Statistical Mechanics of Weakly Coupled Oscillators Presenting Stochasticity Thresholds.

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The problem of understanding the way in which turbulence (or chaos, or stochasticity) blows up in dynamical systems constitutes one of the main present themes of research in the field of pure dynamics. Quite naturally one is then led to take into consideration the possibility that the key concepts dominating the dynamical aspects of the problem should have their counterpart in statistical mechanics, in as much as the latter has indeed to be founded, at least partially, on dynamics.

Thus, for example, just in this spirit RUELLE and TAKENS (1) proposed to understand turbulence in fluids in terms of strange attractors, which indeed dominate the dynamics of dissipative systems, and could not be imagined before the mathematical work of Smale (2) and the numerical work of Lorenz (3).

Something analogous is proposed here for conservative systems, on the basis of the present general understanding suggested by the mathematical work of Siegel, Kolmogorov, Moser and Arnol'd (4), who were able to master the problem of small denominators, and the numerical work of the distinguished astronomers CONTOPOULOS, HÉNON and FROESCHLÉ (5). Indeed, taking into account, for definiteness, Hamiltonian systems of weakly coupled oscillators (such as typically the vibration modes of a solid or of a black body), the present knowledge on dynamics may be considered to suggest that, instead of the formerly usual hypothesis of metrical ergodicity (or of mixing), one

(1) D. RUELLE and F. TAKENS: *Commun. Math. Phys.*, **20**, 167 (1971); **23**, 343 (1971); **64**, 35 (1978).
(2) S. SMALE: *Bull. Am. Math. Soc.*, **73**, 747 (1967).
(3) E. N. LORENTZ, *J. Atmos. Sci.*, **20**, 130 (1963).
(4) C. L. SIEGEL: *Nachr. Akad. Wiss. Gott. Math. Phys. Kl.*, 21 (1952); A. N. KOLMOGOROV: *Dokl. Akad. Nauk SSSR*, **98** (4), 527 (1954); J. MOSER: *Akad. Wiss. Gott. Math. Phys. Kl.*, IIa. No. 1, 1 (1962); V. I. ARNOL'D: *Russ. Math. Surv.*, **18** (5), 9 (1963); **18** (6), 91 (1963). See also C. L. SIEGEL and J. MOSER: *Lectures on Celestial Mechanics* (Berlin, 1971); J. MOSER: *Stable and Random Motions in Dynamical Systems* (Princeton, N. J., 1973); V. I. ARNOL'D and A. AVEZ: *Ergodic Problems of Classical Mechanics* (New York, N. Y., and Amsterdam, 1968).
(5) G. CONTOPOULOS: *Astron. J.*, **68**, 1 (1963); M. HÉNON and C. HEILES: *Astron. J.*, **69**, 73 (1964); C. FROESCHLÉ: *Astrophys. Space Sci.*, **14**, 110 (1971).

should put forward the hypothesis that a transition to stochasticity occurs through sharp energy thresholds. The latter hypothesis is shown here to lead in classical statistical mechanics to a possible removal of the so-called ultraviolet catastrophe, by following a line of thought which can quite naturally be attributed to BOLTZMANN himself (6).

Let us consider a system of a large number N of harmonic oscillators of the same frequency ν, and take Lebesgue measure as defining the *a priori* probability in the phase space of the system. If total energy is the only known quantity, standard considerations (*i.e.* the law of large numbers) then show that in the so-called thermodynamic limit the initial data are distributed in phase space according to Gibb's law; thus, in particular, the energy E of any single oscillators is a positive random variable distributed according to the Maxwell-Boltzmann law, namely with probability density $p(E)$ given by

$$p(E) = \frac{1}{kT} \exp\left[-E/kT\right], \tag{1}$$

k and T being positive parameters interpreted as Boltzmann's constant and absolute temperature, respectively. One has then

$$\int_0^\infty p(E)\,\mathrm{d}E = 1, \tag{2}$$

$$\bar{E} \equiv \int_0^\infty E p(E)\,\mathrm{d}E = kT, \tag{3}$$

so that for the initial data one has equipartition of energy (*i.e.* the average energy $\bar{E}(\nu, T)$ is independent of frequency).

Equipartition of energy was considered in a first approximation as a good result because it explained the observed specific heats for some material bodies at large enough temperatures (law of Dulong and Petit for solids, and the analogous one for some gases). On the other hand, difficulties occured for low temperatures and for high frequencies, as the average energy was then found not to be proportional to temperature. In particular, BOLTZMANN was particularly acute in pointing out a difficulty of principle, remarking (6) that the molecules of a gas should be conceived not as rigid bodies, but rather as systems with internal motions of high frequencies (as is well known today); the problem was then that of understanding why the high-frequency motions did not contribute to the specific heat, behaving as if they had no internal energy at all and were, so to say, frozen. This difficulty was enhanced in the case of a continuous system such as a black body (7,8), where oscillators of arbitrary high frequencies are involved,

(6) L. BOLTZMANN: *Nature (London)*, **51**, 413 (1895); quoted in A. BARACCA: *Manuale critico di meccanica statistica* (Catania, 1981).
(7) J. W. RAYLEIGH: *Philos. Mag.*, V, **49**, 539 (1900); J.-H. JEANS: *Philos. Mag.*, VI, **10**, 91 (1905); H. A. LORENTZ *Nuovo Cimento* **5**, 16 (1908).
(8) P. LANGEVIN and M. DE BROGLIE (Editors): *La théorie du rayonnement et les quanta*, reports and discussions of the *1911 Solvay Conference* (Paris, 1912).

and one would have in principle an infinite contribution to the specific heat (ultraviolet catastrophe).

In the same very vivid paper BOLTZMANN envisaged the possibility of a solution by exploiting a dynamical hypothesis, namely that the high-frequency oscillators perform motions of a very stable character, with respect to the very unstable motions of the low-frequency oscillators, thus distinguishing between an « ideal internal energy », to with all oscillators equally contribute, and what can be called an effective thermodynamic energy, to which only the low-frequency oscillators should contribute. In his words (6): « ... the *vis viva* of the internal (*i.e.* high frequency) vibrations is transformed into progressive and rotatory (*i.e.* low frequency) motion so slowly, that when a gas is brought to a lower temperature the molecules may retain for days, or even for years, the higher *vis viva* of their internal vibrations corresponding to the original temperature. This transference of energy, in fact, takes place so slowly that it cannot be perceived amid the fluctuations of temperature of the surrounding bodies ».

However, this distinction between stable high-frequency motions and unstable low-frequency motions had no clear dynamical basis and could be considered as rather artificial. These ideas were somehow pushed forward by JEANS (9), without success.

The Boltzmann idea of identifying with the thermodynamic internal energy only a fraction of the « ideal internal energy » NkT, on the basis of suitable stability properties of the corresponding motions, can instead be implemented in a quite clear way if one makes use of a hypothesis of dynamical character which can be explicitly found in a paper of Nernst (10). This was probably suggested to him by a combination of Planck's conception of zero-point energy (11), of his personal understanding of it as ordered energy in virtue of his « new heat theorem » (10), and of a remembrance of Boltzmann's idea (12).

Hypothesis (by NERNST): There exists a critical energy $\varepsilon(\nu)$ such that oscillators of frequency ν perform ordered (*i.e.* highly stable) motions, if they have energy $E < \varepsilon(\nu)$ and disordered (*i.e.* chaotic or highly unstable) motions, if they have energy $E > \varepsilon(\nu)$.

In other words, if one looks at a single oscillator of frequency ν in its phase space, it would rotate uniformly on a circle if it were isolated; the interaction with the other ones can then be described (possibly in the thermodynamic limit) as having on the single oscillator the effect of perturbing its motion in a quite different way according as to whether it is inside or outside the circle corresponding to the energy $\varepsilon(\nu)$. In the first case the oscillator should be conceived as still performing essentially uniform rotations with very small amplitude fluctuations, while in the latter case enormous amplitude fluctuations should occur, any trace of a regular rotation being lost.

Such a kind of behaviour is indeed observed in dynamical systems. For mappings this was first clearly seen by FROESCHLÉ (5), who extended to systems of more than two degrees of freedom the observations of a sharp transition to stochasticity first made by HÉNON (5) for two oscillators. For oscillators, some observations almost exactly

(9) J.-H. JEANS: *Philos. Mag.*, VI, **17**, 229, 773 (1909); VI, **18**, 209 (1909); and ref. (6), p. 53.
(10) W. NERNST: *Verh. Dtsch. Phys. Ges.*, **18**, 83 (1916), especially pages 87 and 91. See also W. NERNST: *Die theoretischen und experimentelle Grundlagen des neuen Wärmesatz* (Halle, 1924) (English translation: *The New Heat Theorem* (New York, N. Y., 1969)).
(11) M. PLANCK: *Ann. Phys. (Leipzig)*, **37**, 642 (1912).
(12) See ref. (6), p. 51.

as described above were made by CAROTTA, FERRARIO and LO VECCHIO ([13]) several years ago; some indications can also be found in ref. ([14]).

Remarks that the stochasticity threshold $\varepsilon(\nu)$ should not be conceived as a barrier; as a consequence of the fluctuations described above, any oscillator could indeed go everywhere in its phase space, and at any temperature a statistical equilibrium should be reached for a distribution of the N oscillators below and above threshold.

Leaving aside any attempts at understanding why NERNST deviated from the line of thought pursued here, we can now implement Boltzmann's idea through the dynamical assumption of Nernst. Indeed, through it we have a well-defined criterion to introduce a partition of the oscillators of any frequency ν into two disjoint ensembles, the stable one (with the oscillators below threshold) and the unstable one (with the oscillators above threshold), only the second one contributing to the thermodynamic internal energy. The analogy with the familiar two-fluid theory of superfluidity should be noted.

Precisely, making use of the Maxwell-Boltzmann probability density (1) for a given temperature T, in virtue of the relation $\int_\varepsilon^\infty p(E)\,\mathrm{d}E = \exp[-\varepsilon/kT]$, we find ([15]) that, among the N oscillators of the considered frequency, exactly Nn_0 and Nn_1 are below and above threshold respectively, where

$$n_0 = 1 - \exp[-\varepsilon(\nu)/kT]\,, \qquad n_1 = \exp[-\varepsilon(\nu)/kT]\,, \qquad n_0 + n_1 = 1\,. \tag{4}$$

Moreover, while NkT is, in the sense of Boltzmann, the «ideal internal energy», only the quantity NU_1, with

$$U_1 = \int_{\varepsilon(\nu)}^{\infty} Ep(E)\,\mathrm{d}E = \frac{\varepsilon(\nu) + kT}{\exp[\varepsilon(\nu)/kT]}\,, \tag{5}$$

constitutes the thermodynamic internal energy, which, in virtue of the instability of the corresponding motions, is the one which is «perceived amid the fluctuations of temperature of the surrounding bodies». To such thermodynamic internal energy, each of the N oscillators is thus seen to contribute with an «effective energy per oscillator» given by U_1.

For the sake of completeness, some further useful formulae are added here ([15]). The energy of the whole stable ensemble (the whole «frozen energy», of oscillators belowe threshold) is evidently given by NU_0, where

$$U_0 = kT - U_1\,. \tag{6}$$

([13]) M. C. CAROTTA, C. FERRARIO, G. LO VECCHIO and L. GALGANI: unpublished; see however *Phys. Rev. A*, **17**, 786 (1978).

([14]) L. GALGANI and G. LO VECCHIO: *Nuovo Cimento B*, **52**, 1 (1979); B. CALLEGARI, M. C. CAROTTA, C. FERRARIO, G. LO VECCHIO and L. GALGANI: *Nuovo Cimento B*, **54**, 463 (1979); P. BUTERA, L. GALGANI, A. GIORGILLI, A. TAGLIANI and H. SABATA: *Nuovo Cimento B*, **59**, 81 (1980). Clearer effects are exhibited in G. BENETTIN, G. LO VECCHIO and A. TENENBAUM, *Phys. Rev. A*, **22**, 1709 (1980); and in G. BENETTIN and L. GALGANI: *Transition to stochasticity in a one-dimensional model of a radiant cavity*, preprint.

([15]) L. GALGANI: *Nuovo Cimento B*, **62**, 306 (1981).

One can also introduce conditional expectations of energy E_0 and E_1, defined by

$$U_0 = n_0 E_0\,, \qquad U_1 = n_1 E_1\,, \tag{7}$$

with $n_0 E_0 + n_1 E_1 = kT$, and one finds

$$E_0 = kT - \frac{\varepsilon(\nu)}{\exp[\varepsilon(\nu)/kT] - 1}\,, \qquad E_1 = \varepsilon(\nu) + kT\,. \tag{8}$$

Let us now come in particular to the consideration of a black body. In such a case the number of oscillators per unit volume with frequency between ν and $\nu + \mathrm{d}\nu$ is well known ([16]) to be given by $N(\nu)\,\mathrm{d}\nu$, where

$$N(\nu) = \frac{8\pi\nu^2}{c^3}\,, \tag{9}$$

c being the light velocity. Moreover, as a consequence of the second law of thermodynamics one has the general Wien's law ([16]), according to which the thermodynamic internal energy per unit volume between ν and $\nu + \mathrm{d}\nu$ is given by $u(\nu, T)\,\mathrm{d}\nu$, where

$$u(\nu, T) = \frac{8\pi\nu^2 kT}{c^3} F(\nu/T) \tag{10}$$

and F is an unknown universal function. In virtue of the Boltzmann-like identification $u(\nu, T) = N(\nu)\, U_1(\nu, T)$, one then deduces from (5), (9) and (10) that for a black body the energy threshold $\varepsilon(\nu)$ is a homogeneous linear function of ν; thus

$$\varepsilon(\nu) = h\nu\,, \tag{11}$$

where h is a universal constant, with the dimensions of an action, which can be possibly identified with Planck's constant.

In such a way, instead of the familiar Planck's form for the radiation law

$$f(\nu, T) = \frac{8\pi\nu^2}{c^3}\,\frac{h\nu}{\exp[h\nu/kT] - 1} = \frac{8\pi}{h^2}\left(\frac{kT}{c}\right)^3 \frac{x^3}{\exp[x] - 1}\,, \tag{12}$$

where

$$x = \frac{h\nu}{kT}\,, \tag{13}$$

the theory envisaged here gives the possible form

$$g(\nu, T) = \frac{8\pi\nu^2}{c^3}\,\frac{h\nu + kT}{\exp[h\nu/kT]} = \frac{8\pi}{h^2}\left(\frac{kT}{c}\right)^3 \frac{x^2 + x^3}{\exp[x]}\,. \tag{14}$$

([16]) M. PLANCK: *Vorlesungen über die Theorie der Wärmestrahlung* (Leipzig, 1923) (English translation: *The Theory of Heat Radiation* (New York, N. Y., 1959)).

By this law, which provides, so to say, a classical analog of Planck's law, the ultraviolet catastrophe is thus removed. As a matter of fact, to quite a surprise it also turns out that it is not easy to discriminate between these two formulae on this basis of the available experimental data. Some comments in this connection are deferred to a forthcoming note [17].

Some remarks follow.

a) In a first approximation, the subdivision of the oscillators of frequency ν into two ensembles may be described by saying that any oscillator can lay only on two energy levels, namely $E_0 < h\nu$ and $E_1 > h\nu$, where $E_0 = kT - h\nu/(\exp[x] - 1)$ and $E_1 = h\nu + kT$ (where $x = h\nu/kT$), with populations $n_0 = 1 - \exp[-x]$ and $n_1 = \exp[-x]$, respectively. It is from the present point of view a rather curious fact that $kT - E_0$ just equals the average energy of one oscillator according to PLANCK. Moreover, the « gap » between the two energy levels is given by

$$E_1 - E_0 = h\nu = \frac{h\nu}{\exp[x] - 1}, \tag{15}$$

so that Planck's formula appears from this point of view as defining the addition of a thermal noise to the unperturbed gap $h\nu$. Finally, as was known to NERNST [10], in virtue of the fact that $h\nu/(\exp[x] - 1) \simeq kT - \frac{1}{2}h\nu$ for $x = h\nu/kT \ll 1$, one has in that limit also $E_0 \simeq \frac{1}{2}h\nu$; this fact could be of interest in connection with the problem of the value of the zero-point energy, which is typically observed in the Casimir effect [18].

b) Coming back to the problem of the freezing of the high-frequency oscillators as foreseen by BOLTZMANN, this is well understood for the black body on the basis of the relation $\varepsilon(\nu) = h\nu$. Indeed this freezing is described by the fact that, at a fixed temperature T, the fraction of frozen oscillators as a function of ν is just given by $n_0 = 1 - \exp[-h\nu/kT]$, which tends to one with increasing ν. The freezing, however, clearly also occurs for any frequency with decreasing temperature.

c) The fact that $kT - E_0$ equals the average energy of one oscillator according to Planck, pointed out in *a*), was well known since the year 1916 to NERNST [10], who tried to understand Planck's law on such a basis [15], thus deviating from Boltzmann's line of thought. Moreover, while Nernst's deduction of formula (8) for E_0 was really ununderstandable to everybody, it is a further curious fact that a deduction of it, exactly equal to that given here, was also known to PLANCK himself [19] in the year 1921, as I came to know quite recently. Apparently, however, PLANCK did not share Nernst's conception of $h\nu$ as a stochasticity threshold, nor did he mention Nernst's work. Finally, it is difficult to understand how NERNST himself did not follow the line of thought of Boltzmann pursued here, if one takes into consideration the theoretical objections he raised [20] in the year 1919 to the 1917 Einstein deduction of Planck's law [21], and

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(17) L. GALGANI: in preparation.
(18) H. B. G. CASIMIR: *Konin. Ned. Akad. Wet.*, **51**, 793 (1949); *J. Chem. Phys.*, **46**, 407 (1949): C. P. ENZ: *Is the zero-point energy real?*, in *Physical Reality and Mathematical Description*, edited by ENZ MEHRA (Dordrecht, 1974).
(19) M. PLANCK: *Acta Math.*, **38**, 387 (1921).
(20) W. NERNST and T. WULF: *Verh. Dtsch. Phys. Ges.*, **21**, 294 (1919).
(21) A. EINSTEIN: *Phys. Z.*, **18**, 121 (1917).

the fact that he was the first to raise serious doubts on the experimental validity of Planck's law [20].

d) The first consideration of the problem of the partition of energy for oscillators on the basis of dynamics was given by FERMI, PASTA and ULAM [22], in the same year (1954) in which KOLMOGOROV [4] announced his theorem on small denominators. These authors found, by numerical computations, no trend towards equipartition. A correct qualitative interpretation of such startling result in terms of energy thresholds of stochasticity for the oscillators (in the sense that only initial data below thresholds had been considered) was first given by IZRAILEV and CHIRIKOV [23]. These authors gave some interesting contributions and, together with FORD [24], made this subject popular in the scientific community. The possible relevance of this kind of problems for a removal of the ultraviolet catastrophe was first envisaged among researchers in the theoretical group around CALDIROLA. In this framework, the conception of an energy threshold $\varepsilon(\nu)$ characteristic for each frequency and proportional to it was introduced by CERCIGNANI on the basis of an analogy of Nernst's type between zero-point energy and ordered motions, independently rediscovered by him under the suggestion of some numerical results I had previously obtained with SCOTTI [25]. The basic idea underlying the present note was thus completely clear to the three of us almost ten years ago [26], and we even knew the formula for E_1, to which only the population factor n_1 had to be added here in order to obtain the formula for the effective energy per oscillator U_1. In fact I was lead to such formula after my interpretation [15] of Nernst's deduction of Planck's law, just because of a dissatisfaction for his lack of consideration of the populations. However, it is possible that in the meantime a deeper appreciation of Froexchlé's results at a dynamical level, together with a greater familiarity with several technical aspects of the problem, acquired through many works with Benettin, Casartelli, Giorgilli, Lo Vecchio and Strelcyn [27], turned out to be essential for this step. Finally, a relevant role towards the present statistical interpretation was played by a recognition of the circumstance, particularly emphasized by CASARTELLI, that the invariant Kolmogorov tori appeared to have vanishing measure in the termodynamic limit.

I have thus accomplished the task of describing how the existence of stochasticity thresholds in the dynamics of weakly coupled oscillators leads in classical statistical mechanics to a possible removal of the ultraviolet catastrophe. Being well aware of the completely heuristic character of the considerations reported here, I like to close then with a further quotation from the already mentioned paper of Boltzmann [6]: « It may be objected that the above is nothing more than a series of imperfectly proved

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[22] E. FERMI, J. PASTA and S. ULAM: Los Alamos Report (1954), reprinted in E. FERMI: *Collected Works* (Roma, and Chicago, Ill., 1965), p. 978.

[23] F. M. IZRAILEV and B. V. CHIRIKOV: *Dokl. Akad. Nauk SSSR*, **166**, 57 (1966).

[24] B. V. CHIRIKOV: *Phys. Rep.*, **52**, 263 (1979); J. FORD: *Adv. Chem. Phys.*, **24**, 155 (1973); J. FORD: in *Fundamental Problems in Statistical Mechanics*, edited by E. G. D. COHEN, Vol. **3** (Amsterdam, 1975).

[25] L. GALGANI and A. SCOTTI: *Phys. Rev. Lett.*, **28**, 1173 (1972).

[26] C. CERCIGNANI, L. GALGANI and A. SCOTTI: *Phys. Lett. A*, **38**, 403 (1972); L. GALGANI and A. SCOTTI: *Riv. Nuovo Cimento*, **2**, 189 (1972).

[27] M. CASARTELLI, E. DIANA, L. GALGANI and A. SCOTTI: *Phys. Rev. A*, **13**, 1921 (1976); G. BENETTIN, L. GALGANI and J.-M. STRELCYN: *Phys. Rev. A*, **14**, 2338 (1976); G. BENETTIN, L. GALGANI, A. GIORGILLI and J.-M. STRELCYN: *C. R. Acad. Sci. Ser. A*, **268**, 431 (1978); *Meccanica*, **15**, 9, 21 (1981); A GIORGILLI and L. GALGANI: *Cel. Mech.*, **17**, 267 (1978); G. BENETTIN, M. CASARTELLI, L. GALGANI, A. GIORGILLI and J.-M. STRELCYN: *Nuovo Cimento B*, **44**, 183 (1978); **50**, 211 (1979); L. GALGANI, A. GIORGILLI and J.-M. STRELCYN: *Nuovo Cimento B*, **61**, 1 (1981).

hypotheses. But granting its improbability, it suffices here that this explanation is not impossible. For then I have shown that the problem is not insolvable and nature will have found a better solution than mine ».

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