26.6 Canonical correlation function

The reader should have realized that the derivation of the fluctuation-response relation for multivariable cases does not work for quantum mechanical cases, because Taylor expansion is not simple due to noncommutativity of the variables (observables); since generally $e^{A+B} \neq e^A e^B$, we cannot write $e^{A+\epsilon B} = e^A(1+\epsilon B+\cdots)$. To obtain the quantum version, we need the following non-commutative Taylor expansion formula:

$$e^{A+a} = e^A \left(1 + \int_0^1 d\lambda\, e^{-\lambda A} a e^{\lambda A} + \cdots \right). \tag{0.0.1}$$

†A formal proof is left to standard textbooks.[1] Here, it is explained how to guess this formula, using *Trotter's formula*[2]

$$e^{A+a} = \lim_{n\to\infty} \left(e^{A/n} e^{a/n}\right)^n. \tag{0.0.2}$$

From this, we obtain

$$\left.\frac{d}{dx} e^{A+xa}\right|_{x=0} \simeq \sum_{j=1}^n \frac{1}{n} e^{A(1-j/n)} a e^{A(j/n)}. \tag{0.0.3}$$

This is a Riemann sum formally converging to the integral in the above formula.

With the aid of (0.0.1) we can Taylor expand as

$$e^{-\beta(A+a)} = e^{-\beta A} \left(1 + k_B T \int_0^\beta d\lambda\, e^{\lambda A} a e^{-\lambda A} + \cdots \right). \tag{0.0.4}$$

If we introduce the Heisenberg picture $A(t) = e^{iHt/\hbar} A e^{-iHt/\hbar}$,

$$e^{\beta H} A e^{-\beta H} = A(-i\beta\hbar), \tag{0.0.5}$$

so

$$e^{-\beta(A+a)} = e^{-\beta A} \left(1 + k_B T \int_0^\beta d\lambda\, a(-i\lambda\hbar) + \cdots \right). \tag{0.0.6}$$

Using this and repeating the calculation just as the classical case, we arrive at

$$\delta X_i = \sum_j \beta \langle \delta \hat{X}_i ; \delta \hat{X}_j \rangle \delta x_j, \tag{0.0.7}$$

where

$$\langle \hat{X} ; \hat{Y} \rangle = k_B T \int_0^\beta d\lambda\, \langle \hat{X}(-i\lambda\hbar) \hat{Y} \rangle_e \tag{0.0.8}$$

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[1] One way is to show:

$$\frac{d}{d\lambda} e^{\lambda(A+a)} e^{-\lambda A} = e^{-\lambda(A+a)} a e^{-x\lambda A}.$$

Integrating this from $t = 0$ to 1, we obtain the desired formula.

[2] ⟪**Trotter's formula**⟫ This formula holds if at least A or a is a bounded operator. See J. Glimm and A. Jaffe, *Quantum Mechanics, a functional integral point of view*, second edition (Springer, 1987), Section 3.2. Its ('infinite' matrix) component representation is the path integral. The idea of Trotter's formula is very important in the quantum Monte Carlo method and in numerical solutions of (nonlinear) partial differential equations. The corresponding formula for finite matrix A is originally due to Lie, so the formula should be called the *Lie-Trotter formula*.

is called the *canonical correlation function*. Here, the suffix e implies the equilibrium average without perturbation. If all the variables commute, this reduces to $\langle \hat{X}\hat{Y} \rangle$ and (0.0.7) reduces to (**??**). It is often the case that if we replace the correlation in classical results with the canonical correlation, we obtain formulas valid in the quantum cases.