Chapter 1

The harmonic oscillator

The one-dimensional harmonic oscillator is arguably the most important elementary mechanical system. Its quantum mechanical description is especially simple using the *ladder operators* introduced in almost every textbook [1]. As these "bosonic" operators play a central role in this book various theoretical concepts are already introduced for the description of properties of the harmonic oscillator. Applying these methods in a familiar context should simplify the process to become familiar with them. Also short introductions to time dependent correlation functions and linear response are presented. Readers familar with these topics should read this only to get used to the notation.

1.1 Groundstate properties and correlation functions

The Hamiltonian of a one-dimensional harmonic oscillator reads

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{\lambda}{2}\hat{x}^2, \tag{1.1}$$

where m is the mass of the particle and λ the spring constant. With the frequency $\omega_0 = \sqrt{\lambda/m}$ one defines the lowering operator $\hat{a}$ and its adjoint $\hat{a}^\dagger$

$$\hat{a} = \sqrt{\frac{m\omega_0}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\hbar\omega_0}}\hat{p}\ ; \quad \hat{a}^\dagger = \sqrt{\frac{m\omega_0}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\hbar\omega_0}}\hat{p}\ , \tag{1.2}$$

which obey the commutation relation $[\hat{a}, \hat{a}^\dagger] = \hat{1}$. The position operator $\hat{x}$ and the momentum operator $\hat{p}$ read in terms of a and $\hat{a}^\dagger$

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega_0}} \left(\hat{a} + \hat{a}^\dagger\right); \quad \hat{p} = -i\sqrt{\frac{m\hbar\omega_0}{2}} \left(\hat{a} - \hat{a}^\dagger\right), \tag{1.3}$$

The Hamiltonian $\hat{H}$, its eigenstates $|n\rangle$ and eigenvalues are given by

$$\hat{H} = \hbar\omega_0 \left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \quad ; \quad |n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle \quad , \quad \epsilon_n = \hbar\omega_0 \left(n + \frac{1}{2}\right). \tag{1.4}$$

The groundstate $|0\rangle$ is annihilated by $\hat{a}$, i.e. $\hat{a}|0\rangle = 0$ holds. In the position representation $\langle x|\hat{a}|0\rangle = 0$ is a linear differential equation which determines the groundstate wavefunction $\phi_0(x) \equiv \langle x|0\rangle$ [1]

$$\phi_0(x) = \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega_0}{2\hbar}x^2\right). \tag{1.5}$$

In order to calculate groundstate expectation values of functions of $\hat{x}$ and $\hat{p}$ one can either use the explicit form of $\phi_0(x)$ or the property $\hat{a}|0\rangle = 0$ only. As an example we consider the operator $\exp(-ik\hat{x})$. Its expectation value is readily calculated in the position representation. It is given by the Fourier transform of $|\phi_0(x)|^2$ which is obtained by a Gaussian integration. Alternatively one can use Eq.(1.3) and the *Baker-Haussdorff(BH)-identity* [15] which will be used frequently in this book. It states that

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{-\frac{1}{2}[\hat{A},\hat{B}]}, \quad \text{if} \quad [\hat{A}, [\hat{A}, \hat{B}]] = 0 = [\hat{B}, [\hat{A}, \hat{B}]]. \tag{1.6}$$

Its proof is outlined in exercise 1. For operators $\hat{A}$ and $\hat{B}$ *linear* in the ladder operators the requirements are fulfilled. With $v \equiv -ik\sqrt{\hbar/(2m\omega_0)}$ one obtains

$$\begin{aligned} \langle 0|e^{-ik\hat{x}}|0\rangle &= \langle 0|e^{v\hat{a}^\dagger + v\hat{a}}|0\rangle \\ &= \langle 0|e^{v\hat{a}^\dagger}e^{v\hat{a}}|0\rangle e^{-\frac{1}{2}v^2[\hat{a}^\dagger,\hat{a}]} \\ &= \exp\left(-\frac{\hbar k^2}{4m\omega_0}\right) \end{aligned} \tag{1.7}$$

Because of $\hat{a}|0\rangle = 0$ which implies $\langle 0|\hat{a}^\dagger = 0$ the expectation value in the second equality equals 1. As a test we recover the groundstate density $w_0(x)$

which is obtained much simpler by squaring $\phi_0(x)$. Using the representation of the Dirac delta function as a Fourier integral one has to perform a Gaussian integration

$$\begin{aligned} w_0(x) &= \langle 0|\delta(x-\hat{x})|0\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\langle 0|e^{-ik\hat{x}}|0\rangle dk \\ &= \left(\frac{m\omega_0}{\pi\hbar}\right)^{1/2} \exp\left(-\frac{m\omega_0}{\hbar}x^2\right) \end{aligned} \tag{1.8}$$

For finite temperatures the corresponding calculation is *simpler* than via the position representation.

The dynamical properties of a system described by the Hamiltonian $\hat{H}$ are encoded in its *time dependent correlation functions* [4]. In the absence of external perturbations the time dependence of operators in the Heisenberg picture is given by [1]

$$\hat{A}(t) = e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar} \; . \tag{1.9}$$

If the operator $\hat{A}$ has no explicit time dependence in the Schrödinger picture $\hat{A}(t)$ obeys the equation of motion

$$i\hbar\frac{d}{dt}\hat{A}(t) = [A, H](t) \; , \tag{1.10}$$

which has to be solved with the initial condition $\hat{A}(0) = \hat{A}$. Groundstate correlation functions are defined as

$$\Phi_{AB}(t,t') \equiv \langle E_0|\hat{A}(t)\hat{B}(t')|E_0\rangle = \langle E_0|\hat{A}(t-t')\hat{B}|E_0\rangle \equiv \Phi_{AB}(t-t') \tag{1.11}$$

where $|E_0\rangle$ is the groundstate of the Hamiltonian and the equality follows from Eq. (1.9) and the fact that the expectation value is taken in an eigenstate of the Hamiltonian.

Correlation functions for the harmonic oscillator are easy to calculate as $[\hat{a}, \hat{H}] = \hbar\omega_0\hat{a}$ implies $\hat{a}(t) = \hat{a}\exp(-i\omega_0 t)$. Again only using $\hat{a}|0\rangle = 0 = \langle 0|\hat{a}^\dagger$ to characterize the groundstate this yields e.g.

$$\langle 0|\hat{x}(t)\hat{x}|0\rangle = \frac{\hbar}{2m\omega_0}\langle 0|(\hat{a}e^{-i\omega_0 t} + \hat{a}^\dagger e^{i\omega_0 t})(\hat{a}+\hat{a}^\dagger)|0\rangle = \frac{\hbar}{2m\omega_0}e^{-i\omega_0 t} \tag{1.12}$$

The Fourier transform of the correlation function $\hat{A} \to \exp(ik\hat{x})$ and $\hat{B} \to \hat{A}^\dagger$ is called the *dynamical structure factor* and determines the scattering of a test particle from the oscillator in Born approximation [2, 12]. It will be discussed for the harmonic chain in the next chapter. The evaluation for the harmonic oscillator is a simple exercise for the use of the BH-identity

$$\langle 0|e^{ik\hat{x}(t)}e^{-ik\hat{x}}|0\rangle = \exp\left[-\frac{\hbar k^2}{2m\omega_0}(1-e^{-i\omega_0 t})\right]. \tag{1.13}$$

Instead of further analyzing groundstate correlation functions we generalize the discussion to the case of thermal equilibrium.

1.2 Finite temperature properties

In this section we describe the harmonic oscillator in thermal equilibrium described by the canonical ensemble with temperature T. As discussed in textboks on statistical mechanics [13] the expectation value of an observable A in thermal equilibrium is given by

$$\langle \hat{A}\rangle = \frac{\mathrm{Tr}(\hat{A}e^{-\beta\hat{H}})}{\mathrm{Tr}e^{-\beta\hat{H}}} = \frac{1}{Z}\sum_n \langle E_n|\hat{A}|E_n\rangle e^{-\beta E_n}, \tag{1.14}$$

where $\beta = 1/(k_B T)$, the $|E_n\rangle$ are the eigenstates of the Hamiltonian and $Z = \mathrm{Tr}e^{-\beta\hat{H}} = \sum_n e^{-\beta E_n}$ is the partition function.

For the harmonic oscillator the eigenstates of $\hat{H}$ are given by the "n-phonon"-states $|n\rangle$ obtained by the n-fold application of $\hat{a}^\dagger$ to the groundstate as described in Eq. (1.4). As only diagonal matrix elements contribute in Eq. (1.14) the thermal expectation values $\langle(\hat{a}^\dagger)^l\hat{a}^n\rangle$ vanish unless $l = n$. We therefore calculate the expectation value of the operators $\hat{A}_n \equiv (\hat{a}^\dagger)^n\hat{a}^n$

$$\begin{aligned}
\langle \hat{A}_n\rangle &= \frac{1}{Z}\mathrm{Tr}(\hat{a}^\dagger)^n\hat{a}^n e^{-\beta\hat{H}} \\
&= \frac{1}{Z}\mathrm{Tr}(\hat{a}^\dagger)^n\hat{a}^{n-1}e^{-\beta\hat{H}}e^{\beta\hat{H}}\hat{a}e^{-\beta\hat{H}} \\
&= \frac{1}{Z}\mathrm{Tr}(\hat{a}^\dagger)^n\hat{a}^{n-1}e^{-\beta\hat{H}}\hat{a}e^{-\beta\hbar\omega_0} \\
&= e^{-\beta\hbar\omega_0}\frac{1}{Z}\mathrm{Tr}\hat{a}(\hat{a}^\dagger)^n\hat{a}^{n-1}e^{-\beta\hat{H}}.
\end{aligned} \tag{1.15}$$

From the second to the third line the result $\hat{a}e^{-\beta\hbar\omega_0}$ for the Heisenberg operator with imaginary argument $\hat{a}(-i\beta\hbar)$ was inserted and in the last equality the cyclic invariance of the trace was used. Next the $\hat{a}$ on the left of creation operators is moved back to the right. With the operator identity

$$\hat{a}(\hat{a}^\dagger)^n = [\hat{a}, (\hat{a}^\dagger)^n] + (\hat{a}^\dagger)^n \hat{a} = n(\hat{a}^\dagger)^{n-1} + (\hat{a}^\dagger)^n \hat{a} \tag{1.16}$$

valid for $n \geq 1$, Eq. (1.15) goes over to the recursion relation

$$\begin{aligned} \langle \hat{A}_n \rangle &= e^{-\beta\hbar\omega_0} \left(n \langle \hat{A}_{n-1} \rangle + \langle \hat{A}_n \rangle \right) \\ &= \frac{n}{e^{\beta\hbar\omega_0} - 1} \langle \hat{A}_{n-1} \rangle \end{aligned} \tag{1.17}$$

for $n \geq 1$. With the trivial starting point $\langle \hat{A}_0 \rangle = 1$ one obtains for $n = 1$ the well known result

$$\langle \hat{a}^\dagger \hat{a} \rangle = \frac{1}{e^{\beta\hbar\omega_0} - 1} \equiv n_B(\omega_0), \tag{1.18}$$

where n_B is the Bose function, and for general $n > 1$ *Wick's theorem* [4] for the harmonic oscillator

$$\langle (\hat{a}^\dagger)^n \hat{a}^m \rangle = \delta_{nm} n! \langle \hat{a}^\dagger \hat{a} \rangle^n. \tag{1.19}$$

In quantum field theory the generalization of Wick's theorem plays an important role.

A simple application used frequently in this book is the expectation value

$$\begin{aligned} \langle e^{\lambda \hat{a}^\dagger} e^{\mu \hat{a}} \rangle &= \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{\lambda^n \mu^m}{n! m!} \langle (\hat{a}^\dagger)^n \hat{a}^m \rangle = \sum_{n=0}^{\infty} \frac{(\lambda\mu)^n}{n!} \langle \hat{a}^\dagger \hat{a} \rangle^n \\ &= e^{\lambda\mu \langle \hat{a}^\dagger \hat{a} \rangle} = e^{\lambda\mu n_B(\omega_0)} \end{aligned} \tag{1.20}$$

Operator products like those on the lhs of Eqs.(1.19) and (1.20) are called "normal ordered" because all lowering operators which in the field theoretical context are called *annihilation* operators are to the right of the *creation* operators $\hat{a}^\dagger$. Products like $(\lambda\hat{a}^\dagger + \mu\hat{a})^2$ are *not* normal ordered. In the calculation of expectation values of operators of this type one uses the commutation relation $[\hat{a}, \hat{a}^\dagger] = \hat{1}$ for normal ordering

$$\langle (\lambda\hat{a}^\dagger + \mu\hat{a})^2 \rangle = \langle \lambda^2 (\hat{a}^\dagger)^2 + \lambda\mu(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger) + \mu^2 \hat{a}^2 \rangle = \lambda\mu(1 + 2n_B). \tag{1.21}$$

This yields the important identity

$$\langle e^{\lambda\hat{a}^\dagger + \mu\hat{a}} \rangle = \langle e^{\lambda\hat{a}^\dagger} e^{\mu\hat{a}} \rangle e^{-[\lambda\hat{a}^\dagger, \mu\hat{a}]/2} = e^{\langle (\lambda\hat{a}^\dagger + \mu\hat{a})^2 \rangle /2}, \tag{1.22}$$

where we have used the BH-identity as well as Eqs.(1.20) and (1.21).
With this identity one can immediately generalize the calculation of the average density in Eq. (1.8) using $\langle \exp(ik\hat{x})\rangle = \exp(-k^2\langle\hat{x}^2\rangle/2)$. This implies that the average density is *Gaussian* for *all* temperatures

$$\langle\delta(x-\hat{x})\rangle = \frac{1}{\sqrt{2\pi\langle\hat{x}^2\rangle}} \exp\left(-\frac{x^2}{2\langle\hat{x}^2\rangle}\right), \tag{1.23}$$

with $\langle\hat{x}^2\rangle = \hbar[1+2n_B(\omega_0)]/(2m\omega_0)$. This smoothly interpolates from the groundstate density for $T=0$ to the Boltzmann distribution $\sim \exp(-\beta\lambda x^2/2)$ for $k_BT \gg \hbar\omega_0$, as $n_B(\omega_0) \to 1/(\beta\hbar\omega_0)$ in this limit.
The relation $\langle e^{\hat{A}}\rangle = e^{\langle\hat{A}^2\rangle/2}$ of Eq. (1.22) is easily generalized to

$$\langle e^{\hat{A}}\ e^{\hat{B}}\rangle = e^{(\langle\hat{A}^2+\hat{B}^2+2\hat{A}\hat{B}\rangle)/2} \tag{1.24}$$

for operators $\hat{A}$ and $\hat{B}$ *linear* in the ladder operators.

1.3 Time dependent correlation functions

Finite temperature dynamical correlation functions Φ_{AB} are defined by replacing $|E_0\rangle$ in Eq. (1.11) by $|E_n\rangle$ and averaging with the canonical probabilities $p_n = \exp(-\beta E_n)/Z$

$$\Phi_{AB}(t) \equiv \frac{1}{Z}\sum_n e^{-\beta E_n}\langle E_n|\hat{A}(t)\hat{B}|E_n\rangle = \frac{1}{Z}\mathrm{Tr}[\hat{A}(t)\hat{B}e^{-\beta\hat{H}}] \equiv \langle\hat{A}(t)\hat{B}\rangle \tag{1.25}$$

An important role for the description of experiments is often played by the Fourier transform $\tilde{\Phi}_{AB}$

$$\tilde{\Phi}_{AB}(\omega) \equiv \int_{-\infty}^{\infty} \Phi_{AB}(t)e^{i\omega t}dt\ . \tag{1.26}$$

Inserting the decomposition of the unity in terms of the eigenstates of the Hamiltonian between $\hat{A}(t)$ and $\hat{B}$ in Eq. (1.25) one obtains the "Lehmann representation"

$$\begin{aligned} \Phi_{AB}(t) &= \frac{1}{Z}\sum_{n,m} e^{-\beta E_n}\langle E_n|\hat{A}|E_m\rangle\langle E_m|\hat{B}|E_n\rangle e^{-i(E_m-E_n)t/\hbar} \qquad (1.27)\\ \tilde{\Phi}_{AB}(\omega) &= 2\pi\frac{1}{Z}\sum_{n,m} e^{-\beta E_n}\langle E_n|\hat{A}|E_m\rangle\langle E_m|\hat{B}|E_n\rangle\delta[\omega-(E_m-E_n)/\hbar]. \end{aligned}$$

The change of the summation variables $n \leftrightarrow m$ and use of the delta-function leads to the *detailed balance relation*

$$\tilde{\Phi}_{BA}(-\omega) = e^{-\beta\hbar\omega}\tilde{\Phi}_{AB}(\omega) \ , \tag{1.28}$$

which will be discussed in the context of inelastic neutron scattering in the next chapter.
For the special case $\hat{B} = \hat{A} = \hat{A}^\dagger$ it follows from Eq.(1.27) cthat $\tilde{\Phi}_{AA}(\omega)$ is a *real* function.
The Lehmann representation is seldom used for practical calculations of correlation functions but plays an important role for their interpretation.

We return to the harmonic oscillator and begin with the finite temperature generalization of Eq.(1.12). With the abbreviation $n_B \equiv n_B(\omega_0)$ one obtains

$$\langle \hat{x}(t)\hat{x}\rangle = \frac{\hbar}{2m\omega_0}\left[(1+n_B)e^{-i\omega_0 t} + n_B e^{i\omega_0 t}\right] . \tag{1.29}$$

Note that in the classical high temperature limit $k_BT \gg \hbar\omega_0$ this correlation function is given by the *real* function $(k_BT/\lambda)\cos(\omega_0 t)$, which for $t = 0$ reduces to the equipartition theorem [13].
The relative weights of the delta peaks at $\omega = -\omega_0$ and $\omega = \omega_0$ in $\tilde{\Phi}_{xx}$ can be read off Eq.(1.29) as $n_B/(1+n_B) = e^{-\beta\hbar\omega_0}$ in accordance with the detailed balance relation Eq. (1.28).
As a second example we use Eq.(1.24) for the finite temperature generalization of Eq.(1.13).

$$\langle e^{ik\hat{x}(t)}e^{-ik\hat{x}}\rangle = \exp\left\{-\frac{\hbar k^2}{2m\omega_0}\left[1 + 2n_B - (1+n_B)e^{-i\omega_0 t} - n_B e^{i\omega_0 t}\right]\right\} . \tag{1.30}$$

A discussion of the corresponding result for the harmonic chain is presented in the next chapter.

1.4 Linear response

In order to experimentally investigate a system often a *small* time dependent external perturbation is introduced which corresponds to a total Hamiltonian $\hat{H}_{tot} = \hat{H} + \hat{V}_t$. For the solution of the Schrödinger equation one works in the *interaction representation*, i.e. the time evolution with $\hat{H}$ is separated $|\psi(t)\rangle = \exp(-i\hat{H}t/\hbar)|\psi_t\rangle$. The state $|\psi_t\rangle$ obeys the equation [1]

$$i\hbar\frac{d}{dt}|\psi_t\rangle = \hat{V}_t(t)|\psi_t\rangle \ , \tag{1.31}$$

where $\hat{V}_t(t) = e^{i\hat{H}t/\hbar}\hat{V}_t e^{-i\hat{H}t/\hbar}$ is the Heisenberg operator as defined in Eq.(1.9), i.e. with respect to the *unperturbed* system Hamiltonian $\hat{H}$. The operator $\hat{V}_t(t)$ has an additional time dependence through its *explicit* time dependence in the Schrödinger picture. The initial condition for Eq.(1.31) is given by $|\psi_{t_0}\rangle = \exp(i\hat{H}t_0/\hbar)|\psi(t_0)\rangle$ for a perturbation switched on at time t_0.
In time dependent perturbation theory [1] the differential equation Eq.(1.31) is converted to an integral equation and iterated. Up to the term *linear* in the perturbation one obtains

$$|\psi_t\rangle = |\psi_{t_0}\rangle - \frac{i}{\hbar}\int_{t_0}^{t}\hat{V}_{t'}(t')dt'|\psi_{t_0}\rangle \ . \tag{1.32}$$

Going back to the Schrödinger picture expectation values of observables up to terms linear in the perturbation are then given by

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle = \langle\psi_{t_0}|\hat{A}(t)|\psi_{t_0}\rangle - \frac{i}{\hbar}\int_{t_0}^{t}\langle\psi_{t_0}|[\hat{A}(t),\hat{V}_{t'}(t')]|\psi_{t_0}\rangle dt' \ . \tag{1.33}$$

We now assume that the initial state $|\psi(t_0)\rangle$ is an eigenstate $|E_n\rangle$ of $\hat{H}$. Averaging over the canonical probabilities $p_n = \exp(-\beta E_n)/Z$ and denoting the average over the $\langle E_n(t)|\hat{A}|E_n(t)\rangle$ by $\langle\hat{A}\rangle_t$ yields for a perturbation $\hat{V}_t = -f(t)\hat{B}$ and $t_0 \to -\infty$

$$\delta\langle\hat{A}\rangle_t \equiv \langle\hat{A}\rangle_t - \langle\hat{A}\rangle = \int_{-\infty}^{\infty}\chi_{AB}(t-t')f(t')dt' \ , \tag{1.34}$$

where the *response function* χ_{AB} is given by the "retarded commutator" [12, 4]

$$\chi_{AB}(t) = \frac{i}{\hbar}\langle[\hat{A}(t),\hat{B}]\rangle\Theta(t) \ , \tag{1.35}$$

with $\Theta(t)$ the unit step function. In the derivation we have used that $\langle[\hat{A}(t),\hat{B}(t')]\rangle$ depends on the time difference only. As the "linear response" on the rhs of Eq.(1.34) is in the form of a *convolution* it is favourable to Fourier transform the equation

$$\delta\langle\hat{A}\rangle_\omega = \tilde{\chi}_{AB}(\omega)\tilde{f}(\omega) = \chi_{AB}^{ret}(\omega + i0)\tilde{f}(\omega) \ , \tag{1.36}$$

where the *retarded* response function

$$\chi^{ret}_{AB}(z) = \frac{i}{\hbar}\int_0^\infty \langle[\hat{A}(t),\hat{B}]\rangle e^{izt}dt \equiv -\langle\langle \hat{A};\hat{B}\rangle\rangle_z \tag{1.37}$$

is an analytic function in the *upper* complex $z-$plane. The fact that $\tilde{\chi}_{AB}(\omega)$ is the limiting function of a complex function in the upper half plane is due the unit step function in Eq.(1.35) which reflects *causality*. The symbol with the double parentheses is due to Zubarev [14] and will also be used in this book. In the following we drop the superscript *ret* whenever it is clear from the argument that it is *not* the time dependent function.
If one also introduces the time dependent commutator *without* the unit step function

$$\chi^{''}_{AB}(t) \equiv \frac{1}{2\hbar}\langle[\hat{A}(t),\hat{B}]\rangle = \frac{1}{2\hbar}\left[\Phi_{AB}(t) - \Phi_{BA}(-t)\right] \ , \tag{1.38}$$

its Fourier transform can be used to obtain the *spectral representation* of the retarded response function. For $\mathrm{Im}(z) > 0$ one obtains

$$\begin{aligned}\chi_{AB}(z) &= 2i\int_0^\infty \chi^{''}_{AB}(t)e^{izt}dt = \frac{i}{\pi}\int_0^\infty \left[\int_{-\infty}^\infty \tilde{\chi}^{''}_{AB}(\omega')e^{-i\omega' t}d\omega'\right]e^{izt}dt \\ &= \frac{1}{\pi}\int_{-\infty}^\infty \frac{\tilde{\chi}^{''}_{AB}(\omega')}{\omega' - z}d\omega' \end{aligned}\tag{1.39}$$

This spectral representation can be used to analytically continue $\chi_{AB}(z)$ to the lower half $z-$plane. This analytic function off the real axis is *discontinous* across it. This follows using

$$\frac{1}{\omega \pm i0} \equiv \lim_{\epsilon\to 0}\frac{1}{\omega \pm i\epsilon} = \frac{P}{\omega} \mp i\pi\delta(\omega) \ , \tag{1.40}$$

where the P denotes that the *principal value* has to be taken when the relation is integrated over. Using this relation in Eq.(1.39) yields

$$\chi_{AB}(\omega \pm i0) = P\!\!\!\!\int_{-\infty}^\infty \frac{\tilde{\chi}^{''}_{AB}(\omega')}{\omega' - \omega}d\omega' \pm i\tilde{\chi}^{''}_{AB}(\omega) \equiv \tilde{\chi}^{'}_{AB}(\omega) \pm i\tilde{\chi}^{''}_{AB}(\omega) \ . \tag{1.41}$$

From the definition Eq. (1.38) and the detailed balance relation Eq. (1.28) the *fluctuation dissipation theorem* (FDT) follows after Fourier transformation

$$\tilde{\chi}^{''}_{AB}(\omega) = \frac{1}{2\hbar}\left[\tilde{\Phi}_{AB}(\omega) - \tilde{\Phi}_{BA}(-\omega)\right] = \frac{1 - e^{-\beta\hbar\omega}}{2\hbar}\tilde{\Phi}_{AB}(\omega) \ . \tag{1.42}$$

The name stems from the fact that the energy $\int \omega\tilde{\chi}''_{BB}(\omega)|\tilde{f}(\omega)|^2 d\omega/(2\pi)$ is transferred to ("dissipated" in) the system initially in thermal equilibrium by the perturbation $\hat{V}_t = -f(t)\hat{B}$ with $f(\pm\infty) = 0$.
The FDT together with the Lehmann representation Eq. (1.27) shows that for a system with a discrete energy spectrum, like a many-body system in a finite box, the non-analyticities of $\chi_{AB}(z)$ on the real axis are first order *poles* at the energy differences $E_m - E_n$, if the the product of the matrix elements $\langle E_n|\hat{A}|E_m\rangle\langle E_m|\hat{B}|E_n\rangle$ is nonzero. In the infinite volume limit the energy spectrum becomes continuous and the non-analyticities are *branch-cuts*.

An approach often used to calculate response functions is the "equation of motion (eom) method" [14]. The basic steps are to multiply Eq. (1.37) with $\hbar z$

$$\hbar z\langle\langle\hat{A};\hat{B}\rangle\rangle_z = -\int_0^\infty \langle[\hat{A}(t),\hat{B}]\rangle\frac{d(e^{izt})}{dt}dt \tag{1.43}$$

and then to perform a partial integration. As $\mathrm{Im}(z) > 0$ only the boundary term at $t = 0$ contributes. The use of the Heisenberg equation of motion Eq. (1.9) then leads to

$$\hbar z\langle\langle\hat{A};\hat{B}\rangle\rangle_z - \langle\langle[\hat{A},\hat{H}];\hat{B}\rangle\rangle_z = \langle[\hat{A},\hat{B}]\rangle\ . \tag{1.44}$$

Repeated application generally leads to an infinite hierarchy of equations which has to be truncated. For simple models and operators one can obtain *closed* sets of equations. For the harmonic oscillator and $\hat{A} \to \hat{a}^{(\dagger)}$ the equations close already in the first step

$$\hbar(z-\omega_0)\langle\langle\hat{a};\hat{a}+\hat{a}^\dagger\rangle\rangle_z = 1, \quad \hbar(z+\omega_0)\langle\langle\hat{a}^\dagger;\hat{a}+\hat{a}^\dagger\rangle\rangle_z = -1\ . \tag{1.45}$$

This implies

$$\langle\langle\hat{x};\hat{x}\rangle\rangle_z = \frac{1}{m(z^2-\omega_0^2)} = -\chi_{xx}(z), \tag{1.46}$$

independent of temperature. The quantum mechanical result for this response function is identical to the classical one, in contrast to the behaviour of the correlation function $\tilde{\Phi}_{xx}$.

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