International Journal for Multidisciplinary Research (IJFMR)

E-ISSN: 2582-2160 • Website: www.ijfmr.com • Email: editor@ijfmr.com

Kinetic Equations for Time Correlation Functions Mori-Zwanzig Chain

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Abstract:

In a number of problems, it is more convenient to follow the evolution of the dynamic variable $A(t)$ in time t of an instantaneous fluctuation

$$\delta A_0(t) = A(t) - < A_0(t) >$$

where the brackets $< \cdots >$ denote the statistical averaging over the equilibrium Gibbs ensemble

$$< A(t) > = \int d\Gamma_N f_N^{(0)}(\Gamma_N) A(\Gamma_N : t)$$

and arrive at an infinite chain of linking kinetic equations.

Keywords: fluctuation, Gibbs ensemble, Lioville equation, correlation, split operator

INTRODUCTIO

In the absence of an explicit time dependence, $\delta A_0(t)$ obeys the Liouville equation

$$\frac{d\delta A_0(t)}{dt} = i\hat{Z}\delta A_0(t) \qquad (1)$$

with a formal solution

$$\delta A_0(t) = \exp\,(i\hat{z}t)\delta A_0 \qquad (2)$$

THEORITICAL APPROACH

Knowledge of (2) is difficult, and gives limited information about the behavior of the fluctuation which is contained in the behavior of the time correlation function

$$a(t) = \frac{<\delta A_0(0)\delta A_0(t)>}{<|\delta A(0)|^2>} \qquad (3)$$

with properties

$$\lim_{t\to 0} a(t) = 1 \;,\; \lim_{t\to\infty} a(t) = 0 \qquad (4)$$

The entry of the normalized $a(t)$ can be represented as the result of the operation of projecting fluctuations $\delta A_0(t)$ onto its initial value $\delta A_0(0)$

$$\delta A_0(t) = \delta A_0{\acute{}}(t) + \delta A_0{''}(t) \,,\; \delta A_0{\acute{}}(t) = \prod \delta A_0(t) \,,$$

$$\delta A_0{''}(t) = P\delta A_0(t)$$

where $\prod + P = 1 \;,\; \prod^2 = \prod \;,\; P^2 = P \;,\; \prod P = P \prod = 0$

$$\prod = \frac{<\delta A_0(0)><\delta A_0^*(0)>}{<|\delta A_0(0)|^2>} \qquad (5)$$

Using [4] , [5] and based on the Liouville equation (1), we first write the equation in two subspaces

$$\frac{d}{dt}\delta A_0{\acute{}}(t) = iz_{1\,1}\delta A_0{\acute{}}(t) + iz_{1\,2}\delta A_0{''}(t)$$

$$\frac{d}{dt}\delta A_0{''}(t) = iz_{2\,1}\delta A_0(\acute{t}) + iz_{2\,2}\delta A_0{''}(t) \qquad (6)$$

where $z_{i\,j}$ are matrix elements of the split operator $\hat{z}$.

Solving together the system (4) for the irreducible part of fluctuations, we get

$$\frac{d}{dt}\delta A_0(t) = i\hat{z}_{1\,1}\delta A_0(t) + i\hat{z}_{1\,2}e^{+i\hat{z}_{2\,2}t}\delta A_0(t) -$$

$$-\int_0^t d\tau \hat{z}_{1\,2} e^{+i\hat{z}_{2\,2}\tau}\, \hat{z}_{2\,1}\delta \acute{A}_0(t-\tau) \qquad (7)$$

By virtue of (4) we have $\delta \acute{A}_0(0) = 0$, so that the inhomogeneous contribution(7) disappears. Passing in (7) from fluctuations to their cross correlation function, we find

$$\frac{da(t)}{dt} = i\omega_0 a(t) - \Omega^2 \int_0^t d\tau M(\tau) a(t-\tau) \quad (8)$$

Here we have introduced the following notation

$$\omega_0 = \frac{<\delta A_0(0)\hat{z}\delta A_0(0)>}{<|\delta A_0(0)|^2>} \ , \ \Omega^2 = \frac{<|A_1|^2>}{<|A_0|^2>}$$
$$A_0 = \delta A_0(0) \ , \ A_1 = (\hat{z} - \omega_0) A_0$$
$$M(\tau) = \frac{<A_1^*(0)\exp(i\hat{z}_{2\,2}\tau)A_1(0)>}{<|A_1(0)|^2>} \quad (9)$$

for the Liouvillian natural frequency ω_0, the principal relaxation frequency Ω and the memory function $M(\tau)$. It is easy to see that the new dynamic variable A_1 is orthogonal to the initial $A_0 = \delta A_0(0)$

$$< A_0^*(0) A_1(0) >= 0 \quad (10)$$

The most interesting thing is that the procedure (3)-(9) can be repeated indefinitely for new normalized cross correlation functions $(n \geq 0)$

$$M_n(t) = \frac{<A_n^*(0)\exp(i\hat{z}^{(n)}t)A_n(0)>}{<|A_n(0)|^2>} \quad (11)$$

and for $n = 0$ we have

$$M_0(t) = a(t) \ , \ A_0(0) = \delta A_0(0) \ , \ \hat{z}^{(0)} = \hat{z} \ , \ \hat{z}^{(1)} = \hat{z}_{2\,2} \ , \ \omega_0^{(0)} = \omega_0$$
$$\hat{z}^{(n)} = \hat{z}_{2\,2}^{(n)} = P_{n-1}P_{n-2} \dots P_0 \hat{z} P_0 \dots P_{n-2}P_{n-1} \ , \ \text{n} \geq 1 \quad (12)$$

Here projection operators of the n-th level are introduced [6]

$$P_n = 1 - \prod_n \ , \ \prod_n \prod_m = \delta_{n,m} \prod_n \ , \ P_n^2 = P_n \ , \ \prod_n P_n = P_n \prod_n = 0 \quad (13)$$
$$\prod_n = \frac{A_n(0)><A_n^*(0)}{<|A_n(0)|^2>} \quad (14)$$

where $\delta_{n,m}$ is the Kronecker symbol.

Projectors (12) act on an arbitrary dynamic variable Y as follows :

$$\prod_n Y = A_n(0)\frac{<A_n^*(0)Y>}{<|A_n(0)|^2>} \ , \ Y\prod_n = A_n^* \frac{<YA_n(0)>}{<|A_n(0)|^2>} \quad (15)$$

Dynamic variables are constructed like this

$$A_n = A_n(0) = (\hat{z} - \omega_0^{(n-1)})A_{n-1} - \Omega_{n-1}^2 A_{n-2} \ , \ \text{n>1} \quad (16)$$

where the designations are introduced for the main Ω_n and natural $(\omega_0^{(0)})$ relaxation frequencies

$$\omega_0^{(n)} = \frac{<A_n^*\hat{z}A_n>}{<|A_n|^2>} \ , \ \Omega_n^2 = \frac{<|A_n|^2>}{<|A_{n-1}|^2>} \quad (17)$$

Repeating the procedure (3)-(10) many times and successively using (11) - (17), we arrive at an infinite chain of linking kinetic equations

$$\frac{dM_n(t)}{dt} = i\omega_0^{(n)} M_n(t) - \Omega_{n+1}^2 \int_0^t dt M_{n+1}(\tau) M_n(t-\tau) \quad (18)$$

Formal solution of (18) using the Laplace transform

$$\tilde{a}(s) = \int_0^\infty dt e^{-st} a(t) \quad (19)$$

leads to an infinite system of algebraic equations

$$\widehat{M}_n(s) = \{s - i\omega_0^{(n)} + \Omega_{n+1}^2 \widehat{M}_{n+1}(s)\}^{-1} \quad (20)$$

CONCLUSION

Although the resulting system of equations (18) almost completely coincides with the well-known Mori-Zwanzig equations [1] , [3]. The method presented here [6] differs in two respects. First, an orthogonal set of dynamic variables is used here

$$< A_n^*(0) A_m(0) >= \delta_{n,m} < |A_n(0)|^2 >$$

form in various subspaces are and an orthogonal set of projectors (13) . Second, the exact matrix representation (6) and the Liouvillian splitting in matrix used.

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