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ON THE ESTABLISHMENT OF THERMAL EQUILIBRIUM IN SIMPLEST MECHANICAL SYSTEMS

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ՋԵՐՄԱՅԻՆ ՀԱՎԱՍԱՐԱԿՇՌՈՒԹՅԱՆ ՀԱՍՏԱՏՈՒՄԸ ՊԱՐԶԱԳՈՒՅՆ ՄԵԽԱՆԻԿԱԿԱՆ ՀԱՄԱԿԱՐԳԵՐՈՒՄ

Աշխատանքում դիտարկված է մարող օսցիլյատորների և ,,ազատ,, մասնիկների ջերմային հավասարակշռումը սև ճառագայթման դաշտի հետ փոխազդեցության ժամանակ: Ուշադրություն է դարձված իրական համակարգերի ոչ փակ լինելու նշանակության և շարժման միկրոսկոպիկ հավասարումների անհակադարձելիության վրա, վիճակագրական Ֆիզիկայի պատճառաբանման հարցում:

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Ar.M. KOTZINIAN

ON THE ESTABLISHMENT OF THERMAL EQUILIBRIUM IN SIMPLEST MECHANICAL SYSTEMS

The process of the establishment of thermal equilibrium of the damping oscillators and a "free" particle in interaction with the blackbody radiation field is considered. A special attention is payed to the principal role of non-closedness of real systems as well as to the irreversibility of the microscopic equations of motion in the question of grounding of the statistical physics.

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Ар.М.КОЦИНЯН

ОБ УСТАНОВЛЕНИИ ТЕПЛОВОГО РАВНОВЕСИЯ В ПРОСТЕЙШИХ МЕХАНИЧЕСКИХ СИСТЕМАХ

В работе рассматривается процесс установления теплового равновесия осцилляторов с затуханием и "свободной" частицы при взаимодействии с полем черного излучения. Обращается внимание на принципиальное значение незамкнутости реальных систем и необратимости микроскопических уравнений движения в вопросе обоснования статистической физики.

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1. Introduction.

The problem of strict grounding of the statistical physics, i.e. the description of irreversible macroscopic behavior of the closed system on the basis of time-reversible microscopic mechanical equations, remains unsolved so far [1] .

Recall briefly the situation. It is considered that the closed system consisting of large number of N interacting particles during the finite time turns into thermodynamical equilibrium state. To describe this process, there is used one of the basic notions, i.e. the notion of the Gibbs ensemble introduced into the statistical physics: instead of one closed system there is considered an infinite number of copies of this system under the same macroscopic conditions. Geometrically, this is reduced to the consideration of a finite region on the energy surface in the 6N-dimensional phase space instead of one representative point. The introduction of the ensemble notion is usually explained by lack of our knowledge of the exact microscopic state of the system (see, e.g. [2]). And there is postulated that the macroscopic characteristics of an individual real system coincide with the mean values of these characteristics with respect to the ensemble. Already at this stage one can see the artificiality of the incorporation of the ensemble for describing a separate closed system, since, irrespective of our knowledge within the scope of the classical mechanics, the system itself possesses exact initial data.

Further, the thermodynamical equilibrium state is described by means of microcanonical distribution for which the postulate of a priori equiprobability holds [2] . According to this postulate, for the equilibrium closed system all the microstates satisfying the given macroconditions are equiprobable.

Consider now the ensemble of closed systems consisting of particles whose interaction potentials are velocity-independent. Let these systems be in nonequilibrium state at an initial instant of time. In a finite time t larger than the relaxation time t_r they have to go over into thermodynamical equilibrium state. Let us choose at this instant of time t some system which subsequently will be in equilibrium state. In the microcanonical ensemble describing the equilibrium state at an instant t, there must be found also a system with the opposite direction of velocity. But this second system, according to the reversible microscopic equations, at an instant 2t will come back into initial nonequilibrium state of the first system.

Thus, at any $t > t_r$, the whole available under given macroconditions phase volume of the ensemble is divided into two equal parts, such that if at the given instant of time the system was in the first part, it will remain in equilibrium state, and if in the second part, it will go over into nonequilibrium state. This conclusion proves the obvious contradictoriness of the postulate about the equiprobability of microstates as well as of the statement that the closed system achieves equilibrium state from nonequilibrium one during finite interval of time.

Note, that all the considerations are referred to strictly closed systems. The possibility of the consideration of closed systems is usually based on the smallness of the surface effects against the volume ones ($N^{-\frac{1}{3}}$).

Here we'd like to emphasize one principal circumstance. Since all macrosystems consist of atoms or ions and electrons, i.e. of charged particles, then the interaction of these particles is accompanied by electromagnetic radiation. Moreover, these interactions take place on the background of always existing field of electromagnetic radiation. Owing to this, all real macrosystems are unclosed, and this unclosedness is of a three-dimensional (volumetric) nature.

Hence, naturally, there arises a problem to describe the relaxation process of unclosed systems being under the action of external random forces.

This problem for the system of linear oscillators was considered by Bogolyubov and Krylov [3] in 1939. They had shown that for the system entropy averaged on phases of external random force, there is fulfilled the law of entropy increase. In the same work, for the mean energy of the system consisting of one oscillator they obtained

$$W(t) \sim t\rho(\omega_0) \qquad (1)$$

where $\rho(\omega_0)$ is the spectral energy density of external field on the oscillator frequency. If as an external random force we consider the equilibrium thermal radiation, then the linear growth of oscillator energy contradicts the second law of thermodynamics in Kelvin's formulation [2], since according to (1), one may unlimitedly derive energy from the thermostat, converting it to the mechanical energy of the oscillator.

In the present work we have calculated the energy of simplest charged systems with attenuation in the external field of equilibrium thermal radiation via direct solution of the stochastic equations of motion.

2. The Charged Oscillator with Attenuation.

Consider the motion equation for the charged oscillator with attenuation in the field of equilibrium thermal radiation:

$$\ddot{\vec{r}} + \gamma \dot{\vec{r}} + \omega_0^2 \vec{r} = \vec{f} \qquad (2)$$

where $\omega_0^2 = \frac{K}{m}$ is the proper frequency of the oscillator;

$$\gamma = \frac{2e^2 \omega_0^2}{3mc^3} \qquad (3)$$

is the Lorentz coefficient of the radiation damping, $\vec{f} = \frac{e}{m} \vec{E}$, and $\vec{E}$ is the vector of the radiation electric field. Since the field $\vec{E}$ is a superposition of large number of independent random fields, then, according to the central limiting theorem of probability theory, it represents normally distributed random field.

Such fields are completely described by two first moments. Note also, that the field of equilibrium thermal radiation possesses the properties of stationarity, homogeneity and isotropy. From these properties immediately follows that the field mean value at any instant of time in an arbitrary point of space is zero:

$$< \vec{f}(t, \vec{r}) > = 0 \qquad (4)$$

Consider also the time correlation function at a given point of space. Owing to the homogeneity, this correlator is r- independent. With respect to stationarity and isotropy, it can be presented as

$$< f_i(t+\tau) f_j(\tau) > = \delta_{ij} \Psi(t) \qquad (5)$$

and $\Psi(t)$ can be expanded into the Fourier cosine-integral:

$$\Psi(t) = \int_0^\infty d\omega\, \varphi(\omega) \cos \omega t \tag{6}$$

To find $\varphi(\omega)$, consider $\Psi(0)$. From the definition (5) there follows

$$\Psi(0) = \frac{e^2}{m^2} < E_i(t) E_i(t) > = \frac{e^2}{3m^2} < \vec{E}^2 > = \frac{4\pi}{3} \frac{e^2}{m^2} W \tag{7}$$

where W is the thermal radiation electromagnetic field energy density given by Planck formula. Comparing (7) and (6) at $t = 0$, we find that

$$\varphi(\omega) = \frac{4e^2\hbar}{3\pi m^2 c^3} \cdot \frac{\omega^3}{e^{\frac{\hbar\omega}{\theta}} - 1} \tag{8}$$

where θ is the temperature in energy units.

The integral (6) can be calculated in the explicit form [4] :

$$\Psi(t) = \frac{4}{3} \frac{e^2\hbar}{\pi m^2 c^3} a^4 \left[\frac{e^{3at} + 4e^{2at} + e^{at}}{2\,(e^{at} - 1)^4} - \frac{3}{a^4 t^4} \right] \tag{9}$$

where $a = \frac{2\pi\theta}{\hbar}$. From (9) one can see that $\Psi(t)$ changes its sign at $t_0 \simeq 1.37 \frac{\hbar}{\pi\theta}$. This value of t_0 determines a characteristic time of correlation: at $t > t_0$ the vector $\vec{E}(t)$ in the mean is directed against the vector $\vec{E}(0)$. To the characteristic correlation time corresponds the characteristic correlation radius $r_0 = ct_0$. At room temperatures $t_0 \sim 10^{-14}$ s, and $r_0 \sim 10^{-4}$ cm.

If now we restrict ourselves to the consideration of oscillations whose amplitude is much less than r_0 , then we may assume that in (2) $\vec{E}$ is $\vec{r}$ -independent. Then the general solution of (2) has the form:

$$\vec{r}(t) = \vec{r}_f(t) + \int_0^t d\tau\, \vec{f}(\tau) H(t - \tau) \tag{10}$$

where $H(t) = e^{-\frac{\gamma}{2}t} \frac{\sin \omega_0' t}{\omega_0'}$ is the response function,

$\vec{r}_f(t) = \vec{A} e^{-\frac{\gamma}{2}t} \cos(\omega_0' t + \varphi_0)$ is the general damping solution of the homogeneous equation, and $\omega_0' = \sqrt{\omega_0^2 - \frac{\gamma^2}{4}}$.

We are interested in the behavior of oscillator at large times $t \gg \frac{1}{\gamma}$ therefore, the term $\vec{r}_f(t)$ may be ignored from the very beginning. With respect to (4) we have

$$\langle \vec{r}(t) \rangle = 0 \ , \qquad \langle \dot{\vec{r}}(t) \rangle = 0 \tag{11}$$

To find out the oscillator energy, we must calculate

$$\begin{aligned} \langle \vec{r}^2(t) \rangle &= 3\int_0^t d\tau \int_0^t d\tau' \Psi(\tau - \tau') H(t-\tau) H(t-\tau') \\ \langle \dot{\vec{r}}^2(t) \rangle &= 3\int_0^t d\tau \int_0^t d\tau' \Psi(\tau - \tau') \dot{H}(t-\tau) \dot{H}(t-\tau') \end{aligned} \tag{12}$$

We'll carry out calculations at $\gamma \ll \omega_0$. Substituting (6) into (12) and using the formula $\frac{\gamma}{\frac{\gamma^2}{4} + (\omega \pm \omega_0')^2} \approx 2\pi\delta(\omega \pm \omega_0')$ · ,

for large times we obtain:

$$\begin{aligned} \langle \dot{\vec{r}}^2(t) \rangle &= \frac{3\pi}{2\gamma} \varphi(\omega_0) \\ \langle \vec{r}^2(t) \rangle &= \frac{3\pi}{2\gamma\omega_0^2} \varphi(\omega_0) \end{aligned} \tag{13}$$

Note, that if from the very beginning we take $\gamma = 0$, then the similar calculations at large t give $\langle \dot{\vec{r}}^2(t) \rangle = \frac{3}{2}\pi t \varphi(\omega_0)$, i.e. the result (1) of Ref. [3] is reproduced.

Let now $\hbar\omega_0 \ll \theta$. This corresponds to the situation when the period of proper oscillations is much larger than the correlation time of the radiation field. In this case, from (13) and (8) we obtain:

$$W_{kin} = \left< \frac{m\dot{\vec{r}}^2(t)}{2} \right> = \frac{3}{2}\theta$$

$$W_{pot} = \left< \frac{\kappa\vec{r}^2(t)}{2} \right> = \frac{3}{2}\theta \qquad (14)$$

Thus we can see that with account of attenuation we come to a correct, from the thermodynamics viewpoint, result. The oscillator energy reaches a finite time-independent value, and here the principle of energy equipartition over degrees of freedom is fulfilled. Note, that the fulfilment of the equipartition principle is provided by the choice of the attenuation factor in the form of (3). This points out a close connection between the classical electrodynamics and statistical physics.

Hence we see that to obtain a correct value of the oscillator energy, we should consider the irreversible equations of motion of oscillator. At the same time, as one can see from the derivation [5] of formula (3), the irreversibility in the equation of motion of the charged particle arises due to the choice of retarded solutions of Maxwell equations. That is finally, the irreversibility occurs because of the account of the causality principle.

The result (14) is readily generalized for the case of N identical linearly interacting charged oscillators fixed at the points spaced from each other at distances many times larger than r_0 . In this case the forces from the radiation field affecting individual oscillators are non-correlated, and after passing to normal coordinates we can show that $W_{N\,kin} = W_{N\,pot} = \frac{3}{2} N\Theta$. Hence here too the principle of energy equipartition over degrees of freedom is valid.

3. "Free" Particle.

The behavior of a "free" particle in an external field of equilibrium radiation is described by the equation:

$$\ddot{\vec{r}} + \gamma'\dot{\vec{r}} = \vec{f} \tag{15}$$

Solving (16) in the same manner as in the previous Section, for the kinetic energy at $t \gg \frac{1}{\gamma'}$ we obtain:

$$< W_{kin}(t) > = \frac{\pi e^2}{3mc^3\hbar}\theta^2 \tag{16}$$

As seen from (16), the principle of equipartition over degrees of freedom is violated. This is due to the circumstance that a free particle executes infinite motion, and we must not therefore ignore the $\vec{r}$-dependence of $\vec{f}$.

Nevertheless, there exists a situation when the spatial region of motion has dimensions many times less than r_0, whereas a characteristic time of motion is many times larger than t_0. Such situation is realized for the external electron of strongly excited ($n \geqslant 30$) atom. The corresponding to (16) frequency shift

$$\Delta\nu = \frac{e^2}{6mc^3\hbar^2}\theta^2 \tag{17}$$

will also depend quadratically on absolute temperature.

Note, that the formula (17) can be obtained also at strict quantum-mechanical calculation [6]. Recently, this shift of levels (by six orders of magnitude less than the Lamb shift) was observed in the experiment [7] which supported the validity of expression (17).

4. Conclusion.

Recently, there appeared a hope to solve the problem of strict grounding of the statistical physics with the help of the mixing property in the nonlinear mechanical systems [8]. However, as was shown in the Introduction, one fails to co-ordinate logically the basic postulates of the statistical physics for the closed systems.

We want to emphasize once again that the basic contradiction arises when considering strictly closed mechanical systems. As already mentioned, the real systems are "volumetrically" unclosed, although the effect induced by blackbody radiation might be extremely small. For example, at room temperature its energy density and pressure are 10^{11}-fold less than in an ideal gas

However the unclosedness of the real systems is, to our mind, of principal significance.

First, it gives rise to a natural substantiation for introducing the notion of the Gibbs ensemble. Namely, the representative point of a separate real system consisting of N particles walks at random in a small layer of the 6N-dimensional phase space near the energy surface already at times less than the characteristic time of collisions. And this walking takes place not only at the initial instant of time, but continuously. Therefore, when neglecting the external perturbations, it is natural to consider the evolution in some region of phase space rather than on one trajectory.

Second, if now we adopt that the real system has a property of local instability (exponential runaway of trajectories), i.e. the "dynamical chaos" takes place, then it becomes evident that the division of the phase space, mentioned in the Introduction, in this case will not take place.

Thus, there are two reasons to "forget" initial values of coordinates and momenta in the system: first, the unclosedness of the real systems, and second, the irreversibility of the microscopic equations of motion. Their relative contribution into the system relaxation rate may be different in different problems. For example, in the systems with mixing the relaxation rate will basically be determined not by attenuation but by such parameters of the system as the cross sections of interaction of molecules, their concentration, etc. But it should be emphasized that even in integrable systems of the linear oscillator type a correct account of unclosedness and attenuation brings to a correct result from the viewpoint of the statistical physics.

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ОБ УСТАНОВЛЕНИИ ТЕПЛОВОГО РАВНОВЕСИЯ В ПРОСТЕЙШИХ МЕХАНИЧЕСКИХ СИСТЕМАХ

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