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A STATISTICAL MECHANICS OF INTERACTING BIOLOGICAL SPECIES

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The system of differential equations proposed by V. Volterra, describing the variation in time of the populations N_r of interacting species in a biological association, admits a Liouville's theorem (when log N_r are used as variables) and a universal integral of "motion." Gibbs' microcanonical and canonical ensembles can then provide a thermodynamic description of the association in the large. The "temperature" measures in one number common to all species the mean-square deviations of the N_r from their average values. There are several equipartition theorems, susceptible of direct experimental test, a theorem on the flow of "heat" (the conserved quantity in an isolated association) between two weakly coupled associations at different temperatures, a Dulong-Petit law for the heat capacity, and an analog of the second law of thermodynamics expressing the tendency of an association to decline into an equilibrium state of maximal entropy. The analog of the Maxwell-Boltzmann law is a distribution of intrinsic abundance for each species which has been successfully used by ecologists for interpreting experimental data. A true thermodynamics develops upon introducing the idea of work done on an association through a variation of the variables (such as physical temperature) defining the physical and chemical environment. An ergodic theorem is suggested by the agreement of ensemble and time averages in the one case where the latter may be found explicitly.

1. *Introduction.*

It has often been noticed that the science of population dynamics ought to be capable of some description in statistical or thermodynamic-like terms such as is provided for the Newtonian mechanics of a system of particles by the theory of statistical mechanics. For example A. J. Lotka (1925) has remarked "... what is needed is an analysis... that shall envisage the units of a biological population as the established statistical mechanics envisage molecules, atoms and electrons; that shall deal with such average effects as population density, population pressure, and the like, after the manner in which thermodynamics deal with the average effects of gas concentration, gas pressures, ..." Some such sort of analysis has indeed found expression in various systems of differential, or integro-differential, or other kinds of equations, which supposedly control the population numbers of the interacting species in a biological association. Notable examples are to be found in the works of V. Volterra (1931, 1937).

Now quite clearly these theories are of the nature of statistical theories in that they lay no claim to a power of detailed and precise prediction about the population numbers of any single well-defined biological association, but at best are concerned with average or most probable numbers. Implicitly they refer to ensembles of similar biological associations and in experimental tests assume that the one system under test is not appreciably different from some kind of most probable system. Thus the theories are characterized at the outset by a high phenomenological content attempting to describe directly the behavior of such a most probable system. This is evidenced by the absence of means of finding fluctuations from most probable population numbers; and by the appearance of numerous parameters, such as "coefficients of self-accretion," which remain unevaluated from any set of first principles but must be found from an experimental observation of test systems, much as the decay constant of a radioactive element remains an empirical constant when there is no underlying quantum theory to account for it.

In short, the theories of population interaction are the statistics, or a part of them, in the form of surmises and empirical laws, without the mechanics. They are loosely thermodynamic-like to this extent, but not at all of a statistical-mechanical nature. This is of course inevitably so because of the colossal complexity of the mechanics over which the statistics must be done.

Yet one might still ask of statistics that it speak further about a biological association. For, starting now with a phenomenological description, such as Volterra's, one finds another order of complexity as soon as the number of interacting species exceeds even a few: the equations are not amenable to explicit solution by available methods. The situation becomes somewhat analogous to that in the classical mechanics of many interacting particles, where between the known laws of motion and the knowledge of the motion hangs a deep mathematical fog, penetrated faintly but importantly by a few conservation laws. It is just in such a state of ignorance that there is room for statistical considerations, for statistical mechanics proper. Can then biological associations of many interacting species as whole entities, like whole mechanical systems of many degrees of freedom, be characterized in their entirety by equilibrium states in the thermodynamical sense? by a tendency to decline into such states? by variables of state, such as temperature and entropy? by an equation of state?

Our object in this note is to point out the possibility of affirmative answers by sketching a construction of statistical mechanics on top of a phenomenological population dynamics taken as given. The tools for this are ready to hand in Gibbs ensemble theory, the population dynamics being that advanced by Volterra (1937).

The Hamiltonian form given to his dynamics by Volterra is what in the first instance suggests a statistical development imitating that familiar in physics.* While such a program can be executed in principle it is in practice formidable and not very profitable. This occurs because of a certain artificiality of the Hamilton formulation. The starting Volterra differential equations in the population numbers, N_r, of the different species r in biological associations are of the first order; these Volterra then makes into second-order equations by writing $N_r = \frac{dX_r}{dt}$ and subsequently introducing a Lagrangian and other apparatus of classical mechanics to arrive again at first-order Hamiltonian equations. These are twice as numerous as the starting equations, but of course half of the "constants of the motion" other than the Hamiltonian are already known. That is, the final differential system comes into existence with a large, but false, amount of information embedded in it.

In studying now the motion of the system point in phase space the extraneous constants of motion are a heavy burden of constraints, leading in this context to appreciable mathematical difficulties. Moreover in erecting a statistical mechanics a separate "temperature" must be introduced for each of the many constants of motion (Grad, 1952) so as to accord them in the statistics their

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*S. Takenaka (1941) has observed that Liouville's theorem holds in Volterra's Hamiltonian formulation; this is just a well-known property of the formulation itself.

due weight as elements of knowledge of the system. Thus the statistical mechanics is cluttered with at least as many statistical parameters as degrees of freedom in the original first-order differential equations; and the purpose of a statistical inquiry is very nearly defeated. The Hamiltonian rendition, in other words, forces us to survey our genuine ignorance through a tangle of confusing and trivial information. Finally, disregarding the excess constants of motion, the Volterra Hamiltonian is structurally complex enough to discourage statistical considerations around it alone, lacking in particular the important feature of being a "sum-function" (Khinchin, 1949).

To proceed at once from the starting Volterra equations is therefore plainly desirable, if not absolutely necessary. Now, the statistical mechanics customary in physics, that form of it elaborated by J. W. Gibbs (1902), rests on the Hamiltonian form of the equations of motion only weakly, almost incidentally, the role of Hamilton's equations being to make evident the two corner-stones of the statistical development: Liouville's theorem and energy conservation. It will appear that the initial Volterra equations readily admit a Liouville's theorem and a universal constant of the "motion" somewhat like the Hamiltonian of classical dynamics; and then a statistical analysis of some simplicity, parallel to Gibbs', becomes feasible. Herewith we find a lesson for physics as well as from physics, an example of how much broader is the statistical side of statistical mechanics than the mechanics which calls it into existence.

There are, clearly, important objections to this proposed program. The description of interacting biological species offered by Volterra is surely only an approximation, probably quite crude, to a very complicated state of affairs, and it may seem improperly speculative to build further on it. However the Volterra equations contain at least qualitatively some important biological truths, and in certain cases a reasonably accurate depiction of experimental findings. Conceivably the position is roughly like that in statistical mechanics or kinetic theory when based on the highly idealized picture of atoms as small Newtonian billiard balls, the picture being not so much incorrect as incomplete, but adequate to give valid concepts and results. It must not be forgotten of course that the equations are already statistical in character, as remarked earlier, so that in using Gibbs' ensembles on top of them we are really contemplating an ensemble of ensembles—some kind of grand ensemble.

More significant perhaps is the objection that no useful purpose is served by a statistical Volterra mechanics, that there is no need for it. For we are not faced in the population-biology, as we are in physics, by macroscopic observables and laws which make compelling an explanation of how they are actuated in terms of the microscopic variables. That is, the population numbers, N_r, in a biological association, or a few of them, are the data which are experimentally determined, and these are the microscopic variables themselves in the proposed scheme. This puts us in the position we would be in in physics if our observations on a gas consisted in measurements of the coordinates or momenta of a few of the gas atoms rather than the gas temperature or pressure.

The analogy here gives some answer to the objection posed: the non-observation of macroscopic variables and laws does not necessarily mean that they do not exist or that it is pointless to invent or discover them. One can easily visualize in the case of a detailed knowledge of the positions of a few gas atoms that there remains point to the introduction of thermodynamic concepts. In effect the behavior of a few microscopic coordinates samples and bears the impress of the operation of the larger system in which they are immersed; in this sense the large system is observable and its statistical workings of legitimate concern.

Though the following considerations have no perfectly firm foundation, and their usefulness be only partly apparent at this juncture, it is hoped that they may exhibit, however crudely, some possibilities for a fresh mode of understanding of biological association.

2. *Volterra's Mechanics.*

The equations proposed by Volterra to describe the behavior in time of n biological species in interaction, having populations $N_1, N_2, \ldots, N_n$, are

$$\frac{dN_r}{dt} = \epsilon_r N_r + \frac{1}{\beta_r} \sum_s \alpha_{sr} N_s N_r. \tag{1}$$

The first term on the right-hand side expresses how each species propagates if left to itself in a given environment and no other species interacts with it. It provides an exponential fall or rise of N_r in time according as the coefficient of self-accretion ϵ_r (natural birth minus death rate) is negative or positive. The remaining terms express the interaction of species r with all other species s, stating that the increase or decrease of N_r per unit time is effectively proportional to the number of encounters per second between r and any s, taken to be measured by the product N_rN_s. To account for the one-sided nature of the encounters, wherein if r gains because of the encounter then s must lose, the interaction parameters α_{sr} are antisymmetric; $\alpha_{rs} = -\alpha_{sr}$. The positive quantities β_r^{-1} are Volterra's "equivalent numbers" such that in the binary encounters r,s the ratio of the number of s's lost (or gained) per second to the number of r's gained (or lost) per second is $\beta_s^{-1}/\beta_r^{-1}$.

A particular interest attaches to the *stationary states* of the biological association, those for which all dN_r/dt vanish and for which the population numbers N_r have the steady values q_r defined by

$$\epsilon_r\beta_r + \sum_s \alpha_{sr}q_s = 0. \tag{2}$$

At some cost in generality we shall assume these equations to have a unique solution with all q_r positive, possible only if the number of species is even and if all ϵ_r do not have the same sign. This is perhaps the most interesting and important case. The more general cases need a separate investigation outside the scope of the present one.

Volterra has shown in an elegant discussion that the N_r are variable between finite positive limits; that at least some, often all of them, fluctuate continually without damping out; and that their time averages are the steady values q_r and so are independent of their initial values. These characteristics are most congenial to our aims.

Let us rewrite equation (1) as

$$\frac{\beta_r}{N_r}\frac{dN_r}{dt} = \epsilon_r\beta_r + \sum_s \alpha_{sr}N_s, \tag{3}$$

and then introduce $\epsilon_r\beta_r$ from equation (2) and also the new dependent variables

$$v_r \equiv \log\frac{N_r}{q_r}; \qquad N_r \equiv q_re^{v_r}, \qquad v_s = \log\frac{N_s}{q_s}.$$

This gives the equations of "motion"

$$\beta_r \dot{v}_r = \sum_s \alpha_{sr} q_s (e^{v_s} - 1), \qquad \dot{v} \equiv \frac{dv}{dt}, \tag{4}$$

in the form we shall use.

An omission in the above equations is a self-interaction term, $\alpha_{rr} N_r^2$, of the Verhulst-Pearl type. Such terms have been shown quite generally by Volterra (1931) to give a kind of frictional damping of the otherwise undamped oscillations about the stationary state. The system dies down to this state eventually; the remote future of the system is foreseeable; and the scope for a statistical analysis is much narrowed. Also, with these terms no constant of the motion is available. We continue to assume them to be negligible, limiting ourselves to systems showing bounded and undamped motions ("conservative" system in Volterra's phrase). The restriction to even numbers of species seems artificial, but as Volterra has noted it is probable that uneven systems decay into even ones.

3. *Statistical Mechanics; Microcanonical Ensembles.*

The purpose of having introduced the particular variables v_r is to secure a Liouville's theorem. Consider a large number of copies, a Gibbs ensemble of biological associations each of the same character and each controlled by the same differential equations (4) but having all variety of initial values of v_r. In the Cartesian space of the v_r (phase space) the configuration of each copy is represented by a point, the ensemble by an ensemble of points. The points are propelled in phase space by the motional equations (4). When taken to be sufficiently numerous the points constitute a fluid of, say, density $\rho(v_1, v_2, \ldots, v_n)$ at a point $(v_1, v_2, \ldots, v_n)$, and velocity $V = (\dot{v}_1, \dot{v}_2, \ldots, \dot{v}_n)$ at this point. Since fluid is neither created nor destroyed we must have the hydrodynamical equation of continuity

$$\frac{\partial \rho}{\partial t} + \operatorname{div} \rho V \equiv \frac{\partial \rho}{\partial t} + \sum \frac{\partial (\rho \dot{v}_r)}{\partial v_r} = 0.$$

Expanding the derivatives under the summation sign gives

$$\frac{\partial \rho}{\partial t} + \sum \dot{v}_r \frac{\partial \rho}{\partial v_r} + \sum \rho \frac{\partial \dot{v}_r}{\partial v_r} = 0.$$

But the latter sum vanished according to equation (4), which tells that $\dot{v}_r$ is independent of $v_r(\alpha_{rr} = 0)$. There follows Liouville's theorem of the conservation of density in phase,

$$\frac{D\rho}{Dt} \equiv \frac{\partial \rho}{\partial t} + \sum \dot{v}_r \frac{\partial \rho}{\partial v_r} = 0, \tag{5}$$

stating that as one goes along with the motion of one system point the density in its neighborhood remains invariable. In particular it may be noted (Tolman, 1938) that a constant density of phase points (uniform ensemble) stays constant; there is no tendency of the motional equations to enrich one part of phase space over another. Another consequence, or equivalence of Liouville's theorem, is Gibbs' principle of conservation of extension in phase, to the effect that an element of volume of phase space, though changing its shape, maintains a uniform size as the motions of its points unfold, so long as its boundaries are marked by the same points.

There are variables other than v_r providing a Liouville's theorem; in fact a large class of them amongst which something resembling the transformation theory of dynamics may be built. But for our present purposes the v_r suffice. A helpful feature of their definition is that their range of variability, unlike the N_r, is over all positive and negative numbers.

Next we reconstruct in v language an important integral of the motion introduced by Volterra. In equation (4) multiply throughout by $q_r(e^{v_r} - 1)$ and sum over all r. Because of the antisymmetry of the α_{rs} there is left only

$$\sum \beta_r q_r \dot{v}_r (e^{v_r} - 1) = 0.$$

With $\tau_r \equiv \beta_r q_r$ for convenience, an integration gives

$$G = \sum \tau_r (e^{v_r} - v_r) = \text{constant}. \tag{6}$$

This is the only general integral that is visible. It is a universal, single-valued constant of the motion. That it is a sum of terms relating to the separate species in association is a considerable advantage, allowing a natural specification of the "components" of the system in the sense usual in statistical mechanics. We shall call G_r the members $\tau_r(e^{v_r} - v_r)$ and refer to "the G" of an association or of a few, or one, of its member species. The equations of motion may be written "canonically" in terms of G as

$$\dot{v}_r = \left(\sum \gamma_{sr} \frac{\partial}{\partial v_s}\right) G, \qquad \left(\gamma_{sr} = \frac{\alpha_{sr}}{\beta_s \beta_r} = -\gamma_{rs}\right),$$

which are loosely reminiscent of the Hamilton equations.

Each G_r has the minimum value τ_r, occuring for $v_r = 0$, and increases monotonically for v_r increasing positively or negatively; the total $G = \Sigma G_r$ has the absolute minimum value $\Sigma \tau_r$ (by a slight change of the variables v_r, it could be arranged that the minimum G is zero). A surface of constant G in phase has all the necessary mathematical properties we need; it encloses a simply-connected region of finite volume and is as smooth as wanted.

We define according to Gibbs an ensemble in statistical equilibrium (stationary ensemble) as one for which $\partial \rho / \partial t = 0$. The properties of such ensembles are then the same at all times. Of special interest are ensembles with densities which are functions of G alone. These are stationary and satisfy Liouville's equation (5) as may be directly verified. The ensemble average of any function $f(v_1, v_2, \ldots, v_n)$ of phase coordinates is defined to be

$$\bar{f} = \frac{\int \rho f d\tau}{\int \rho d\tau}, \tag{7}$$

the integrals being over all of phase space. ρ is thus of the nature of a probability density.

Let us admit at this point the fundamental statistical hypothesis that, for purposes of finding expected values of variables of interest for an association about which there is only limited knowledge, equal extensions in phase corresponding equally well to this knowledge be assigned equal *a priori* probabilities. This is simply to say that for a statistical survey we contemplate all possible copies of a system compatible with what information we have about it, and in ignorance beyond this point weigh all copies equally; the phase space appropriately populated with system points is then just machinery for conducting the survey. It may be noted that a separate statistical hypothesis is not needed for some purposes if an ergodic theorem, ensuring the equality of time averages over a single system and phase averages over a suitable ensemble of systems, can be established (ter Haar 1954, 1955). We shall later have an indication that there may be such a theorem.

Suppose now that our knowledge of a biological association is only that its G is constant at some value G_0. Then to equal regions on the surface $G = G_0$ we give equal probability, that is, we choose

$$\rho = \rho_0 \, \delta(G - G_0),$$

where δ stands for the delta function, zero everywhere except at the point where its argument vanishes and there so large that an integral of δ over a region containing this point is unity (ρ_0 is an unimportant numerical constant). This defines the microcanonical ensemble of Gibbs. In a well-known computation we may represent an element of volume $d\tau$ as $dSdn$ = element of area on a surface of constant G × increment of length normal to the surface; the latter is $dG/|\nabla G|$ where dG is the difference in G-values of two neighboring constant-G surfaces; thence equation (7) specializes to

$$\begin{aligned} \bar{f} &= \int f\delta(G - G_0)\, dS \frac{dG}{|\nabla G|} \Big/ \int \delta(G - G_0) \frac{dSdG}{|\nabla G|} \\ &= \int_{G_0} f \frac{dS}{|\nabla G|} \Big/ \int_{G_0} \frac{dS}{|\nabla G|} \qquad (8) \end{aligned}$$

$$\left(|\nabla G|^2 = \sum \left(\frac{\partial G}{\partial v_r}\right)^2\right).$$

The integrals are surface integrals over $G = G_0$.

Taking for example f to be

$$T_r = v_r \frac{\partial G}{\partial v_r} = \tau_r \left(\frac{N_r}{q_r} - 1\right) \log \frac{N_r}{q_r},$$

we note first that since

$$\nabla G = \sum \frac{\partial G}{\partial v_r} \hat{v}_r = |\nabla G| \, \hat{n}$$

($\hat{v}_r$ denoting a unit vector in the v_r direction and $\hat{n}$ a unit normal vector to the surface G = constant), the direction cosines of $\hat{n}$ are

$$\hat{n} \cdot \hat{v}_r = \frac{\partial G}{\partial v_r} \Big/ |\nabla G|$$

so that

$$v_r \frac{\partial G}{\partial v_r} \frac{dS}{|\nabla G|} = v_r(\hat{n} \cdot \hat{v}_r)\, dS = \hat{n} \cdot \mathrm{v}_r\, dS$$

[v_r denoting the vector to the point $(0, \ldots, 0, v_r, 0, \ldots .\, 0)$]. Then, calling the denominator in equation (8) Δ_0, the ensemble average of T_r is

$$\overline{T}_r = \frac{1}{\Delta_0} \int \hat{n} \cdot \mathrm{v}_r\, dS = \frac{1}{\Delta_0} \int \mathrm{div}\ \mathrm{v}_r\, d\tau = \frac{\tau_0}{\Delta_0}$$

for all r, here we have used Gauss' divergence theorem and represented the volume enclosed by G_0 as τ_0.

This result is analogous to the equipartition theorem of physics. In words, the mean T for any species is the same as for any other; or, the total T of the biological association in the mean is equally distributed amongst all species. Were the association ergodic, "mean" here would refer to "time average for one association." Unlike the situation in physics, this equipartition result should be susceptible of experimental test. The quantity T will be recognized to be a loose analog of kinetic energy.

Another interesting result follows from the calculation of the average of

$$D_r = \frac{\partial G}{\partial v_r} = \tau_r\left(\frac{N_r}{q_r} - 1\right).$$

By a manipulation similar to the previous one we get

$$\overline{D}_r = \frac{1}{\Delta_0} \int \hat{n} \cdot \hat{v}_r\, dS = \frac{1}{\Delta_0} \int \mathrm{div}\ \hat{v}_r\, d\tau = 0.$$

The ensemble average of N_r is q_r.

As has been mentioned, the *time* average of N_r is also q_r. This follows at once from equation (3) upon integrating from time 0 to time t,

$$\frac{\beta_r}{t} \log \frac{N_r(t)}{N_r(0)} = \epsilon_r\beta_r + \sum \alpha_{sr}\left(\frac{1}{t} \int_0^t N_s(t)\, dt\right),$$

whence taking t large and remembering that N_r remains bounded, it is seen that

$$\text{time averages of the } N_s = \lim_{t\to\infty} \frac{1}{t} \int_0^t N_s(t)\,dt$$

all satisfy the same equation (2) as the q_s.

The suggestion is that the system under study may be ergodic, a single system point in general travelling over the surface G_0 comprehensively enough as eventually to cover nearly all parts of it, so that looking at it for a long time is tantamount to looking at a Gibbs ensemble covering the surface at one time. The suggestion is strengthened by a glance at Poincaré's recurrence theorem in mechanics (Chandrasekhar, 1943) stating that under quite general conditions, satisfied here, the system point starting at a given point will wander back to this point arbitrarily closely (not exactly) and infinitely often. This seems at least necessary for ergodicity; otherwise there would be regions of phase space that would be avoided relative to others during the long-time motion.

A valuable consequence of Poincaré's theorem in the present context is that *all* species, not just some as proven by Volterra, must in general exhibit undamped oscillations; for the only alternative to continual oscillation is a tendency of the N toward finite limits, and such a tendency in any N clearly will not permit the system point to return near a given starting point. In Volterra's discussion of small oscillations of an association about its stationary state is found a case in point.

It will be evident, from the fact that experimental data relate to perhaps a few selected species whose populations are observed as a function of time, that an ergodic theorem in the population dynamics has even a more important position than in classical mechanics. We shall adopt the surmise that biological associations are ergodic.

4. *Canonical Ensembles.*

We may ask now about the behavior of a part, or component, consisting in, say, only ν of the total n species, of an association. The component does not have its G constant throughout time but exchanges G with the rest of the association, only the total G being conserved. Corresponding to the points on the surface $G = G_0$

in the microcanonical distribution are points in the sub-space of dimension ν representing configurations of the component.

How are these component points distributed? The answer is a basic proposition in statistical mechanics: they are distributed according to the law

$$\rho_\nu = e^{\frac{\psi - G_\nu}{\theta}},$$

defining Gibbs' canonical ensemble. The factor (Gibbs' phase integral)

$$e^{-\frac{\psi}{\theta}} \equiv Z = \int e^{-\frac{G_\nu}{\theta}}\, d\tau_\nu$$

is just such as to normalize the distribution,

$$\int \rho_\nu\, d\tau_\nu = 1.$$

$\rho_\nu(v_1, v_2, \ldots, v_\nu)\, d\tau_\nu$ represents the probability that a member of the ensemble (which is in statistical equilibrium) chosen at random will be found in the volume element $d\tau_\nu$ around $(v_1, v_2, \ldots, v_\nu)$. For the mean value of any function of phase we have

$$\bar{f} = \int f \rho_\nu\, d\tau_\nu.$$

The distribution is characterized by the constant θ, its *modulus*, rather than by G (which here is not constant) as in the microcanonical distribution.

The importance of the canonical ensemble in physics comes from the fact that it is a representative ensemble with a capacity for describing not isolated systems with a fixed energy but those which are in thermal equilibrium with their surroundings, continually exchanging energy with them. In the theoretical construction the residual system, that of $n - \nu$ degrees of freedom left over from the original one when the component ν is separated for individual study, holds the position of being the "heat bath" in which the component is immersed. The modulus θ represents the thermodynamic temperature, and ψ the free energy of a system in thermodynamic equilibrium. Through this same door we enter into a 'thermodynamic' description of biological association. It is interesting to see that in our case the decomposability of G does not lead to the awkwardness of introducing some "small" G of interaction between components to provide G-exchange between them, as occurs in mechanics when the Hamiltonian is split into parts. This is inherent in the Volterra equations; the rigorous separation into components in general does not keep them from interacting. It is not implied of course that a weak interaction cannot be introduced between otherwise noninteracting associations.

Another important feature of the canonical ensemble is that when the number of degrees of freedom of its members is large a great preponderance of them have G's in the immediate vicinity of $\bar{G}$ (the canonical mean G), and, not unexpectedly, canonical averages are substantially the same as microcanonical ones on the surface $G = \bar{G}$. This is easy to prove in a familiar computation if G is sufficiently small, when

$$G_r = \tau_r(e^{v_r} - v_r) \simeq \tau_r(1 + \tfrac{1}{2} v_r^2)$$

and G = constant is an ellipsoid; for larger G an approximate computation shows the same thing (effectively what is involved is a sufficiently rapid ascent of the volume enclosed by successively larger constant-G surfaces). The canonical ensemble thus also has the aspect of a mathematical strategem to simplify the calculation of microcanonical averages. Under the adopted ergodic hypothesis we can then regard canonical averages as time averages also. Of course the number of biological degrees of freedom seldom will rival the number of mechanical ones commonly encountered. But it may nonetheless be substantial; when insubstantial the canonical approximation to the microcanonical ensemble weakens and a more precise analysis of component systems is needed; or, for isolated systems with an insubstantial number of degrees of freedom the microcanonical ensemble, and the thermodynamic description provided by *it*, may be employed.

We must in any event emphasize the importance in the present statistical mechanics of fluctuations from expectation values. It will be appreciated also that time averages and relaxation times for attainment of equilibrium, practically speaking, refer here to intervals of time of a completely different order of magnitude than those frequently met in physics.

Dropping now the subscript ν we compute the canonical average of D_r,

$$\overline{D_r} = \int \frac{\partial G}{\partial v_r} e^{-\frac{G}{\theta}} dr \Big/ \int e^{-\frac{G}{\theta}} dr$$

$$= -\theta \int \frac{\partial}{\partial v_r} \left(e^{-\frac{G_r}{\theta}}\right) dv_r \Big/ \int e^{-\frac{G_r}{\theta}} dv_r$$

$$= -\theta \left[\exp - r_r(e^{v_r} - v_r)\right]_{-\infty}^{+\infty} \Big/ \int e^{-\frac{G_r}{\theta}} dv_r$$

$$= 0.$$

As before, the mean N_r is appropriately q_r. Similarly, for the average of T_r we find

$$\overline{T_r} = \int v_r \frac{\partial G}{\partial v_r} e^{-\frac{G}{\theta}} dr \Big/ \int e^{-\frac{G}{\theta}} dr$$

$$= \left\{ -\theta \left[v_r\, e^{-\frac{G_r}{\theta}}\right]_{-\infty}^{+\infty} + \theta \int e^{-\frac{G_r}{\theta}} dv_r \right\} \Big/ \int e^{-\frac{G_r}{\theta}} dv_r$$

$$= \theta.$$

This gives not only the earlier result of equipartition of T but an insight into the meaning of the 'temperature' θ of biological association.

A more perspicuous view of θ comes from the average of D_r^2,

$$\overline{D_r^2} = r_r^2 \overline{\left(\frac{N_r}{q_r} - 1\right)^2} = \int \left(\frac{\partial G}{\partial v_r}\right)^2 e^{-\frac{G}{\theta}} dr \Big/ \int e^{-\frac{G}{\theta}} dr$$

$$= \left\{ -\theta \left[\frac{\partial G_r}{\partial v_r} e^{-\frac{G_r}{\theta}}\right]_{-\infty}^{+\infty} + \theta \int e^{-\frac{G_r}{\theta}} \frac{\partial^2 G_r}{\partial v_r^2} dv_r \right\} \Big/ \int e^{-\frac{G_r}{\theta}} dv_r,$$

but, since $\frac{\partial^2 G_r}{\partial v_r^2} = \frac{\partial G_r}{\partial v_r} + \tau_r$, this becomes

$$\overline{D_r^2} = \theta \left(\int e^{-\frac{G_r}{\theta}} \frac{\partial G_r}{\partial v_r} dv_r \Big/ \int e^{-\frac{G_r}{\theta}} dv_r \right) + \theta \tau_r$$

$$= \theta \tau_r,$$

or, *for all species r*,

$$\theta = \frac{\overline{D_r^2}}{\tau_r} = \tau_r \frac{\overline{(N_r - \overline{N}_r)^2}}{\overline{N}_r^2} = \frac{\beta_r}{q_r} \overline{(N_r - q_r)^2}.$$

In other words the temperature measures, in one number common to all species, the mean square deviations of the populations from their stationary values q_r, and *vice-versa*. Zero temperature corresponds to the completely "quiet" stationary state of biological association. The temperature is, so to speak, a kind of indicator of the level of excitation of the association from its stationary state. Its greater significance is, according to an established theorem, that it tells the preferred direction of flow of G from one association to another weakly coupled to it: on the average the association with higher θ will lose G and decrease its θ, and inversely for the low-θ association. This result, perhaps in the quantitative form following from a knowledge of the "heat" capacities (see below), but at least qualitatively, may be amenable to experimental test.

We might perhaps here conveniently introduce a definition of the thermodynamic state of equilibrium of an association as that for which the mean D_r^2/τ_r has the same value for all species.

Together with ΣT_r, the $\Sigma D_r^2/\tau_r$ is partitioned equally among all species on the average.

The Gibbs phase integral is, with $\alpha \equiv \frac{1}{\theta}$,

$$Z = \int \exp\left(-\alpha \sum G_r\right) d\tau = \Pi \int_{-\infty}^{+\infty} e^{-\alpha G_r} dv_r$$

$$= \Pi \int_0^{\infty} \left(\frac{N_r}{q_r}\right)^{\alpha \tau_r} e^{-\alpha \beta_r N_r} \frac{dN_r}{N_r}$$

$$= \Pi (\tau_r \alpha)^{-\tau_r \alpha} \Gamma(\tau_r \alpha) \equiv \Pi\, Z_r.$$

What is the probability that one species will have its v_r in v_r, $v_r + dv_r$? From either an integration over all coordinates but v_r, or from taking a component to be the one species r, this is

$$P_r dv_r = \frac{e^{-\frac{G_r}{\theta}} dv_r}{Z_r},$$

or, in terms of $n_r \equiv N_r/q_r$.

$$P(n_r)\, dn_r = \frac{n_r^{\alpha\tau_r - 1} e^{-\alpha\tau_r n_r} dn_r}{\alpha\tau_r^{-\alpha\tau_r} \Gamma(\alpha\tau_r)}.$$

This is analogous to the Maxwell-Boltzmann distribution law. It is exactly the distribution of the 'intrinsic abundance' of a species assumed by Corbet, Fisher, and Williams (1943; also Kendall, 1948) to deduce the probability

$$p_i = \left(\frac{at}{1 + at}\right)^i \Bigg/ i \log \left(1 - \frac{at}{1 + at}\right)^{-1} \tag{9}$$

that a catch of individuals in time t contains just i individuals, in the limit that

$$\overline{N} \longrightarrow 0, \ \alpha r \longrightarrow 0, \qquad \frac{\overline{N}}{\alpha r} = a = \text{finite}.$$

These authors found it necessary to take this limit to comprehend the experimental data on catches of butterflies and moths; some meaning of the then obscure but important shape-determining parameter αr(k in Kendall's notation) and of the limit $\alpha r \longrightarrow 0$ ($\theta >> r$) here becomes clear. We may say, perhaps, that the observations were on species of low "intrinsic temperature" r compared to that (θ) of the equilibrium state (one evolved over a long period of time) of the encompassing biological association; quite possibly θ was bigger than a great many r's for different species of that association. The remarkable success of the result (9) would seem to be in some measure an experimental verification of the present scheme.

The moments of order p of n_r are

$$\overline{n_r^p} = \frac{\Gamma(\alpha\tau_r + p)}{\Gamma(\alpha\tau_r)} (\alpha\tau_r)^{-p},$$

and in particular $\overline{N_r}/q_r = 1$ again. In the limit $\theta \longrightarrow 0$ ($\alpha \longrightarrow \infty$) these moments all are unity, expressing, as is necessary, that

$$P(n_r) \longrightarrow \delta(n - 1)$$

When $\alpha r_r > 1$ the most probable n_r, call it $[n_r]$, is

$$[n_r] = 1 - \frac{1}{\alpha r_r} = 1 - \frac{\theta}{r_r},$$

which always is less than $\bar{n}_r$. For $\alpha r_r \leqslant 1$ the most probable n_r is 0, indeed $P(n_r = 0) = \infty$ $(\alpha r_r < 1)$. The distribution in general assigns appreciable weight to N's less than q_r. This is understandable in view of the fact that the surfaces of constant G have a relatively large lobe in the region of $v_r < 0$ compared to the smaller lobe for all $v_r > 0$; then under the ergodic hypothesis we expect phases points generally to spend more time in the first region than the second. The importance of having introduced the "canonical" variables v_r is here apparent.

By ordering the species according to the sequence

$$r_1 \leqslant r_2 \leqslant \ldots \leqslant r_\nu,$$

we may distinguish two categories. At a given temperature θ the lower group having r's less than θ have predominantly very low populations most probably; the upper group with r's exceeding θ most probably have appreciably higher populations.

Turning now to the evaluation of the conventional thermodynamic variables we have for the "free energy" ψ

$$- \psi\, \alpha = \log Z,$$

$$\psi = \sum r_r \log r_r\, \alpha - \frac{\log \Gamma(r_r\, \alpha)}{\alpha} \equiv \sum \psi_r,$$

or, with $x_r \equiv r_r\, \alpha$,

$$\frac{\psi_r}{r_r} = \log x_r - \frac{\log \Gamma(x_r)}{x_r}.$$

The "internal energy (G)" is

$$\bar{G} = - \frac{\partial \log Z}{\partial \alpha}$$

$$= \sum r_r \log r_r\, \alpha + r_r - r_r\, \varphi(r_r\, \alpha) \equiv \sum \bar{G}_r$$

$$\frac{\bar{G}_r}{r_r} = \log x_r + 1 - \varphi(x_r),$$

where $\varphi(x) = d \log \Gamma(x)/dx$ is the digamma function.

The "heat (G) capacity" is

$$C = \frac{\partial \overline{G}}{\partial \theta} = -\alpha^2 \frac{\partial \overline{G}}{\partial \alpha}$$

$$= \sum x_r^2 \varphi'(x_r) - x_r \equiv \sum C_r,$$

$\varphi'(x)$ denoting $d\varphi/dx$, the trigamma function. The "entropy" is

$$\overline{S} = \frac{\overline{G - \psi}}{\theta} = \log Z - \alpha \frac{\partial}{\partial \alpha} \log Z$$

$$= \sum - x_r \varphi(x_r) + x_r + \log \Gamma(x_r) \equiv \sum \overline{S}_r.$$

The behavior of the single-species contributions to these variables as functions of $\frac{1}{x} = \frac{\theta}{r}$ or of x are shown in the figures (Figures 1-4). All but ψ_r/r_r increase monotonically with increasing temperature. C_r alone tends for large θ asymptotically to a limit, $C_r = 1$,—whence an analog to the Dulong-Petit law,—and comes to the value $\frac{1}{2}$ linearly as θ vanishes, whence no analog to the Nernst heat theorem. $\overline{S}_r$ increases in magnitude without bound in the limits of both small and large θ, the state of lowest ($-\infty$) entropy being the stationary state of association, $\theta = 0$.

In the limit of high temperatures,

$$\frac{\overline{G_r}}{r_r} \longrightarrow \frac{\theta}{r_r} - \log \frac{\theta}{r_r} + 1 - \varphi(1) = \frac{\theta}{r_r} \left(1 - O\left(\frac{\log \theta}{\theta}\right)\right).$$

Therefore in this limit G is equipartitioned amongst all species. At small θ,

$$\frac{\overline{G_r}}{r_r} \longrightarrow 1 + \frac{1}{2}\frac{\theta}{r_r}, \qquad \overline{G_r} - r_r \longrightarrow \frac{1}{2}\theta,$$

so that

$$\sum G_r - G_{r\,\min} \qquad (G_{r\,\min} \equiv r_r)$$

is equipartitioned. Altogether then $\sum G_r - G_{r\,\min}$ is equipartitioned

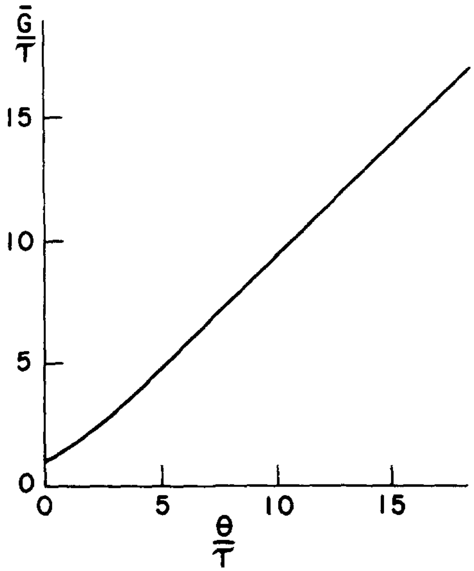

FIGURE 1a. Single-species contribution to internal energy, giving $\bar{G}$ as function of association temperature θ for fixed intrinsic temperature τ.

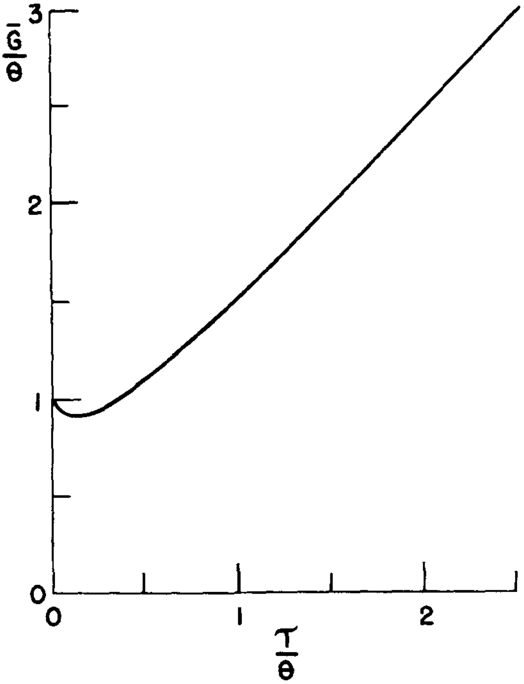

FIGURE 1b. Single-species $\bar{G}$ as function of τ for fixed θ.

for low temperatures at $\frac{1}{2}\,\theta$ per degree of freedom and for high temperatures at θ per degree of freedom. We may note also that the general rule of mixing,

$$\int_{\theta_1}^{\theta} C_A \, d\theta = \overline{G_A}(\theta) - \overline{G_A}(\theta_1) = \overline{G_B}(\theta_2) - \overline{G_B}(\theta) = \int_{\theta}^{\theta_2} C_B \, d\theta,$$

giving the final equilibrium temperature θ of two equilibrium associations A and B at initial temperatures θ_1 and $\theta_2 > \theta_1$ when placed in weak interaction, has the corollary

$$\nu_A \, (\theta - \theta_1) = \nu_B \, (\theta_2 - \theta), \qquad \theta = \frac{\nu_B \, \theta_2 + \nu_A \, \theta_1}{\nu_B + \nu_A},$$

for all temperatures sufficiently high or all sufficiently low (ν_A and ν_B denoting the number of species in each association).

The entropy, as in conventional statistical mechanics, measures higher for systems in equilibrium, represented by the canonical ensemble, than the corresponding quantity ($-\log \rho$) for other states of the systems (represented by other than canonical ensembles)

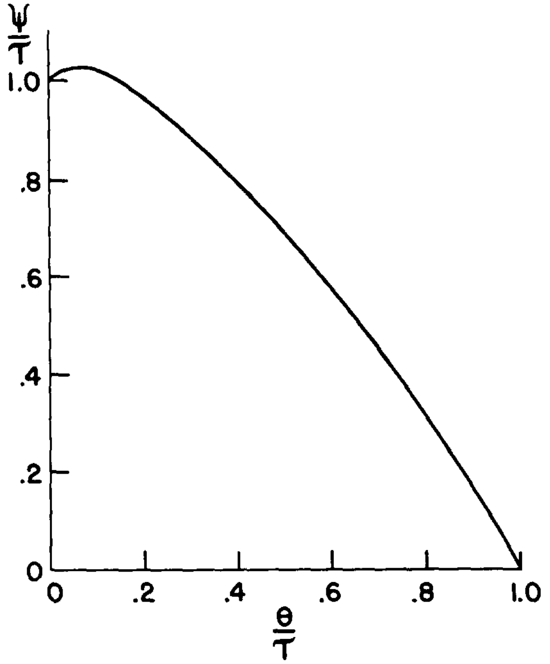

FIGURE 2a. Free energy per species for fixed r and variable θ.

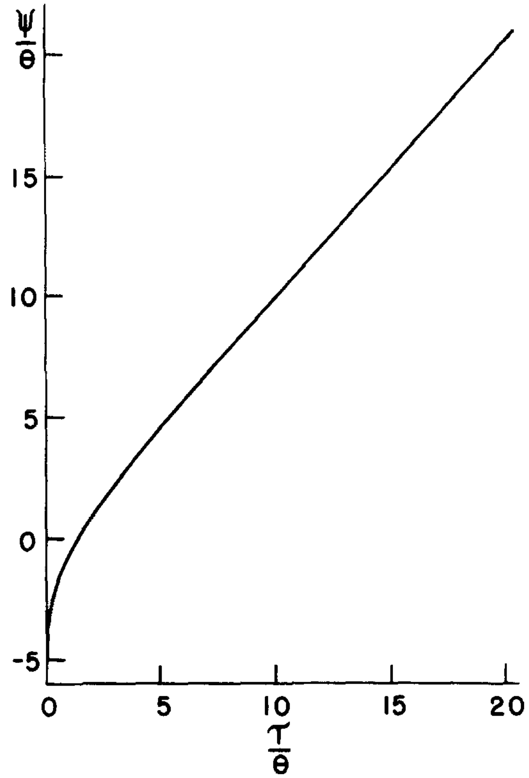

FIGURE 2b. Free energy per species for fixed θ and variable τ.

having the same mean G. And in the well-known sense of Gibbs' coarse-grained view of the density in phase, non-equilibrium states tend to decline into equilibrium ones of maximal entropy. It must not be forgotton here that, because the number of degrees of freedom in a biological association is not so enormously large as that of physical systems studied by the same methods, the tendency toward equilibrium may be expected to be somewhat obscured by noticeable fluctuations.

We have thermodynamic variables but no thermodynamics as yet. The previous considerations are really calorimetric rather than thermodynamic in character, as the only independent variable of state is the temperature θ and the only process contemplated is "heat" (G) transfer from one system to another. The thing that is missing is the concept of *work*.

In mechanics the Hamiltonian is laden with "external parameters" such as the volume of the system and strengths of external gravitational or other fields acting on its parts; when altered these pro-

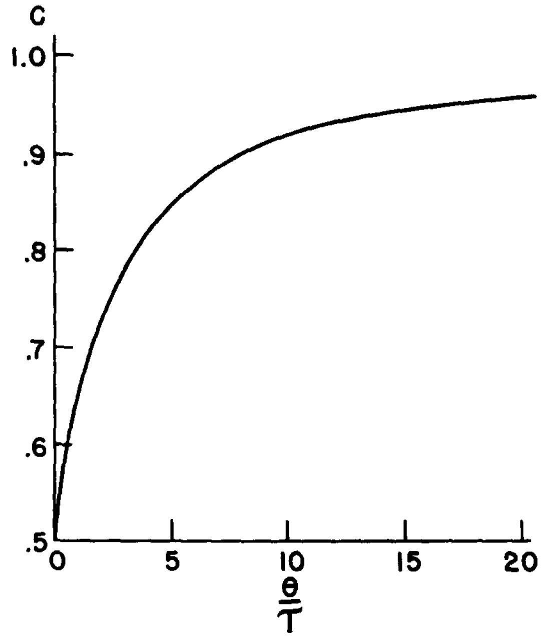

FIGURE 3. Heat capacity per species as function of association temperature θ.

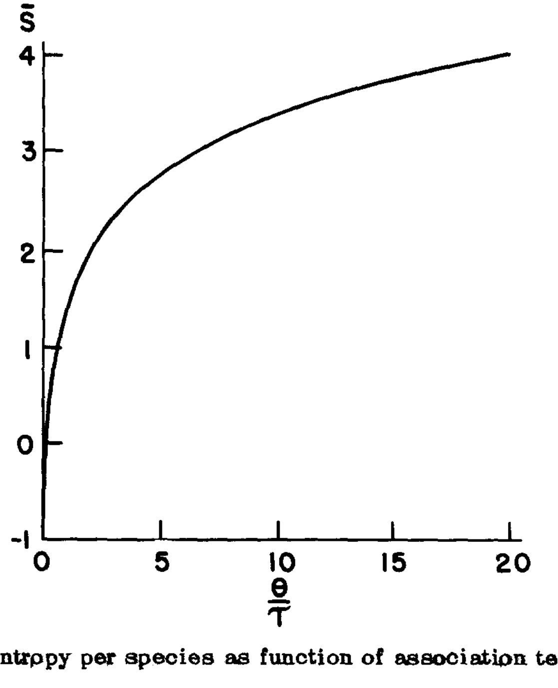

FIGURE 4. Entropy per species as function of association temperature θ.

duce alterations in the state of the system, in fact they alter the system itself, and so are variables of state. What, in Schrödinger's phrase (1952), are these "screws, pistons, and what not" by which we can squeeze on a biological association? What indeed are the observables other than the population numbers? They are the real physical and chemical variables of the *milieu exterieur*: physical temperature, pressure, radiation and other field strengths, and chemical abundances. Physical temperature particularly has a preeminent place, being like the volume in thermodynamics, a universal type of external parameter and playing a universally important role.

Consider therefore that the τ_r are functions of these exterior variables, say a_i, and through them so is the G of an association. In the customary way, define the generalized forces,

$$F_i = -\frac{\partial G}{\partial a_i} = -\sum_r \frac{\partial \tau_r}{\partial a_i}(e^{v_r} - v_r).$$

Then the canonical mean F_i is

$$\begin{aligned} \overline{F_i} &= -\frac{\partial \psi}{\partial a_i} = -\sum_r \frac{\partial \psi_r}{\partial a_i} = \sum_r \overline{F_{ir}} \\ \overline{F_{ir}} &\equiv -\frac{\partial \tau_r}{\partial a_i}(\log x_r + 1 - \varphi(x_r)), \end{aligned} \tag{10}$$

and plainly

$$\frac{\overline{G_r}}{\tau_r} = -\frac{\overline{F_{ir}}}{\dfrac{\partial \tau_r}{\partial a_i}}; \qquad \overline{F_{ir}} = -\overline{G_r}\frac{\partial}{\partial a_i}\log \tau_r.$$

Equations 10 are loosely analogous to Dalton's law of partial pressures and constitute a system of equations of state. If there be a single equation of state it is perhaps equation (10) with a_i = physical temperature T. When the association temperature θ is large, because of the equipartition of $\overline{G}$ we have

$$\overline{F_T} = -\theta \sum \frac{\partial}{\partial T} \log \tau_r.$$

For the sake of illustration only we might suppose, in a crude but not impossible approximation that each $\tau_r(T) = b_r T^{-\lambda_r}$ over some limited range of T; then the equation of state reads

$$\overline{F_T}\,T = \lambda\nu\theta, \quad \left(\lambda = \sum \lambda_r\right),$$

ν being the number of degrees of freedom in the association. This is analogous to the gas law $PV = NkT$, with $\overline{F_T}, T, \theta$ the analogs of P, V, T, though $\overline{F_T}$ of course is not a single datum of direct experience as is P.

It is evident at this point that we are carried into thermodynamics proper but without an adequate experimental frame of reference. To proceed further into a discussion of cycles (like Carnot's) in a T,θ plane, of transport processes (like conduction of G in physical space, under some kind of Fourier conduction law), in short to elaborate further the interplay in the large of the biological and physical worlds, seems perhaps possible but now premature.

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