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A NEW CONCEPT OF THE CORRELATION FUNCTION

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Abstract: In this paper we defined correlation function by generalizing the concept of finite equation of motion. For one-dimensional motion we derived differential equation for correlation function. Further, we discussed the special case of harmonic motions and calculated some expectation values by using the method of correlation function. We used the results of this calculation to get some results of the theory of specific heat.

1. Introduction

Let $X = X(t)$ be finite equation of motion of a particle; (in this paper we shall restrict ourselves to one-dimensional motion. The generalization to many-dimensional case is easy but for our present purposes unnecessary). Obviously, the coordinate X can be expressed as function of the coordinate of a free motion which is linear and homogenous in time and of unit velocity i. e. $x = at + b$, $a = 1$, $b = 0$. The second motion we shall call fundamental and the first motion correlated motion. Hence, the coordinate of an arbitrary motion can be expressed as function of the coordinate of just defined fundamental motion

$$X = X(x). \tag{1}$$

Let us consider a slightly less trivial example. If $x = x(t)$ is the finite equation of motion of a totally isolated particle which moves periodically in the interval (a, b), then

$$P(x) = \mathrm{Const} \int_a^x \frac{\mathrm{d}x}{|\dot{x}|}, \quad \dot{x} \equiv \frac{\mathrm{d}x}{\mathrm{d}t} \tag{2}$$

is the distribution function of the coordinate x. As the distribution function (2) satisfies differential equation

$$\ddot{P}(x) = 0 \tag{3}$$

we can interpret the periodic motion as fundamental and distribution function as the correlated »free motion«.

We shall now slightly generalize these two examples. Let $x = x(t)$ and $X = X(t)$ finite equations of motion of two particles of masses m and M, respectively. At each instant t, the coordinates of these particles define a point (x, X) of the space $R \times R$, where R is the set of all real numbers. The set of all points (x, X) for different t defines a subset in $R \times R$, i. e. a (generally multivalued) function F in R. This function we shall call correlation function. Hence,

$$X = F(x). \tag{4}$$

The motions $x = x(t)$ and $X = X(t)$ we shall call fundamental and correlated motion, respectively.

Let $x = x(t)$ be finite equation of the fundamental motion and $g(x)$ the force acting on the particle of mass m in the fundamental motion.

Let

$$M\ddot{X} = G \tag{5}$$

be differential equation of correlated motion and G the force acting in the correlation motion. In order to find the finite equation of correlated motion we can either integrate the equation (5) or find the correlation function F. We shall solve this problem by finding correlation function F.

2. *Differential equation for correlation function*

Let $h(x)$ be kinetic energy of fundamental motion. Then

$$h'(x) = g(x), \quad h' \equiv \frac{\mathrm{d}h}{\mathrm{d}x}. \tag{6}$$

On the other side we have

$$M\ddot{F}(x) = M[\dot{x}^2 F''(x) + \ddot{x} F'(x)] = G. \tag{7}$$

If we put $M = \mu m$, then we have finally

$$2\mu\, h(x) F''(x) + \mu\, h'(x) F'(x) - G = 0, \tag{8}$$

which is the required differential equation for correlation function F. If fundamental motion is fixed, then the solution of the differential equation (8) is equivalent to the solution of the differential equation (5). If $x = at$, $a = 1$, then (8) becomes (5). If the correlated motion is free motion, then $G = 0$ and (8) becomes

$$2h(x)\,F''(x) + h'(x)\,F(x) = 0. \tag{9}$$

The solution of (9) is, obviously, given by (2).

The integration of differential equation (8) can be performed by standard methods. If the force acting in the correlated motion depends on the coordinate of correlated motion (as we supposed for fundamental motion), then the integration of (8) is very easy. After we have multiplied the equation (8) by $F'(x)$, the integration gives

$$\mu h(x)\,[F'(x)]^2 = \int G(F)\,\mathrm{d}F + \text{const.} \tag{10}$$

As the variables in (10) can be separated, the final step in integration of (8) can be performed without difficulty.

In the derivation of differential equation (8) we assumed that the force acting on the particle in fundamental motion was dependent upon the coordinate only. But, since the first derivative of the kinetic energy with respect to coordinate is always equal to the force, we should be able to derive differential equation for more general case.

After deriving differential equation for correlation function we shall proceed to investigate a special case of correlation of harmonic with harmonic motion.

3. *Correlation of harmonic with harmonic motion*

Let the fundamental as well as the correlated motion be harmonic, or more precisely, let the fundamental motion be given by

$$x = a \cos \omega t \tag{11}$$

and the force acting in correlated motion by

$$G = -M\,\Omega^2\,F(x). \tag{12}$$

If we put $\Omega = \lambda\,\omega$ and again $M = \mu\,m$, then the equation (10) becomes

$$(a^2 - x^2)\,[F'(x)]^2 + \lambda^2\,F^2(x) = \text{const.} \tag{13}$$

If $A = \alpha a$ is the amplitude of correlated motion, then for $F(x) = \pm \alpha a$ we have $[\dot{F}(x)]^2 = \omega^2 (a^2 - x^2) [F'(x)]^2 = 0$ and (13) becomes

$$(a^2 - x^2) [F'(x)]^2 = \lambda [\alpha^2 a^2 - F^2(x)]. \tag{14}$$

The equation (14) has two linearly independent solutions

$$F_{\alpha,\lambda}(x) = \alpha a \cos \left(\lambda \arccos \frac{x}{a} \right), \tag{15}$$

$$G_{\alpha,\lambda}(x) = \alpha a \sin \left(\lambda \arccos \frac{x}{a} \right). \tag{16}$$

We shall devide all correlated motions in two classes. If the fundamental motion is a special case of correlated motion, then we shall call it correlated motion of the first kind. Otherwise, we shall call it correlated motion of the second kind. In (15) we have, obviously, a correlated motion of the first kind ($\alpha = \lambda = 1$) and in (16) a correlated motion of the second kind.

For $\alpha = 1$, $a = 1$ and $\lambda = n$, $n = 1, 2, 3, \ldots$, the solutions (15) and (16) are Tschebyscheff's functions of the first and second kind, respectively. The equations (14) and (15) give two relations for Tschebyscheff's functions (polynomials) of the first kind $T_n(x)$ (the relations are valid for $n = 0$, too)

$$(1 - x^2) [T_n'(x)]^2 = n^2 [1 - T_n^2(x)], \tag{17}$$

$$T_n [T_m(x)] = T_m [T_n(x)] = T_{mn}(x). \tag{18}$$

An equation similar to (17) is valid for Tschebyscheff's functions of second kind. We mentioned (16), (17) and (18) firstly, for the sake of completness and secondly, because we had not found the relations (17) and (18) published in Ref1).

After we succeeded to express the coordinate of an arbitrary harmonic motion as function of the coordinate of a fixed harmonic motion, we shall proceed to calculate some expectation values of correlated motion as function of corresponding expectation values of fundamental motion.

4. *Calculation of expectation values*

For the purpose of proposed calculations we shall put the equation (14) in the form

$$| \dot{F}_{\alpha,\lambda}(x) | = \lambda \omega \sqrt{\alpha^2 a^2 - F^2_{\alpha,\lambda}(x)}. \tag{19}$$

Then, for a function of the coordinate of correlated system $\Phi(F_{\alpha,\lambda}(x))$ we have the expectation value

$$\langle\Phi(F_{\alpha,\lambda}(x)\rangle_{\alpha,\lambda}=\frac{\lambda\omega}{\varkappa}\int\limits_{-A}^{+A}\Phi(F_{\alpha,\lambda}(x))\frac{\mathrm{d}F_{\alpha,\lambda}}{|\dot{F}_{\alpha,\lambda}(x)|}=\frac{1}{\delta}\int\limits_{-A}^{+A}\Phi(F_{\alpha,\lambda}(x))\frac{\mathrm{d}F_{\alpha,\lambda}}{\sqrt{\alpha^2a^2-F^2_{\alpha,\lambda}(x)}}=$$

$$=\frac{\omega}{\varkappa}\int\limits_{-a}^{+a}\Phi(\alpha x)\frac{\mathrm{d}x}{|\dot{x}|}=\langle\Phi(\alpha,x)\rangle_{1,1}, \tag{20}$$

(the expectation values on the left and right side of (20) are calculated with respect to the distribution function of the coordinate of correlated and fundamental system, respectively).

Take

$$\Phi_1(F_{\alpha,\lambda}(x))=F^2_{\alpha,\lambda}(x), \tag{21}$$

$$\Phi_2(F_{\alpha,\lambda}(x))=m^2_{\alpha,\lambda}\lambda^2\omega^2(\alpha^2a^2-F^2_{\alpha,\lambda}(x))=m^2_{\alpha,\lambda}[\dot{F}_{\alpha,\lambda}(x)]^2, \tag{22}$$

where $m_{\alpha,\lambda}$ is the mass of the correlated system. Then, by (20) we have

$$\langle F^2_{\alpha,\lambda}(x)\rangle_{\alpha,\lambda}=\alpha^2\langle x^2\rangle_{1,1}, \tag{23}$$

$$\langle m^2_{\alpha,\lambda}[\dot{F}_{\alpha,\lambda}(x)]^2\rangle_{\alpha,\lambda}=\alpha^2\lambda^2\mu^2\langle m_{1,}\dot{x}^2\rangle_{1,1}, \tag{24}$$

where $m_{1,1}$ is the mass of the fundamental system. The equations (23) and (24) give the expectation values of the square of coordinate and impulse of correlated particle by means of the corresponding expectation values of fundamental particle. Since dispersions of coordinate and impulse are just the expectation values of the square of coordinate and impulse, we have

$$D\,P_{\alpha,\lambda}\,D\,F_{\alpha,\lambda}=\alpha^4\lambda^2\mu^2\,D\,P_{1,1}\,D\,F_{1,1}. \tag{25}$$

From (23) and (24) we get for total energy of correlated motion

$$E_{\alpha,\lambda}=\langle\frac{1}{2}m_{\alpha,\lambda}[\dot{F}_{\alpha,\lambda}(x)]^2\rangle_{\alpha,\lambda}+\langle\frac{1}{2}m_{\alpha,\lambda}\Omega^2F^2_{\alpha,\lambda}(x)\rangle_{\alpha,\lambda}=\alpha^2\lambda^2\mu E_{1,1}.$$

We shall end our discussion of calculation of expectation values with the problem of finding among all possible classical oscillators of equal mass ($\mu=1$) a countable set of »almost quantum« oscillators. This can be done, for instance, by taking the amplitudes and frequencies such that they satisfy the following conditions

$$\sqrt{\frac{DP_{a,\lambda}\,DF_{a,\lambda}}{DP_{1,1}\,DF_{1,1}}} = \frac{E_{a,\lambda}}{E_{1,1}} = 2n+1, \tag{27}$$

where $n = 0, 1, 2, \ldots$. The equations (27) are, in the frame of classical mechanics, ad hoc assumptions but as they are of quantum mechanical origin we can expect that the set of oscillators satisfying (27) might reproduce some quantum mechanical results better than any other set of classical oscillators. From the equations (25), (26) and (27) we can easily see that the set consists of oscillators of equal frequencies ($\lambda_n = 1$) and of amplitudes $\mu_n = \sqrt{2n+1}$). Hence, equal frequencies are a consequence of »quantumlikeness« of the system of oscillators. And this was an assumtion of Einstein's theory of specific heat. In fact, if our oscillators are in thermal equilibrium then the expectation value of energy is

$$\langle E \rangle_{\mathrm{th\cdot cq.}} = \frac{\sum\limits_{n=0}^{\infty} (2n+1)\,E_{1,1}\,e^{-(2n+1)\frac{E_{1,1}}{KT}}}{\sum\limits_{n=0}^{\infty} e^{-(2n+1)\frac{E_{1,1}}{KT}}} = E_{1,1}\,\mathrm{cotg}\,h\,\frac{E_{1,1}}{KT}. \tag{28}$$

The expectation value (28) differs from the corresponding one of Einstein's theory by a constant. Therefore, both formulas give the same dependence of specific heat on absolute temperature. The difference, however, lies in the fact that for $T \to 0$ the equation (28) gives $\langle E \rangle_{\mathrm{th\cdot cq.}} = E_{1,1}$ instead of $\langle E \rangle_{\mathrm{th\cdot cq.}} = 0$ of the Einstein model, if it is adapted in such a way that the ground state energy is discarded, as it is done, for instance, in the Ref.[2] of Einstein's theory.

5. *Concluding remarks*

At the end we shall make some final remarks. We developed the concept of correlation function for one-dimensional motion because we have had constantly in mind statistical mechanics where many models are basically one-dimensional. But the method may be useful in many-dimensional motion as well. Further, we believe that the method can be applied in Mechanics for integration of differential equations of motion. Finally, we can get some results of pure methematical interest as we have shown in the paper. We illustrated the method by simple examples in order to show how the methods works and not to find some new physical results.

References

1) H. Bateman, Higher transcendental functions, vol. II N. YORK, 1953, p. 183;
2) C. Kittel, Introduction to solid state Physics, N.YORK, 1966, p. 168.

O JEDNOM NOVOM POJMU KORELACIONE FUNKCIJE

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Sadržaj

Ako se koordinata X čestice (ograničićemo se na jednodimenziono kretanje) može izraziti kao funkcija koordinate x neke druge čestice, onda funkciju nazivamo korelacionom funkcijom, prvo kretanje korelisanim a drugo kretanje fundamentalnim kretanjem. Ako je data konačna jednačina fundamentalnog kretanja a takođe i sila koja dejstvuje u korelisanom kretanju, onda se može izvesti diferencijalna jednačina (8) koju zadovoljava korelaciona funkcija. Rešenje ove jednačine ekvivalentno je rešenju diferencijalne jednačine (5) korelisanog kretanja. Ako sila kod korelisanog kretanja zavisi samo od koordinate, onda jedn. (10) daje prvi integral diferencijalne jednačine (8). Pošto se promenljive u (10) mogu razdvojiti to se druga integracija može izvesti bez teškoća.

Ako je fundamentalno kretanje harmonijsko (11) a korelisano kretanje takođe harmonijsko (12), onda su dva linearno nezavisna rešenja diferencijalne jednačine (8) date jednačinama (15) i (16). Korelaciona funkcija (15) u specijalnom slučaju ($\alpha = \lambda = i$) daje koordinate fundamentalnog kretanja. Takve korelacione funkcije nazivamo korelacionim funkcijama prve vrste. Korelaciona funkcija (16) nema tu osobinu i nju nazivamo korelacionom funkcijom druge vrste. U specijalnom slučaju $\alpha = 1$, $\alpha = 1$ i $\lambda = n$, $n = 1, 2, \ldots$ korelacione funkcije (15) i (16) postaju Čebiševljeve funkcije prve odn. druge vrste za koje možemo da pokažemo da važe relacije (17) i (18). (Za Čebiševljeve funkcije druge vrste važi samo prva relacija.)

Pošto su u (15) nađene korelacione funkcije u sledećem koraku se pokazuje kako se mogu izraziti očekivane vrednosti proizvoljne funkcije koordinate osnovnog kretanja u funkciji odgovarajuće očekivane vrednosti osnovnog kretanja (20). Koristeći se jednačinom (20) izračunali smo proizvod disperzije impulsa i koordinate (25) i energiju (26) korelisanog kretanja u funkciji odgovarajućih veličina fundamentalnog kretanja.

Jednačine (25) i (26) iskoristili smo da među svim mogućim klasičnim linearnim oscilatorima jednakih masa izaberemo prebrojiv skup koji će po svojim osobinama biti najsličniji sistemu kvantnih oscilatora. Za određivanje parametara α i x iskoristili smo dva uslova (27), u suštini kvantnog porekla. Kao rezultat smo dobili da oscilatori moraju biti jednakih frekvencija što je bila jedna od pretpostavki Ajnštajnove teorije specifičnih toplota. Izračunavanjem očekivane vrednosti energije (28) tako izabranih klasičnih oscilatora i pod pretpostavkom toplotne ravnoteže, dobili smo vrednost koja se od Ajnštajnove razlikuje za konstantu što znači da daje isto ponašanje specifičnih toplota u funkciji apsolutne temperature. Formula (28), međutim, razlikuje, se u suštini, samo po tome što za $T \to 0$ daje vrednost različitu od nule nasuprot nuli u Ajnštajnovoj teoriji.