notations since $\tilde{\xi}_{BA}$ and $\tilde{C}_{BA}$ only depend on the time differences involved,

$$i\hbar \tilde{\xi}_{BA}(t) = -\frac{1}{\pi} \frac{d \tilde{C}_{BA}(t)}{dt} \log \left| \coth \frac{\pi t}{2\beta \hbar} \right|.$$  \hspace{1cm} (3.2)

\(^2\) See the remarks in Section 2.2.
an expression equivalent to Eq. (2.8). Thus, at any temperature, the dissipative part of the response function (i.e. the function $\tilde{\xi}_{BA}(t)$) appears to be proportional to the convolution product taken with respect to $t$ of the functions $d\tilde{C}_{BA}(t)/dt$ and $\log|\coth(\pi t/2\beta\hbar)|$. This latter function is very peaked around $t = 0$ at high temperature while it becomes more and more spread around this value as the temperature decreases.

### 3.2. The classical limit
In the classical limit, making use of the property (A.14), that is

$$\log|\coth ax| \sim_{|a| \to \infty} \frac{\pi^2}{4|a|} \delta(x),$$

with $a = \pi/2\beta\hbar$, one shows that Eq. (3.2) reduces to

$$i\hbar \tilde{\xi}_{BA}(t) = -\beta\hbar \frac{d\tilde{C}_{BA}(t)}{dt},$$

which yields for the associated response function $\tilde{\chi}_{BA}(t, t')$ the expression

$$\tilde{\chi}_{BA}(t, t') = \beta \Theta(t - t') \frac{\partial \tilde{C}_{BA}(t', t)}{\partial t'}.$$ (3.5)

Eq. (3.5) constitutes the expression of the classical equilibrium fluctuation-dissipation theorem in the time domain [3].

### 3.3. Illustration: the harmonic oscillator
One easily checks that Eq. (3.4) is actually verified by the functions $\tilde{\xi}_{xx}(t)$ as given by Eq. (2.19) and $\tilde{C}_{xx}(t)$ as given by the classical limit of Eq. (2.20), namely

$$\tilde{C}_{xx}(t) = \frac{kT}{m\omega_0^2} \cos \omega_0 t.$$ (3.6)

### 4. The zero temperature case

#### 4.1. The zero-temperature fluctuation-dissipation theorem
As the temperature decreases, the function $\log|\coth(\pi t/2\beta\hbar)|$ becomes more and more spread around $t = 0$. At $T = 0$, coming back to the formulation (2.16) of the FDT, one gets

$$i\hbar \tilde{\xi}_{BA}(t) = \frac{1}{\pi} \tilde{C}_{BA}(t) * \text{vp} \frac{1}{t}, \quad \tilde{C}_{BA}(t) = -\frac{1}{\pi} i\hbar \tilde{\xi}_{BA}(t) * \text{vp} \frac{1}{t},$$

that is

$$-i\hbar \tilde{\xi}_{BA}(t) = \frac{1}{\pi} \text{vp} \int_{-\infty}^{\infty} \tilde{C}_{BA}(t') \frac{1}{t' - t} dt',$$ (4.1)
and
\[ \tilde{C}_{BA}(t) = -\frac{1}{\pi} \text{vp} \int_{-\infty}^{\infty} \frac{(-i\hbar \xi_{BA}(t'))}{t' - t} \, dt'. \]  
(4.3)

Interestingly enough, these Hilbert transformation relations, which constitute the formulation of the fluctuation-dissipation theorem in the time domain at zero temperature, are formally similar to the usual Kramers-Kronig relations between the real and imaginary parts of the generalized susceptibility, except for the evident fact that they hold in the time domain and not in the frequency domain. Otherwise stated, at \( T = 0 \), the quantities \( \tilde{C}_{BA}(t) \) and \(-i\hbar \tilde{\xi}_{BA}(t)\) must constitute respectively the real and imaginary parts of an analytic signal \( \tilde{Z}_{BA}(t) \) with only positive frequency Fourier components \([9]-[10]\).

4.2. The zero-temperature analytic signal

Following these lines, consider the signal \( \tilde{Z}_{BA}(t) = \langle B(t)A \rangle \). One has
\[ \tilde{Z}_{BA}(t) = \tilde{C}_{BA}(t) + \hbar \tilde{\xi}_{BA}(t), \]  
(4.4)
which displays the fact that \( \tilde{Z}_{BA}(t) \) has for real part \( \tilde{C}_{BA}(t) \) and for imaginary part \(-i\hbar \tilde{\xi}_{BA}(t)\). By Fourier transformation, one gets
\[ Z_{BA}(\omega) = C_{BA}(\omega) + \hbar \xi_{BA}(\omega). \]  
(4.5)

At \( T = 0 \), the fluctuation-dissipation relations (2.15) reduce to
\[ \xi_{BA}(\omega) = \frac{1}{\hbar} \text{sgn}(\omega) C_{BA}(\omega), \]  
(4.6)
with
\[ \text{sgn}(\omega) = \begin{cases} +1, & \omega > 0, \\ -1, & \omega < 0, \end{cases} \]  
(4.7)
so that one gets, as expected,
\[ Z_{BA}(\omega) = \begin{cases} 2C_{BA}(\omega), & \omega > 0, \\ 0, & \omega < 0. \end{cases} \]  
(4.8)

Actually, at \( T = 0 \), the function \( \tilde{Z}_{BA}(t) = \langle B(t)A \rangle \) has only positive frequency components and thus possesses the characteristics of an analytic signal \([9]-[10]\). This implies that the integral definition \( \tilde{Z}_{BA}(\tau) = \int_{0}^{\infty} Z_{BA}(\omega)e^{-i\omega\tau} \, d\omega/2\pi \) can then be extended in the whole lower half of the complex \( \tau \)-plane\(^3\) (i.e. \( \Im \tau \leq 0 \)).

In the same way, consider the function \( \tilde{Y}_{BA}(t) = \langle AB(t) \rangle \). One has:
\[ \tilde{Y}_{BA}(t) = \tilde{C}_{BA}(t) - \hbar \xi_{BA}(t). \]  
(4.9)

\(^3\) This is in accordance with the above noted fact that at finite temperature the prolongation to the region \(-\beta \leq \Im \tau \leq 0 \) of the complex \( \tau \)-plane of the correlation function \( \langle B(\tau)A \rangle \) is analytic.
At $T = 0$, making use of the fluctuation-dissipation relations (2.15), one gets

$$Y_{BA}(\omega) = \begin{cases} 0, & \omega > 0, \\ 2C_{BA}(\omega), & \omega < 0. \end{cases} \quad (4.10)$$

Thus, the function $\tilde{Y}_{BA}(t) = \langle AB(t) \rangle$ possesses only negative frequency components. The integral definition $\tilde{Y}_{BA}(\tau) = \int_0^\infty Y_{BA}(\omega)e^{-i\omega\tau}d\omega/2\pi$ can be extended in the whole upper half of the complex $\tau$-plane (i.e. $\Im \tau \geq 0$).

### 4.3. Other representations of the analytic signal

Let us here focus on the analytic signal $\tilde{Z}_{BA}(t)$ of positive frequency components (similar considerations can be made for $\tilde{Y}_{BA}(t)$).

For $\Im \tau \leq 0$, one can write, taking advantage of Eqs. (4.6) and (4.8),

$$\tilde{Z}_{BA}(\tau) = \frac{1}{2\pi} \int_0^\infty d\omega \, 2\hbar \xi_{BA}(\omega) e^{-i\omega \tau}. \quad (4.11)$$

This yields the following representation of $\tilde{Z}_{BA}(\tau)$ for $\Im \tau \leq 0$ in terms of the dissipative part $\xi_{BA}(t)$ of the response function:

$$\tilde{Z}_{BA}(\tau) = \frac{1}{\pi} \int_{-\infty}^{\infty} dt' \left(-i\hbar \xi_{BA}(t')\right) \frac{1}{\tau - t'}. \quad (4.12)$$

Note that, when $\Im \tau = 0$, the integral in Eq. (4.12) must be understood as a principal value.

Eq. (4.12) can in turn be used as a definition of $\tilde{Z}_{BA}(\tau)$ in the upper half of the complex $\tau$-plane (i.e. $\Im \tau > 0$), where the integral definition $\tilde{Z}_{BA}(\tau) = \int_0^\infty Z_{BA}(\omega)e^{-i\omega\tau}d\omega/2\pi$ cannot be used. It verifies the property

$$Z_{BA}^*(\tau) = Z_{BA}(\tau^*). \quad (4.13)$$

### 4.4. Illustration: the harmonic oscillator

Let us consider once again the harmonic oscillator of mass $m$, angular frequency $\omega_0$ and displacement $x$, in thermal equilibrium at $T = 0$.

At $T = 0$, the equilibrium correlation functions $\tilde{Z}_{xx}(t) = \langle x(t)x \rangle$ and $\tilde{Y}_{xx}(t) = \langle xx(t) \rangle$ are given by

$$\tilde{Z}_{xx}(t) = \frac{\hbar}{2m\omega_0} e^{-i\omega_0 t} \quad (4.14)$$

and

$$\tilde{Y}_{xx}(t) = \frac{\hbar}{2m\omega_0} e^{i\omega_0 t}. \quad (4.15)$$

Thus $\tilde{Z}_{xx}(t)$ is a monochromatic signal of angular frequency $\omega_0$ and of Fourier spectrum

$$Z_{xx}(\omega) = \frac{\hbar}{m\omega_0} \pi \delta(\omega - \omega_0), \quad (4.16),$$
while, similarly, \( \tilde{Y}_{xx}(t) \) is a monochromatic signal of angular frequency \(-\omega_0\) and of Fourier spectrum
\[
Y_{xx}(\omega) = \frac{\hbar}{m\omega_0} \pi \delta(\omega + \omega_0).
\] (4.17)

The Hilbert transformation relations (4.1) between \( \tilde{C}_{xx}(t) \) and \(-i\hbar \tilde{\xi}_{xx}(t)\) read:
\[
\sin \omega_0 t = \frac{1}{\pi} \cos \omega_0 t * \text{vp} \frac{1}{t}, \quad \cos \omega_0 t = -\frac{1}{\pi} \sin \omega_0 t * \text{vp} \frac{1}{t}.
\] (4.18)

The representation (4.12) of \( \tilde{Z}_{xx}(\tau) \) in the complex \( \tau \)-plane reads:
\[
\tilde{Z}_{xx}(\tau) = \begin{cases} 
\frac{\hbar}{2m\omega_0} e^{i\omega_0 \tau}, & \Re \tau > 0, \\
\frac{\hbar}{2m\omega_0} e^{-i\omega_0 \tau}, & \Re \tau \leq 0.
\end{cases}
\] (4.19)

5. Discussion and conclusion

Clearly, the time domain formulation of the equilibrium fluctuation-dissipation theorem is completely equivalent to the widely used frequency form of the theorem. In the classical limit, the time domain formulation establishes a proportionality relation between the dissipative part of the response function and the derivative of the equilibrium correlation function. At zero temperature, it takes the form of Hilbert transformation relations between the dissipative part of the response function and the symmetrized equilibrium correlation function.

The time domain formulation is of considerable help in discussing out-of-equilibrium phenomena. A good illustration of that can be found in the discussion of aging effects. For instance, in a recent paper [8], we have studied these effects as displayed by the correlation function of the displacement \( x(t) - x(t_0) \) of a free quantum Brownian particle with respect to its position at a given time \( t_0 \). Indeed, since diffusion is going on, the variable \( x(t) - x(t_0) \) never attains equilibrium. For any times \( t \) and \( t' \) such that \( t_0 \leq t \leq t' \), the displacement correlation function \( C_{xx}(t, t'; t_0) \) depends both on the time difference \( t - t' \) and on the waiting time or age \( t_w = t' - t_0 \). Since the particle displacement cannot be viewed as corresponding to a stationary stochastic process, Fourier analysis and the Wiener-Khintchine theorem cannot be used in order to compute \( C_{xx}(t, t'; t_0) \). This quantity must thus be obtained through a double time integration of the velocity correlation function \( C_{vv}(t_1, t_2) \) (which only depends on the time difference \( t_1 - t_2 \) since the Brownian particle velocity thermalizes and does not age).

In this situation, for any temperature of the thermal bath, one can write a modified FDT relating the displacement response function \( \chi_{xx} \) to the partial derivative \( \partial C_{xx}(t, t'; t_0) / \partial t' \), this latter quantity taking into account even those fluctuations of the particle displacement which take place during the waiting time (the FDT being valid with no modifications only when \( t_w = 0 \), i.e. when one wants...
to relate $\chi_{xx}$ and $\partial C_{xx}(t, t'; t_0)/\partial t'_0|_{t_0=t'}$. This is rendered possible through the introduction of an associated effective inverse temperature $\beta_{\text{eff.}}$ (or, equivalently, of a violation factor $X$) depending on both time arguments $t - t'$ and $t_w$ [8].

The above considerations, which solely rely on the consideration of time-dependent quantities, can be extended to other out-of-equilibrium dynamic variables of dissipative systems, classical or quantal [5]-[6].
Appendix A : some useful Fourier transforms and convolution relations

A.1. Fourier transform of \( \tanh \beta \hbar \omega/2 \)

Let us set

\[
I_1 = \int_0^\infty d\omega \sin \omega t \tanh \frac{\beta \hbar \omega}{2}.
\]  

(A.1)

Using the expansion

\[
\tanh \frac{\pi x}{2} = \frac{4x}{\pi} \sum_{k=1}^{\infty} \frac{1}{(2k-1)^2 + x^2},
\]  

(A.2)

with \( \omega = (\pi/\beta \hbar)x \), one gets

\[
I_1 = 2\pi \frac{\beta \hbar}{\pi} \sum_{k=1}^{\infty} e^{-(2k-1)\pi t/\beta \hbar}, \quad t > 0,
\]  

(A.3)

which yields the final result, valid whatever the sign of \( t \):

\[
I_1 = \begin{cases} 
\frac{\pi}{\beta \hbar} \sinh \frac{\pi t}{\beta \hbar}, & t \neq 0, \\
0, & t = 0.
\end{cases}
\]  

(A.4)

One thus has:

\[
\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \tanh \frac{\beta \hbar \omega}{2} = -\frac{i}{\pi} I_1.
\]  

(A.5)

A.2. Fourier transform of \( \coth \beta \hbar \omega/2 \)

Similarly, let us set

\[
I_2 = \int_0^\infty d\omega \sin \omega t \coth \frac{\beta \hbar \omega}{2}.
\]  

(A.6)

Using the expansion

\[
\coth \frac{\pi x}{2} = 2 \frac{\pi x}{\pi x} + \frac{4x}{\pi} \sum_{k=1}^{\infty} \frac{1}{(2k)^2 + x^2},
\]  

(A.7)

with \( \omega \) defined as above, one gets

\[
I_2 = \frac{\pi}{\beta \hbar} + 2\pi \frac{\beta \hbar}{\beta \hbar} \sum_{k=1}^{\infty} e^{-2k\pi t/\beta \hbar}, \quad t > 0,
\]  

(A.8)
which yields the final result, valid whatever the sign of $t$:

$$I_2 = \begin{cases} \pi \beta \coth \frac{\pi t}{\beta \hbar}, & t \neq 0, \\ 0, & t = 0, \end{cases} \quad (A.9)$$

One thus has:

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \ e^{-i\omega t} \coth \frac{\beta \hbar \omega}{2} = -\frac{i}{\pi} I_2. \quad (A.10)$$

A.3. From the relation

$$\tanh \frac{\beta \hbar \omega}{2} \coth \frac{\beta \hbar \omega}{2} = 1, \quad (A.11)$$

one deduces, by Fourier transformation and use of the above Fourier formulas (Eqs. (A.5) and (A.10)), the convolution relation

$$\frac{\pi}{\beta \hbar} \text{vp} \frac{1}{\sinh \frac{\pi}{\beta \hbar} t} * \frac{\pi}{\beta \hbar} \text{vp} \coth \frac{\pi t}{\beta \hbar} = -\pi^2 \delta(t). \quad (A.12)$$

At $T = 0$, Eq. (A.12) reduces to

$$\text{vp} \frac{1}{t} * \text{vp} \frac{1}{t} = -\pi^2 \delta(t). \quad (A.13)$$

A.4. Some useful relations

One has

$$\log |\coth ax| \sim_{|a| \to \infty} \frac{\pi^2}{4|a|} \delta(x) \quad (A.14)$$

and

$$\frac{a}{\sinh ax} \sim_{|a| \to \infty} -\frac{\pi^2}{2|a|} \delta'(x). \quad (A.15)$$

Formula (A.14) can be demonstrated in a standard fashion by considering $\log |\coth ax|$ as a distribution. Indeed, for any well-behaved function $\phi(x)$, the integral $\int_{-\infty}^{\infty} \log |\coth ax| \phi(x) \, dx$ tends towards $(\pi^2/4|a|) \phi(0)$ in the limit $|a| \to \infty$.

Formulas (A.14) and (A.15) can be used to study the classical limit of the convolution relation (A.12). Indeed, in the classical limit, using Eq. (A.15) with $a = \pi/2\beta \hbar$, the l.h.s. of Eq. (A.12) is seen to reduce to $-(\pi^2/2) \delta'(t) \ast \text{sgn}(t)$, that is, to $-\pi^2 \delta(t)$, as it should.
Appendix B: the harmonic oscillator case

B.1. The first fluctuation-dissipation relation

The first fluctuation-dissipation relation (2.21) expresses for the harmonic oscillator the displacement response function in terms of the displacement correlation function. The convolution product in the r.h.s. can be easily calculated – and Eq. (2.22) easily checked – by making use of the expansion

\[
\frac{1}{\sinh \frac{\pi t}{\beta \hbar}} = 2 \sum_{k=1}^{\infty} e^{- (2k-1) \pi t / \beta \hbar}, \quad t > 0,
\]  

and computing separately each convolution product of the series.

In spite of their oscillating character, it is not necessary here to treat the oscillator displacement response and correlation functions as distributions. Correspondingly, due to the fact that the function \(1/\sinh(\pi t/\beta \hbar)\) involved in the computation of the integral \(I\) (Eq. (2.2)) tends towards zero for large values of its argument, the contour integration on the contour \(\Gamma\) described in Section 2.1 can be carried out without problems, even in the limit \(R \to \infty\).

B.2. The second fluctuation-dissipation relation

The second fluctuation-dissipation relation (2.22) expresses for the harmonic oscillator the displacement correlation function in terms of the displacement response function. In order to compute the convolution product in the r.h.s., it is convenient to write

\[
\coth \frac{\pi t}{\beta \hbar} = \text{sgn}(t) + \left( \coth \frac{\pi t}{\beta \hbar} - \text{sgn}(t) \right),
\]  

with

\[
\text{sgn}(t) = \begin{cases} 
+1, & t > 0, \\
-1, & t < 0,
\end{cases}
\]  

and to make use of the expansion

\[
\coth \frac{\pi t}{\beta \hbar} - \text{sgn}(t) = \begin{cases} 
2 \sum_{k=1}^{\infty} e^{-2k\pi t / \beta \hbar}, & t > 0, \\
-2 \sum_{k=1}^{\infty} e^{2k\pi t / \beta \hbar}, & t < 0.
\end{cases}
\]  

The first contribution to the r.h.s., namely the convolution product

\[
-\frac{1}{\pi} \sin \omega_0 t * \frac{\pi}{\beta \hbar} \text{sgn}(t),
\]  

is...
only makes sense as a relation between distributions. One has:

\[-\frac{1}{\pi} \sin \omega_0 t \ast \text{sgn}(t) = \frac{2}{\beta \hbar \omega_0} \cos \omega_0 t. \quad (B.6)\]

As for the second contribution to the r.h.s., namely the convolution product

\[-\frac{1}{\pi} \sin \omega_0 t \ast \frac{\pi}{\beta \hbar} \left( \coth \frac{\pi t}{\beta \hbar} - \text{sgn}(t) \right), \quad (B.7)\]

it can be easily calculated by making use of the expansion (B.4) and computing separately each convolution product of the series. One thus gets:

\[-\frac{1}{\pi} \sin \omega_0 t \ast \frac{\pi}{\beta \hbar} \left( \coth \frac{\pi t}{\beta \hbar} - \text{sgn}(t) \right) = \left( \coth \frac{\beta \hbar \omega_0}{2} - \frac{2}{\beta \hbar \omega_0} \right) \cos \omega_0 t. \quad (B.8)\]

Gathering together results (B.6) and (B.8), one obtains Eq. (2.22). Note that, interestingly enough, it is only in the computation of the first contribution to the r.h.s. of Eq. (2.22), that is, of the convolution product (B.5), that the consideration of the oscillator displacement response and correlation functions as distributions is required.

Coming back to the computation of the contour integral \( J \) (Eq. 2.9)), one writes, for finite \( R \),

\[ J = 2i\pi \tilde{C}_{xx}(t - t') + J_a + J_b. \quad (B.9)\]

In Eq. (B.9), \( 2i\pi \tilde{C}_{xx}(t - t') \) is the contribution of the two small semicircles centered in \( t' \) and \( t' - i\hbar \beta \), and \( J_a \) denotes the contribution to \( J \) of the two vertical segments of abscissas \( R \) and \(-R \) (Fig. 1). As for \( J_b \), it is defined by

\[ J_b = \text{vp} \int_{-R}^{R} dt'' \left[ \langle x(t'')x(t) \rangle - \langle x(t)x(t'') \rangle \right] \frac{\pi}{\beta \hbar} \coth \frac{\pi(t'' - t')}{\beta \hbar}. \quad (B.10)\]

Interestingly enough, while \( J_a \) and \( J_b \), considered separately, do not tend towards a limit when \( R \to \infty \) but display instead an oscillatory behaviour, the sum \( J_a + J_b \) possesses a well defined limit. Indeed one has, for \( R \) finite but such that \( R \gg t', \beta \hbar \),

\[ J_a \simeq -\frac{2i\pi}{m_0^2 \beta} \cos \omega_0 R \cos \omega_0 t, \quad (B.11)\]

This amounts to say that the oscillating functions \( \sin \omega_0 t \) and \( \cos \omega_0 t \) have to be defined through the usual limiting procedures, namely

\[ \sin \omega_0 t = \lim_{\epsilon \to 0^+} \sin \omega_0 t e^{-\epsilon |t|}, \quad \cos \omega_0 t = \lim_{\epsilon \to 0^+} \cos \omega_0 t e^{-\epsilon |t|}. \]
and
\[ J_b \simeq \frac{2i\pi}{m\omega_0^2\beta} \cos \omega_0 R \cos \omega_0 t - \frac{2i\pi}{m\omega_0^2\beta} \cos \omega_0 (t - t') \]
\[ + i \frac{\hbar}{m\omega_0} \text{vp} \int_{-R}^{R} \sin \omega_0 (t - t'') \frac{\pi}{\beta\hbar} \left( \coth \frac{\pi (t'' - t')}{\beta\hbar} - \text{sgn}(t'' - t') \right). \quad (B.12) \]

When \( R \to \infty \), the sum \( J_a + J_b \) possesses a well-defined limit, namely
\[ J_a + J_b = -\frac{2i\pi}{m\omega_0^2\beta} \cos \omega_0 (t - t') \]
\[ + i \frac{\hbar}{m\omega_0} \text{vp} \int_{-\infty}^{\infty} \sin \omega_0 (t - t'') \frac{\pi}{\beta\hbar} \left( \coth \frac{\pi (t'' - t')}{\beta\hbar} - \text{sgn}(t'' - t') \right). \quad (B.13) \]

Using then formula (B.5), and the fact that \( J = 0 \), together with the expression (2.20) for \( \tilde{C}_{xx}(t) \), one checks again, as expected, the fluctuation-dissipation relation (2.22).
Figure caption

Fig. 1
Integration contour for the calculation of the integrals $I$ (Eq. (2.2)) and $J$ (Eq. (2.9)).
References

1. H.B. Callen and T.A. Welton, Phys. Rev. 83, 34 (1951).
2. H.B. Callen and R.F. Greene, Phys. Rev. 86, 702 (1952).
3. R. Kubo, J. Phys. Soc. Japan 12, 570 (1957).
4. R. Kubo, Rep. Prog. Phys. 29, 255 (1966).
5. L.F. Cugliandolo, J. Kurchan and G. Parisi, J. Phys. 4, 1641 (1994).
6. J.-P. Bouchaud, L.F. Cugliandolo, J. Kurchan and M. Mézard, in Spin-glasses and random fields, A.P. Young Ed. (World Scientific, 1997).
7. L.F. Cugliandolo and G. Lozano, Phys. Rev. Lett. 80, 4979 (1998); Phys. Rev. B 59, 915 (1999).
8. N. Pottier and A. Mauger, preprint cond-mat/9912028, to appear in Physica A.
9. J.W. Goodman, Statistical optics, Wiley (1985).
10. L. Mandel and E. Wolf, Optical coherence and quantum optics, Cambridge University Press (1995).
11. S.W. Lovesey, Condensed matter physics: dynamic correlations, The Benjamin/Cummings Publishing Company (1980).
Figure 1