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FDT for fluctuations of a special perturbated harmonic oscillator and its application in q-deformed Harmonic Oscillator

Huangcheng Yin

School of Mathematics and Physics, Xi'an Jiaotong-Liverpool University, Suzhou, China.

Corresponding author's e-mail: Huangcheng.Yin20@student.xjtlu.edu.cn

Abstract. In this paper, we will use fluctuation dissipation theorem on the harmonic oscillator with time correlation creation annihilation operator as the perturbated term and through calculation, we find that the exact value of the dissipation associated Imχ of this special perturbation harmonic oscillator is exactly equal to π. Next, we give its potential application in the q-deformed harmonic oscillator, which means connect the q-deformed harmonic oscillator with fluctuation dissipation.

1. Introduction

The fluctuation-dissipation theorem (FDT) is a well-established result, first formulated by Nyquist [1] and later proved by Callen and Welton [2]. It connects the fluctuations of the product of two operators with the dissipation expressed through the imaginary part of their response function. In this article, we will fluctuation dissipation of simple harmonic oscillator with time correlation creation annihilation operator as perturbation term, then calculate the susceptibility function and the average over fluctuation. During the calculation, it is found that Im(χ(ω)) is a constant π. In the third part, we will discuss the practical application of this form of perturbation, which is an analogy of q-deformed Hamiltonian [3].

2. Fluctuation dissipation of simple harmonic oscillator with time correlation creation annihilation operator as perturbation term

The pure quantum harmonic oscillator can be described by the Hamiltonian $\hat{H}_0 = (\hat{a}^\dagger \hat{a} + 1/2)\hbar\omega$ where $\hat{a}^\dagger$, $\hat{a}$ correspond to the non-deformed annihilation and creation operators, respectively [4]. Let us consider the Hamiltonian perturbed by a term

$$\hat{H} = \hat{H}_0 + \hat{H}' = (\hat{a}^\dagger \hat{a} + 1/2)\hbar\omega - \hat{a}^\dagger$$

(Remark: It is not self-adjoint on account of $\hat{a}^\dagger(t)$. This term breaks the self-adjointness of the Hamiltonian and, therefore, nonphysical. However, we can see it's potential application in section 3.) $\hat{a}^\dagger(t)$ is an operator in the Heisenberg picture, related to its Schrodinger representation through

$$\hat{a}^\dagger(t) = exp(\frac{i\hat{H}_0 t}{\hbar})\hat{a}_s^\dagger exp(\frac{-i\hat{H}_0 t}{\hbar})$$

and $\hat{H}_0$ is the unperturbed Hamiltonian.

Under the condition $t \to -\infty \Rightarrow \hat{H}' \to 0$, expanding the Dyson series, and the eigenstates of the total Hamiltonian become

$$|\phi_n\rangle = |n\rangle - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, \hat{H}'(t')|n\rangle = |n\rangle - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, \hat{a}^\dagger(t')|n\rangle$$

where the last line corresponds to first-order perturbation theory, and $|n\rangle$ is a state of the unperturbed Hamiltonian with energy E_n (i.e., $\hat{H}_0|n\rangle = E_n|n\rangle$).
The expected value of another arbitrary operator $\hat{p}(t)$ is simply given by [5] [6]

$$\langle \hat{p}(t)\rangle = \frac{1}{Z}\sum_m \langle \phi_m|\hat{p}(t)|\phi_m\rangle\, e^{-\frac{E_m}{k_B T}}$$

$$\langle \hat{p}(t)\rangle = \frac{1}{Z}\sum_m \{\langle m|\hat{p}(t)|m\rangle + \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, \varphi(t')\langle m|[\hat{p}(t), \hat{q}(t')]|m\rangle\} e^{-\frac{E_m}{k_B T}}$$

Where $Z = \sum_m e^{-\frac{E_m}{k_B T}}$ is the partition function at temperature T [7].
Thus in the above Hamiltonian, given the $\varphi = 1$, and has the intrinsic energy of the simple harmonic oscillator is $E_m = \hbar\omega(m + 1/2)$, and if let the another operator $\hat{p}(t) = \hat{a}(t)$, thus

$$\langle \hat{a}(t)\rangle = \frac{1}{Z}\sum_m \{\langle m|\hat{a}(t)|m\rangle + \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, \langle m\big|[\hat{a}(t), \hat{a}^\dagger(t')]\big|m\rangle\} e^{-\frac{\hbar\omega(m+1/2)}{k_B T}}$$

The first term reduced to $\langle m|\hat{a}(t)|m\rangle = \langle m|\hat{a}_S|m\rangle$, recast it as

$$\langle \delta\hat{a}(t)\rangle = \langle \hat{a}(t) - \hat{a}(-\infty)\rangle = \int dt'\, \chi(t - t')$$

where susceptibility function is [5]

$$\chi(t - t') = \frac{i}{\hbar Z}\theta(t - t')\sum_m \langle m\big|[\hat{a}(t), \hat{a}^\dagger(t')]\big|m\rangle\, e^{-\frac{\hbar\omega(m+1/2)}{k_B T}}$$

Using the closure relation $|n\rangle\langle n| = I$, we can write

$$\langle m\big|[\hat{a}(t), \hat{a}^\dagger(t')]\big|m\rangle = \sum_n \{\langle m|\hat{a}_S|n\rangle\langle n\big|\hat{a}_s^\dagger\big|m\rangle - \langle m\big|\hat{a}_s^\dagger\big|n\rangle\langle n|\hat{a}_S|m\rangle\}\, e^{i\omega(m-n)(t-t')}$$

taking the time Fourier transform to work in frequency space, here we have

$$\int_0^\infty dt\, e^{i\omega' t} = \frac{i}{\omega' + i\epsilon}$$

Thus

$$\chi(\omega') = \int dt\, \chi(t) e^{i\omega' t}$$

After calculation, we can get

$$\chi(\omega') = \frac{-1}{Z}\sum_{m,n} \langle m|\hat{a}_S|n\rangle\langle n\big|\hat{a}_s^\dagger\big|m\rangle$$

In fact, by changing the frequency of the simple harmonic oscillator such that $\omega' = \omega$

$$\chi(\omega) = \frac{-1}{Z}\sum_{m,n} \langle m|\hat{a}_S|n\rangle\langle n\big|\hat{a}_s^\dagger\big|m\rangle \frac{e^{-\hbar\omega(m+1/2)/k_B T} - e^{-\hbar\omega(n+1/2)/k_B T}}{\hbar\omega(m - n + 1) + i\epsilon}$$

the dissipation associated to χ can be written

$$\mathrm{Im}(\chi(\omega)) = (1 - e^{-\hbar\omega/k_BT})\frac{\pi}{Z}\sum_{m,n}\langle m|\hat{a}_S|n\rangle\langle n|\hat{a}_s^{\dagger}|m\rangle\, e^{-\hbar\omega(m+1/2)/k_BT}\delta(m-n+1)$$

We can make reasonable settings $\hat{a}_S = \hat{a}$ and $\hat{a}_s^{\dagger} = \hat{a}^{\dagger}$ when $\mathrm{t} = 0$ Thus

$$\mathrm{Im}(\chi(\omega)) = (1 - e^{-\hbar\omega/k_BT})\frac{\pi}{Z}\sum_{m}\langle m|\hat{a}|m+1\rangle\langle m+1|\hat{a}^{\dagger}|m\rangle\, e^{-\hbar\omega(m+1/2)/k_BT}$$

Notice the identity

$$\hat{a}|m+1\rangle = \sqrt{m+1}|m\rangle$$
$$\hat{a}^{\dagger}|m+1\rangle = \sqrt{m+1}|m+1\rangle$$

Insert the two identity in $\mathrm{Im}(\chi(\omega))$

$$\mathrm{Im}(\chi(\omega)) = (1 - e^{-\hbar\omega/k_BT})\frac{\pi}{Z}\sum_{m}(m+1)\, e^{-\hbar\omega(m+1/2)/k_BT}$$

Let's do some math skills, Multiply $e^{-\hbar\omega/2k_BT}$ on both numerator and denominator

$$\mathrm{Im}(\chi(\omega)) = (1 - e^{-\hbar\omega/k_BT})\frac{\pi}{e^{-\hbar\omega/2k_BT}Z}\sum_{m}(m+1)\, e^{-\hbar\omega(m+1)/k_BT}$$

Absorbing $\mathrm{m}+1$ into the differential form

$$\mathrm{Im}(\chi(\omega)) = (1 - e^{-\hbar\omega/k_BT})\frac{\pi}{e^{-\hbar\omega/2k_BT}Z}\sum_{m}\frac{k_BT}{-\hbar}\frac{de^{-\hbar\omega(m+1)/k_BT}}{d\omega}$$

$$\mathrm{Im}(\chi(\omega)) = (1 - e^{-\hbar\omega/k_BT})\frac{\pi}{e^{-\hbar\omega/2k_BT}Z}\frac{d\sum_m e^{-\hbar\omega(m+1)/k_BT}}{d\omega}\frac{k_BT}{-\hbar}$$

Let's look at the denominator now

$$e^{-\hbar\omega/2k_BT}Z = \sum_{\mathrm{m}} e^{-\hbar\omega(m+1)/k_BT}$$

Reverse Taylor expansion

$$\sum_{\mathrm{m}} e^{-\hbar\omega(m+1)/k_BT} = \mathrm{e}^{-\hbar\omega/k_BT}\frac{1}{1-\mathrm{e}^{-\hbar\omega/k_BT}} = \frac{1}{\mathrm{e}^{\hbar\omega/k_BT}-1}$$

Notice this is the Bose-Einstein distribution function [7]. Let's denote it as

$$\mathrm{n}(\omega) = \frac{1}{\mathrm{e}^{\hbar\omega/k_BT}-1}$$

Thus $\mathrm{Im}(\chi(\omega))$ can be written a

$$\mathrm{Im}(\chi(\omega)) = \frac{\mathrm{e}^{\hbar\omega/k_BT}-1}{\mathrm{e}^{\hbar\omega/k_BT}}\frac{\pi}{\mathrm{n}(\omega)}\frac{\mathrm{dn}(\omega)}{\mathrm{d}\omega}\frac{k_BT}{-\hbar} = \frac{1}{\mathrm{e}^{\hbar\omega/k_BT}}\frac{\pi}{n(\omega)^2}\frac{dn(\omega)}{d\omega}\frac{k_BT}{-\hbar}$$

$$\Rightarrow \mathrm{Im}(\chi(\omega)) = \frac{\pi}{\mathrm{d}\mathrm{e}^{\hbar\omega/k_BT}/\mathrm{d}\omega}\frac{\mathrm{d}\dfrac{1}{\mathrm{n}(\omega)}}{\mathrm{d}\omega}$$

$$\Rightarrow \mathrm{Im}(\chi(\omega)) = \pi\frac{\mathrm{d}\dfrac{1}{\mathrm{n}(\omega)}}{\mathrm{d}\mathrm{e}^{\hbar\omega/k_BT}} = \pi$$

So under the such Hamiltonian, the $\mathrm{Im}(\chi(\omega))$ is a constant π. Notice the definition of the average over fluctuations is

$$S(t-t') = \langle \hat{a}(t)\hat{a}^{\dagger}(t')\rangle = \int \frac{d\omega}{2\pi} S(\omega) e^{-i\omega(t-t')}$$

$$S(\omega) = 2\hbar(n(\omega)+1)\mathrm{Im}(\chi(\omega))$$

Thus insert $\mathrm{Im}(\chi(\omega)) = \pi$ into $S(\omega)$

$$S(\omega) = 2\pi\hbar(n(\omega)+1) = h(n(\omega)+1)$$

where h is Planck constant.
Therefore, we can calculate the average value of the generated annihilation operators over time

$$\langle \hat{a}(\omega_1)\hat{a}^{\dagger}(\omega_2)\rangle = \int dt_1 dt_2\, e^{i\omega_1 t_1 + i\omega_2 t_2}\langle \hat{a}(t_1)\hat{a}^{\dagger}(t_2)\rangle = 2\pi\delta(\omega_1+\omega_2)S(\omega_1)$$

$$\langle \hat{a}(\omega_1)\hat{a}^{\dagger}(\omega_2)\rangle = 2\pi h(n(\omega_1)+1)\delta(\omega_1+\omega_2)$$

Using the same way, the Fourier transform of the fluctuation $\langle \hat{a}^{\dagger}(\omega_2)\hat{a}(\omega_1)\rangle$

$$\langle \hat{a}^{\dagger}(\omega_2)\hat{a}(\omega_1)\rangle = 2\pi h n(\omega_1)\delta(\omega_1+\omega_2)$$

Note that the amount we can observe is only Hermitian, and the symmetrized product is Hermitian.

$$\frac{1}{2}\langle \hat{a}(\omega_1)\hat{a}^{\dagger}(\omega_2) + \hat{a}^{\dagger}(\omega_2)\hat{a}(\omega_1)\rangle = 2\pi h(n(\omega_1)+\frac{1}{2})\delta(\omega_1+\omega_2)$$

Similarly, annihilation operator as perturbation term can be made

$$\hat{H} = \hat{H}_0 + \hat{H}' = (\hat{a}^{\dagger}\hat{a} + 1/2)\hbar\omega - \hat{a}(t)$$

3. Application of Hamiltonian of the above form

When a q-deformation is applied to the above system, the Hamiltonian is modified to the form [3]:

$$\hat{H}_q = \frac{1}{2}(\hat{A}^{\dagger}\hat{A} + \hat{A}\hat{A}^{\dagger})$$

where $\hat{A}$ and its adjoint $\hat{A}^{\dagger}$ are the deformed annihilation and creation operators, respectively, the oscillator described by the Hamiltonian $\hat{H}_q$ is called the q-deformed harmonic oscillator.
The operators $\hat{A}$ and $\hat{A}^{\dagger}$ obey the deformed commutation relation

$$\hat{A}\hat{A}^{\dagger} - q^2\hat{A}^{\dagger}\hat{A} = I$$

where $0 < q < 1$.
I hope to use the fluctuation dissipation theorem, so rewrite the above form

$$\hat{H}_q = \frac{1}{1+q^2}\hat{H}_0 = \frac{1}{1+q^2}(\hbar\omega(\hat{a}^{\dagger}\hat{a} + \frac{1}{2}))$$

Perform Taylor expansion and remove the higher-order terms

$$\hat{H}_q = \frac{1}{1+q^2}\hat{H}_0 = \hat{H}_0 - q^2\hat{H}_0$$

Notice if q is much smaller than 1, $\hbar\omega q^2/2$ can be ignored. Thus

$$\hat{H}_q = \frac{1}{1+q^2}\hat{H}_0 = \hat{H}_0 - q^2\hbar\omega\hat{a}^{\dagger}\hat{a}$$

Notice $\hat{H}_q$ not equals $\hat{H}_q^\dagger$, thus this is also nonphysical. Therefore, we can consider the following disturbance forms:

$$\hat{H} = \hat{H}_0 - \lambda \hat{a}^\dagger(t)\hat{a}(t)$$

The operation steps are similar to deal with $\hat{H} = (\hat{a}^\dagger \hat{a} + 1/2)\hbar\omega - \hat{a}^\dagger$.

4. Conclusion

By focusing on $\hat{H} = (\hat{a}^\dagger \hat{a} + 1/2)\hbar\omega - \hat{a}^\dagger$, this paper finds that the results of this form of fluctuation dissipation are not complicated, and even unexpectedly simple and clear, at the same time, an application of this $\hat{H} = (\hat{a}^\dagger \hat{a} + 1/2)\hbar\omega - \hat{a}^\dagger$ is illustrated, that is, $-\lambda \hat{a}^\dagger(t)\hat{a}(t)$ simulated from the q-deformed Harmonic Oscillator.

5. Appendix

Kramers-Kronig Relations [5] [6]:

$$\chi_{B,A}(\omega) = \frac{-1}{Z}\sum_{m,n}\langle n|B|m\rangle\langle m|A|n\rangle \frac{e^{-E_n/k_BT} - e^{-E_m/k_BT}}{\hbar\omega + E_n - E_m + i\epsilon}$$

as $\chi_{B,A}(\omega)$ is also a complex-valued function along the real axis, so accordingly

$$\chi_{B,A}(\omega) = \chi'_{B,A}(\omega) + i\chi''_{B,A}(\omega)$$

And

$$\chi'_{B,A}(\omega) = \frac{1}{\hbar} PV \int d\omega' \frac{\chi''_{B,A}(\omega')}{\omega' - \omega}$$

$$\chi''_{B,A}(\omega) = -\frac{1}{\hbar} PV \int d\omega' \frac{\chi'_{B,A}(\omega')}{\omega' - \omega}$$

Here

$$PV \int d\omega' = \int_{-}^{\omega-0} d\omega' + \int_{\omega+0}^{\infty} d\omega'$$

is called the (Cauchy) principal value integral, and the above relations follow immediately from

$$\chi_{B,A}(\omega) = \frac{1}{\pi}\int d\omega' \frac{\chi''_{B,A}(\omega')}{\omega' - z} = \frac{1}{2\pi i}\int d\omega' \frac{\chi_{B,A}(\omega' + i\epsilon) - \chi_{B,A}(\omega' - i\epsilon)}{\omega' - z}$$

which in turn follows from the Residue Theorem because of the mentioned analytical and asymptotic properties of the susceptibility $\chi_{B,A}(\omega)$.

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