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Note

## Green's Function for the Classical System

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Bogoliubov and Sadovnikov<sup>1</sup> were the first to introduce the Green's function formalism into the statistical mechanics of classical systems. The aim of this work is to present a slightly different approach of its introduction and to describe the decoupling of Green's function hierarchy by the moment conserving method.

With the formal approach<sup>1</sup> ( $\hbar \rightarrow 0$ ) from quantum mechanical description to the classical one the following spectral representation can be obtained:

$$\langle [A(t), B(t')] \rangle = -\frac{i}{KT} \int_{-\infty}^{+\infty} I(\omega) e^{-i\omega(t-t')} d\omega \quad (1)$$

$$\langle\langle A; B \rangle\rangle_E^{r,a} = \frac{1}{2\pi KT} \int_{-\infty}^{+\infty} I(\omega) \omega \frac{d\omega}{E - \omega \pm i\varepsilon} \quad (2)$$

The symbols and the notation are the conventional ones<sup>1,2</sup>. The equation of motion for the dynamic quantity

$$A(t) = A\{q_1(t) \dots q_N(t); p_1(t) \dots p_N(t)\}$$

is

$$\frac{dA}{dt} = [A, H] \quad (3)$$

where  $[ ]$  denotes a Poisson bracket. In analogy with the quantum mechanical approach the following equation results:

$$\frac{dG(t, t')}{dt} = \delta(t-t') \langle [A(t), B(t')] \rangle + \langle\langle [A, H]; B \rangle\rangle \quad (4)$$

or with

$$G(t, t') = \int_{-\infty}^{+\infty} G(E) e^{-iE(t-t')} dE$$

$$-iE \langle\langle A; B \rangle\rangle_E = \frac{1}{2\pi} \langle [A, B] \rangle + \langle\langle [A, H]; B \rangle\rangle_E \quad (5)$$

The evaluation of the right side of eq. (5) gives

$$\langle\langle A; B \rangle\rangle_E = \frac{1}{2\pi} \left\{ \frac{i \langle [A, B] \rangle}{E} + \frac{i^2}{E^2} \langle\langle [A, H], B \rangle\rangle + \right. \\ \left. + \frac{i^3}{E^3} \langle\langle [ [A, H], H ], B \rangle\rangle + \dots \right\} \quad (6)$$

With the notation

$$M_0 = \langle [A, B] \rangle \quad M_1 = \langle [[A, H], B] \rangle \quad \text{etc.}$$

the eq. (5) takes the form

$$\langle\langle A; B \rangle\rangle_E = \frac{1}{2\pi} \left\{ \frac{i}{E} M_0 + \frac{i^2}{E^2} M_1 + \frac{i^3}{E^3} M_2 + \dots \right\} \quad (7)$$

The moments  $M_n$  at time  $t = t'$  can be generated from eq. (1)

$$M_0 = \langle [A, B] \rangle = -\frac{i}{KT} \int_{-\infty}^{+\infty} I(\omega) \omega \, d\omega$$

by differentiation. Thus

$$M_n = \frac{(-i)^{n+1}}{KT} \int_{-\infty}^{+\infty} I(\omega) \omega^{n+1} \, d\omega$$

Introducing

$$m_n = \int_{-\infty}^{+\infty} I(\omega) \omega^{n+1} \, d\omega$$

the eq. (7) takes the form

$$\langle\langle A; B \rangle\rangle_E = \frac{1}{2\pi KT} \left[ \frac{m_0}{E} + \frac{m_1}{E^2} + \dots + \frac{m_n}{E^{n+1}} + \dots \right] \quad (8)$$

The procedure for decoupling eq. (8) known<sup>3</sup> as the moment conserving method *via* Pade approximants can be used. To show the utility of this approach we used the Pade approximant [2,1] known as the geometric approximation. The moments  $m_1, m_3$  of the transform of the correlation function are known<sup>4,5</sup>

$$m_1 = \frac{k^2}{m\beta}$$

and

$$m_3 = 3 \frac{k^4}{m^2 \beta^4} + \frac{k^2 n}{m^2 \beta} \int \frac{\partial^2 V}{\partial z^2} g(r) (1 - \cos kz) \, dr = \frac{k^2}{\beta m} \left( 3 \frac{k^2}{m\beta} + W_k^2 \right)$$

The index  $k$  determines the *quasi*-discrete levels and was previously omitted from eq. (4).

As an example we want to describe the geometric approximation as applied to plasma oscillation.  $W_k^2$  in this case is the plasma frequency<sup>5</sup>  $W_k^2 = \frac{4\pi^2 l^2 n}{m}$ . The geometric approximation gives the dispersion relation:

$$E(k) = \sqrt{W_k^2 + \frac{3k^2}{m\beta}}$$

which is a well known result first obtained by Vlasov<sup>6</sup>. The above described procedure can be of some use in the study of liquid state to discuss the problem as collective motion in it.

## REFERENCES

1. N. N. Bogoliubov, Jr. and B. I. Sadovnikov, *Zh. Eksp. Teor. Fiz.* **43** (1962) 677.
2. D. N. Zubarev, *Usp. Fiz. Nauk* **71** (1960) 71.
3. O. Goscinski and B. Lukman, *Chem. Phys. Lett.* **7** (1970) 573.
4. P. G. DeGennes, *Physica* **25** (1959) 825.
5. J. Hubbard and J. L. Beeby, *J. Phys.* **C2** (1969) 561.
6. A. A. Vlasov, *Zh. Eksp. Teor. Fiz.* **8** (1938) 85.

## IZVLEČEK

**Greenove funkcije klasičnega sistema delcev**

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V delu so zapisane gibalne enačbe Greenovih funkcij za klasični sistem delcev. Z uporabo momentov in Padejevo aproksimacijo je izračunana energijska disperzijska relacija za geometrijski približek razklopitve sistema Greenovih funkcij.

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