THE UNIVERSALITY HYPOTHESIS IN CLASSICAL STATISTICAL MECHANICS

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A broad class of models amenable to the methods of classical statistical mechanics is presented. A formal verification of a certain aspect of the universality hypothesis for critical phenomena is obtained within this context.

The universality hypothesis [1,2] suggests that there is a wide class of systems in which critical exponents [3] are determined uniquely by the spatial dimensionality d of the system and the dimensionality n of the underlying order parameter [3,4]. A characteristic property of an n-dimensional order parameter – which will be important below – is that, in the absence of any ordering field, its probability distribution has the symmetry of an $(n-1)$-sphere. If this symmetry is spontaneously broken, ordering occurs. At a critical point spontaneous ordering vanishes continuously.

Much of the work which supports this hypothesis is concerned with classical spin assemblies [5,6]. These are generalisations of idealized magnetic systems and they have order parameters which are vectors in the space of all ordered n-tuples of real numbers equipped with the usual notion of length. (Some notion of length is necessary if one is to characterize an $(n-1)$-sphere as the set of all points at a given distance from some fixed point.)

Suppose that the dimension d is fixed. Consider a system in which the order parameter and the associated notion of length are not of the classical spin type. Suppose that the order parameter – which might be a function, matrix, polynomial, etc., etc. – is a vector in an abstract n-dimensional vector space furnished with some notion of length. Then, according to the universality hypothesis, if the system displays critical behaviour, this should be of the same type as that found in a classical spin assembly with the same value of n. The details should be irrelevant.

There is some evidence which supports the above view. This comes mainly from approximate studies of isotropic and anisotropic classical and quantum spin models [3–10] and from arguments of a physical nature involving block-spin and other renormalization group approaches [8–10]. However, there seems to have been little in the way of formal studies. The purpose of this note is to rectify this and to present results which amount to the formal verification of the above aspect of the universality hypothesis for a broad class of models amenable to the methods of classical statistical mechanics.

Consider an assembly of N identical but distinguishable microsystems. Suppose that the state of the ith microsystem corresponds to a vector ξ_i in an abstract n-dimensional vector space $\mathcal{V}$ in which real numbers play the role of scalars. Suppose that the hamiltonian H of the assembly is the sum of pair interactions. In addition, suppose that the interaction energy $E_{ij}(\xi_i, \xi_j)$ of the arbitrary pair i, j of micro-systems has the following properties:

$$E_{ij}(\xi_i, \xi_j) = -2J_{ij}F(\xi_i, \xi_j)\,, \tag{1}$$

where J_{ij} is a constant and, quite generally,

$$F(\xi_1, \xi_2) = F(\xi_2, \xi_1)\,, \tag{2}$$

$$F(\alpha\xi_1 + \beta\xi_1', \xi_2) = \alpha F(\xi_1, \xi_2) + \beta F(\xi_1', \xi_2)\,, \tag{3}$$

$$F(\xi, \xi) \geqslant 0\,, \tag{4}$$

α and β being scalars and the equality in eq. (4) holding if and only if ξ is the zero vector. Any F satisfying eqs. (2)–(4) is acceptable. Such F's correspond to inner products on $\mathcal{V}$ [11]. Furthermore, if one puts

$$\|\xi\| = \sqrt{F(\xi, \xi)}\,, \tag{5}$$

for all ξ, then $\|\cdot\|$ serves as a length on $\mathcal{V}$ [11].

The motivation for eqs. (1)–(4) comes from the standard microscopic form of the classical n-vector model. In this, the states ξ_i, ξ_j are "spins" or n-tuples $\boldsymbol{s}_i, \boldsymbol{s}_j$ of real numbers and the pair interaction energies have the form $-2J_{ij}\boldsymbol{s}_i \cdot \boldsymbol{s}_j$ where $\cdot$ denotes the usual inner product for such real n-tuples. Eqs. (1)–(4) are all satisfied in this case and eq. (5) corresponds to the notion of length familiar from Pythagoras's theorem. Thus the above scheme represents a broad generalization of the standard situation.

The fact that spin assemblies are included as a special case helps one to proceed with the theory. It suggests that, in the general case, one should couple an ordering field h – which is a vector in $\mathcal{V}$ – to the system by adding to the hamiltonian the one-body terms $-m_i F(h, \xi_i)$ where the m_i are real constants. It also indicates that one should expect the quantity $N^{-1}\Sigma m_i \xi_i$ to serve as an order parameter. (A spin $\boldsymbol{s}_i$ has an energy $-m_i \boldsymbol{H}\cdot \boldsymbol{s}_i$ in a magnetic field $\boldsymbol{H}$ where m_i is the magnetic moment per spin. In a spin assembly the spontaneous magnetization $N^{-1}\Sigma m_i \boldsymbol{s}_i$ is an order parameter.)

The calculation of physical properties proceeds, in the general case, via integrals of the form

$$I(A) = \int_S A \exp(-H/kT)\,\mathrm{d}\sigma\,, \tag{6}$$

where A is a real valued function of the state $(\xi_1, ..., \xi_N)$ of the assembly, k is Boltzmann's constant and T is the absolute temperature. In eq. (5), S denotes the set of all states of the assembly satisfying $\|\xi_1\| = 1, ..., \|\xi_N\| = 1$. Since – as is shown in ref. [11] – eqs. (1)–(5) imply that

$$|F(\xi_1, \xi_2)| \leqslant \|\xi_1\| \times \|\xi_2\|\,, \tag{7}$$

this restriction to S yields pair interaction emergies which are bounded. Furthermore, in the special case of real n-tuples, the restriction is equivalent to the standard constraint $\boldsymbol{s}_1 \cdot \boldsymbol{s}_1 = 1, ..., \boldsymbol{s}_N \cdot \boldsymbol{s}_N = 1$;

Eq. (6) appears to involve a surface integral. There are often theoretical difficulties associated with such integrals. Volume integrals are usually free of these. The natural measure-theoretic notion of integration in $\mathcal{V}$ leads to volume integrals in the state space of the assembly. Thus it is convenient to define eq. (6) via an integral over the set of all $(\xi_1, ..., \xi_N)$ satisfying $1 \leqslant \|\xi_1\| \leqslant 1+\epsilon, ..., 1 \leqslant \|\xi_N\| \leqslant 1+\epsilon$. The definition involves dividing this integral by ϵ^N and taking the limit as $\epsilon \to 0$. It is convenient to regard A and H as taking the same value at $(\xi_1, ..., \xi_N)$ as at the point $(\xi_1/\|\xi_1\|, ..., \xi_N/\|\xi_N\|)$ of S. One can check directly that, in the case of real n-tuples, one obtains, in this way, the standard integration over products of hyperspheres [5,6].

Two results remain to be established. First, one must show that the probability distribution of the order parameter in the general model has the appropriate symmetry. Second, one must show that the critical exponents of an arbitrary case of the general model are the same as those displayed by some classical spin assembly with the same value of n.

The question of symmetry can only be tackled if a length can be ascribed to the order parameter $N^{-1}\Sigma m_i \xi_i$. Thus it is important that $N^{-1}\Sigma m_i \xi_i$ is a vector in $\mathcal{V}$. This means that the length of eq. (5) is available.

Let U be the set of all vectors of the form μe_1, where μ is any scalar satisfying $M \leqslant \mu \leqslant M + \Delta$ with M and Δ constant and e_1 is a vector in $\mathcal{V}$ with the property that $\|e_1\| = 1$. Let V be as U but with the unit vector f_1 in place of e_1. The probability that the order parameter $N^{-1}\Sigma m_i \xi_i$ takes a value in U is given by the integral

$$P(U) = \int_S \chi_U \exp(-H/kT)\,\mathrm{d}\sigma\,, \tag{8}$$

where $\chi_U = 1$ if $N^{-1}\Sigma m_i \xi_i \in U$ and $\chi_U = 0$ otherwise. To establish the symmetry discussed above one needs to show that, in the absence of the ordering field h, $P(U) = P(V)$. Extend e_1 and f_1 to the orthonormal bases $(e_1, ..., e_\alpha, ..., e_n)$ and $(f_1, ..., f_\alpha, ..., f_n)$ respectively of $\mathcal{V}$. (This can always be done via the extension theorem and the Gramm–Schmidt process [11].) Let σ be the linear transform defined here by $f_\alpha = \sigma e_\alpha$. The idea is to use σ to "change coordinates" in eq. (8). One can check directly that σ followed by χ_U is χ_V and that, in zero field, H is unchanged when coupled with σ. The second result follows from the invariance of inner products under σ. This invariance means that lengths are preserved so that the measure used in integration is also preserved. One therefore finds that

$$P(U) = \int_S \chi_V \exp(-H/kT)\,\mathrm{d}\sigma = P(V)\,, \qquad (9)$$

which is the required symmetry condition.

Attention can now be turned to the question of how the physics of an assembly depends on the nature of the vectors ξ_i and the inner product F. The perspective established above leads one to choose, as standard, the case where the vectors are real n-tuples $\boldsymbol{s}_1, ..., \boldsymbol{s}_i, ..., \boldsymbol{s}_j, ..., \boldsymbol{s}_N$ and where $F(\boldsymbol{s}_i, \boldsymbol{s}_j) = \boldsymbol{s}_i \cdot \boldsymbol{s}_j$ and attempt to relate all other cases to this. A key concept turns out to be an isometry which is a one–one linear transformation between vector spaces equipped with inner products which preserves these inner products. (The map σ between $\mathcal{V}$ and $\mathcal{V}$ used above is an isometry.)

Choose a basis $(e_1, ..., e_\alpha, ..., e_n)$ of $\mathcal{V}$ which is orthonormal with respect to the given inner product F. (It has already emerged that such a choice is always possible.) Write any vector ξ as $e_1 s_1 + ... + e_n s_n$. It is easy to see that the correspondence $\xi \leftrightarrow (s_1, ..., s_n)$ between abstract vectors and F and real n-tuples and $\cdot$ is an isometry. The idea is again to "change variables" – but this time to do it in eq. (6) and to use the above correspondence υ.

In the abstract model the natural notion of measure derives from F via the length introduced at eq. (5). In the space of real n-tuples, one uses the corresponding notion based on $\cdot$ and this is equivalent to adopting the standard procedures of multi-variable calculus. Because υ is an isometry, it follows that a set of abstract vectors and the set of real n-tuples corresponding to it have the same measure. This means that on changing variables one finds that the definition adopted for eq. (6) yields

$$I(A) = \lim_{\epsilon \to 0} \epsilon^{-N} \int_1^{1+\epsilon} \mathrm{d}r_1 \ldots \int_1^{1+\epsilon} \mathrm{d}r_N$$

$$\times \int_{S_1} \mathrm{d}\Omega_1 \ldots \int_{S_N} \mathrm{d}\Omega_N\, A' \exp(-H'/kT)\,, \qquad (10)$$

where $\mathrm{d}\Omega_1, ..., \mathrm{d}\Omega_N$ denote elements of surface area on the unit $(n-1)$-spheres $S_1, ..., S_N$ and A' and H' are obtained from A and H by using υ to replace $\xi_1, ..., \xi_N$ by n-tuples $\boldsymbol{s}_1, ..., \boldsymbol{s}_N$. Because of the way A and H are determined off S in the definition of eq. (6), A' and H' are independent of $r_1, ..., r_N$. This means that one has proved that

$$I(A) = \int_{S_1} \mathrm{d}\Omega_1 \ldots \int_{S_N} \mathrm{d}\Omega_N\, A' \exp(-H'/kT)\,, \qquad (11)$$

where H' is obtained from H by replacing each term $-2J_{ij}F(\xi_i, \xi_j)$ by $-2J_{ij}\boldsymbol{s}_i \cdot \boldsymbol{s}_j$ and each term $-m_i F(h, \xi_i)$ by $-m_i \boldsymbol{H} \cdot \boldsymbol{s}_i$, where $\boldsymbol{H}$ and h correspond via υ. (Of course A' may be obtained similarly.)

The right-hand side of eq. (11) is in the usual form in which statistical mechanical properties of classical spin assemblies are expressed. This means that one has proved that the statistical mechanical properties of an arbitrary case of the general model are the same as those of a certain classical spin assembly with the same value of n. If one takes $A = 1$ – which yields $A' = 1$ – one finds that, in particular, this result applies to the partition function and corresponding thermodynamic properties of the assembly.

The fact that "the physics" is the same for all the above models of course implies a fortiori that, in particular, critical exponents have the same values. When one combines this result with the symmetry property of the order parameter established above, one finds that one has, as promised, formally verified a certain aspect of the universality hypothesis.

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