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LETTER TO THE EDITOR

Rigorous results in equilibrium statistical mechanics of terrestrial ecosystems

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Abstract. Equilibrium statistical mechanics of terrestrial ecosystems is briefly outlined and rigorous results are stated.

In this brief report on recent results in statistical mechanics of a certain class of many-body open systems, we extend the ideas of Kerner (1957, 1959, 1972) (see also Goel *et al* 1971), who applied statistical physics to Volterra-Lotka subsystems. We are studying instead ecosystems in more generality, and investigate a more general type of subsystem dynamics suited to general ecosystems, and attempt to clarify the notion of a Gibbs state on these subsystems, which are composed of biological species and inorganic substances. From a very abstract but useful point of view, terrestrial ecosystems are defined here to be maps of subsets of a base manifold into C^* -dynamical systems of the C^* -algebra generated from the Banach space of continuous functions on the phase space as common in classical statistical mechanics (see, e.g. Ruelle 1974), together with a semigroup of automorphisms (see, e.g. Emch 1972). They are mathematically special cases of sheaves of C^* -dynamical systems. The phase space is a manifold of biotic observables q_j , e.g. the logarithms of the biomasses, in tensor product with the manifold of abiotic factors, e.g. the logarithms of chemical masses or climatic factors. States on the C^* -dynamical systems are in algebraic statistical mechanics (see, e.g. Emch 1972) elements of the topological dual of the algebra, i.e. they are linear, normalized, positive continuous functionals, or measures, often absolutely continuous measures, given by a \mathcal{L}_1 distribution function as weight function. The time evolution acts on the algebra and induces, by duality, a time evolution on the state space which describes the dynamics of the terrestrial ecosystem.

Subsystems are cells or compartments of the ecosystem, which are large compared to the mean free intermolecular collision path, but small compared to the dimension of the terrestrial ecosystem. They are therefore assumed to be locally in thermodynamic equilibrium with respect to molecular physics. The dynamics of these, e.g. $2n$ cells, is assumed to be given by a Hamiltonian flow on the phase space elements $q_j, j = 1, \dots, 2n$. Consequently it is of the form

$$\frac{d}{dt} q_i = - \sum_{j=1}^{2n} (\Gamma^{-1})_{ij} \frac{\partial U}{\partial q_j} = F_i \quad (1)$$

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where Γ is an antisymmetric, non-singular matrix and U is a many-body, or more generally, many-cell biophysical interaction energy. This is the most general form of Hamilton's equations, because Γ induces a symplectic structure on the phase space by a similarity transformation (see, e.g. Gantmacher 1966). From biological reasoning it is straightforward that the biophysical interaction energy U is permutation invariant, and, if one-cell potentials are considered only, should diverge linearly in $|q|$ for large negative q and diverge for large positive q (Goel *et al* 1971, Kerner 1957, 1972, Messer 1992a, b). Since nonlinear oscillations should be essential, one can give a reasonable approximation of the general form of the many-cell biophysical interaction energy

$$U(q_1, \dots, q_{2n}) = \sum_{k=1}^{2n} \sum_{1 \leq i_1 < \dots < i_k \leq 2n} V^k(q_{i_1}, \dots, q_{i_k}) \quad (2)$$

by one-cell potentials through the biophysical anharmonic oscillator interaction energy

$$U = - \sum_{j=1}^{2n} \tau_j (q_j - e^{q_j}). \quad (3)$$

For very general, but differentiable many-cell potentials, e.g., as in (2), we have:

Lemma 1. U is an integral of motion.

The equations of motion (1) are the Euler-Lagrange equations of a straightforward generalization of Kerner's Lagrangian (Kerner 1959). Therefore, the canonical momentum and the observables q_j are linearly dependent, and this can be considered as an additional conservation law. Thus, we suggest

$$\mathfrak{H}((p), (q)) = \alpha \{ U(\alpha^{-1} \Gamma^{-1}(p)) + U((q)) \} \quad (4)$$

with $\alpha \in \mathbb{R}$, $\alpha > 0$, but otherwise arbitrary, as Hamiltonians. The system is described by doubling the 'configuration space' and introducing momentum variables in the second space by the above-mentioned linear relation between momenta and observables. The $4n$ -dimensional tensor product of these two spaces is a possible true phase space on which the Hamiltonian dynamics act and confines the motion to a $(2n-1)$ -dimensional hypersurface.

We are able to prove:

Lemma 2. \mathfrak{H} is a Hamilton function. The Hamilton equations and the equations of motion are identical.

Lemma 3. There are $2n+1$ integrals of motion in \mathbb{R}^{4n} , $\{\mathfrak{H}, \mathfrak{C}_j; j=1, \dots, 2n\}$, with

$$\mathfrak{C}_j = q_j - \sum_{k=1}^{2n} (\Gamma^{-1})_{jk} p_k \quad (5)$$

and

$$\{\mathfrak{H}, \mathfrak{C}_j\} = 0 = \{\mathfrak{H}, \mathfrak{H}\} \quad (6)$$

$$\{\mathfrak{C}_i, \mathfrak{C}_j\} = 2(\Gamma^{-1})_{ij}. \quad (7)$$

More details will be presented in a forthcoming article (Messer 1992b).

A second method to introduce a possible true phase space, uses, as already described above, the fact that half of a suitable linear combination of the subsystem observables q_j are configurations, whereas the other half are canonical momenta, and Γ as an antisymmetric matrix already induces the symplectic structure (see, e.g. Gantmacher 1966). This theory is an extension of a later theory of Kerner (1964).

The canonical ensemble is defined by the Gibbs state of the Hamiltonian. The Gibbs measure is associated with the weight function

$$Z^{-1} \exp(-\beta \mathcal{H}((p), (q))). \quad (8)$$

At this point our presentation deviates from Kerner's scheme. He has, at first (Kerner 1957), simply taken

$$\tilde{Z}^{-1} \exp(-\beta U((q))) \quad (9)$$

as the weight function for Volterra-Lotka interactions, not taking into account the fact that the biophysical energy function $U((q))$ does not satisfy the Hamilton equations of motion.

We are able to give two rigorous theories of the canonical state in applying the two possible correct phase spaces introduced above.

Lemma 4. If $U(q_1, \dots, q_{2n}) = \sum_{j=1}^{2n} u_j(q_j)$ with

$$u_j(q) = \tau_j(e^q - q) \quad (10)$$

i.e. the one-cell potential of a Volterra-Lotka interaction system, then the partition function is

$$Z = Z_0^2 |\det \Gamma|^{-1} \quad (11)$$

with

$$Z_0 = \prod_{j=1}^{2n} Z_{1j} \quad (12)$$

and

$$Z_{1j} = \int_{-\infty}^{\infty} dq \exp(-\beta u_j(q)) = (\tau_j \beta)^{-\tau_j \beta} \Gamma(\tau_j \beta). \quad (13)$$

The free energy $F_\infty(\beta)$, in the limit of an infinite number of cells, is given by

$$\beta F_\infty(\beta) = \int_0^\infty ((\tau \beta) \ln(\tau \beta) - \ln \Gamma(\tau \beta)) Z(\tau) d\tau \quad (14)$$

with $Z(\tau)^{-1} = d\tau/dj$ and whereby $\Gamma(z)$ denotes the gamma function at z . Similar expressions exist for the derived thermodynamic functions of the canonical ensemble (Messer 1992b).

The thermodynamic functions and the probability distribution for the observables q_j , after tracing out the momenta, are essentially identical to Kerner's expressions for both of our two rigorous theories.

Apart from the very particular Volterra-Lotka interactions, used in lemma 4, one has for very general potentials the following results.

Theorem 5. If the interaction is composed of stable and weakly tempered many-body or many-cell potentials, which are elements of the metric cone $(\mathcal{H}_{S,WT}, d_\rho(\cdot, \cdot))$, introduced by Messer (1977, 1979), then the free energy per cell converges in the thermodynamic limit, where $n \rightarrow \infty$ and the 'logarithmic biomass volume' diverges in the sense of Fisher; however, the ratio approaches the density ρ .

The proofs of this and related theorems are given by Messer (1992b). We have used topological arguments following equicontinuity with respect to a metric cone of interactions introduced by Messer (1977, 1979).

For the thermodynamic limit of the correlation functions, one has at first the particular result:

Lemma 6. If U is composed of Volterra-Lotka one-cell potentials, as defined in lemma 4, or, more generally, if U is composed out of one-cell potentials only, but with finite one-cell partition functions, then there exists the thermodynamic limit of the correlation functions in the sense of Fisher for every thermodynamic parameter, and coincides with those of the product state.

In the general case one cannot expect convergence, because of the possible existence of phase transitions. However, we have succeeded (Messer 1992b) in proving a weak version of the Gibbs phase rule, using the topological techniques of metric cones of interactions (Messer 1977, 1979).

Theorem 7. If the potential is a superstable, lower regular and weakly tempered many-body, or many-cell potential, element of the metric cone $(\mathcal{H}_{SS,LR,WT}, d_\rho(\cdot, \cdot))$, introduced by Messer (1977, 1979), then the mean canonical correlation functions converge weakly, and in the sense of Fisher with respect to a net of diverging 'logarithmic biomass volumes', d_ρ -almost everywhere.

The last theorem is not stated in full precision; however, it will be formulated and explained in more detail in a forthcoming article (Messer 1992b).

Empirical curves and forestal measurement data have been compared with the theoretical equilibrium distributions (Messer 1992b). From these data one may conclude that selection forests are in equilibrium states of the above type.

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