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Eigenvalue Degeneracy as a Possible "Mathematical Mechanism" for Phase Transitions*

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Some years ago Ashkin and Lamb noted that the phase transition in the two-dimensional Ising model with nearest-neighbor interaction was characterized mathematically by an asymptotic degeneracy of the largest eigenvalue of a linear operator. More recently Kac and Thompson showed this eigenvalue degeneracy also characterized the phase transition in the Kac model (with weak, long-range forces), suggesting that this "mathematical mechanism" is not restricted to systems with short-range forces. However both the Kac model and the Ising model consider the "spins" to be one-dimensional unit vectors assuming only the *discrete* values +1 and −1. We are therefore led to consider the nature of the phase transition in one of the few exactly soluble models in which the spins can assume an entire continuum of orientations—the closed linear chain of classical spins of arbitrary spin dimensionality interacting isotropically through the Hamiltonian

$$\mathcal{H}_\nu = -\sum_{i=1}^{N} J_{i,i+1}\mathbf{S}_i^{(\nu)}\cdot\mathbf{S}_{i+1}^{(\nu)},$$

where the exchange constants $J_{i,i+1}$ are arbitrary numbers. We find for all spin dimensionalities ν that the two-spin correlation function may be expressed as $\rho_N^{(\nu)}(r) = (\lambda_1^{(\nu)}/\lambda_0^{(\nu)})^r$, where $\lambda_0^{(\nu)}$ and $\lambda_1^{(\nu)}$ are the largest and next-largest eigenvalues of a certain linear operator. Thus the onset of long-range order, $\lim_{r\to\infty}\rho_N^{(\nu)}(r)\neq 0$, is characterized by the degeneracy of $\lambda_0^{(\nu)}$ and $\lambda_1^{(\nu)}$. This onset of long-range order occurs at a critical temperature $T_c^{(\nu)}=0$, for all values of spin dimensionality ν.

Considerable attention has focussed recently on the question of whether there might be some universal "mathematical mechanism" characteristic of phase transitions in a wide variety of soluble model systems. For example, it has been appreciated for some time that the phase transition in the Ising model is characterized by the asymptotic degeneracy of the eigenvalue spectrum of an appropriate linear operator. Specifically, the asymptotic degeneracy of the largest eigenvalue of the transfer matrix was shown by Ashkin and Lamb,[1] almost three decades ago, to provide the mathematical mechanism for the onset of long-range order in the Ising model,

$$\mathcal{H}_I \equiv -J\sum_{\langle i,j\rangle} S_i^{(1)}S_j^{(1)}, \qquad (1)$$

where the summation in (1) is restricted to nearest-neighbor pairs of sites $\langle i,j\rangle$.

Recently Kac and Thompson[2] asked the question whether the eigenvalue degeneracy mechanism was restricted to systems with nearest-neighbor interactions. To this end, they were led to consider a soluble example of a system which possesses long-range interactions, the "Kac model",

$$\mathcal{H}_K \equiv -\gamma J\sum_{i,j}\exp(-\gamma\,|\,i-j\,|)\,S_i^{(1)}S_j^{(1)}, \qquad (2)$$

where here the summation is over all N sites i and j in the entire lattice. They found that the mathematical mechanism associated with the onset of long-range order in the Kac model (with weak, long-range forces) was essentially the same as that in the Ising model (with strong, short-range forces), thereby suggesting that the eigenvalue degeneracy mechanism is not restricted to a particular type of force range.

We are naturally led to question to what extent this "eigenvalue degeneracy mechanism" is restricted in generality, since for both Hamiltonians (1) and (2),

(a) the spins are allowed to assume only the discrete values +1 and −1, and

(b) the spin "dimensionality" is unity—i.e., the spins are simple one-dimensional scalar quantities.

A very recent calculation by Thompson[3] is relevant to point (a). Specifically, Thompson has shown that the eigenvalue degeneracy mechanism is responsible for the onset of long-range order in the spherical model[4] for lattice dimensionality $d=1$, 2, and 3. The spherical model is generally defined[4] as a "continuum modification of the $S=\frac{1}{2}$ Ising model" in which the one-dimensional spins $S_i^{(1)}$ in Eq. (1) are no longer restricted to the discrete values $+1$ and -1, but instead are allowed to assume any values whatsoever so long as the sum of their squares is equal to the total number of spins in the system. To the extent that the spherical model can also be regarded[5] as a model in which the spins are "infinite-dimensional isotropically interacting unit vectors", Thompson's calculation[3] is also relevant to point (b), suggesting perhaps that the eigenvalue degeneracy mechanism has a greater generality. In this note we present additional evidence in support of this conjecture, by considering another exactly soluble system, namely a linear chain of N classical spins $\mathbf{S}_i^{(\nu)}$ of arbitrary dimensionality ν which are interacting isotropically with one another as described by the Hamiltonian[6]

$$\mathcal{H}_\nu \equiv -J\sum_{i=1}^{N} \mathbf{S}_i^{(\nu)}\cdot\mathbf{S}_{i+1}^{(\nu)}, \tag{3a}$$

where $\mathbf{S}_{N+1}\equiv\mathbf{S}_1$. Thus the "spins" are essentially unit vectors; if $[\sigma_1(i), \sigma_2(i), \cdots, \sigma_\nu(i)]$ are the Cartesian components of spin $\mathbf{S}_i$, we require that

$$\sum_{n=1}^{\nu} \sigma_n^2(i)=1. \tag{3b}$$

We observe that the Hamiltonian (3) reduces for $\nu=1$, 2, and 3 respectively to the $S=\frac{1}{2}$ Ising, plane rotator, and classical Heisenberg models respectively. Also in the limit $\nu\rightarrow\infty$, the thermodynamic properties of (3) are essentially those of the Berlin–Kac spherical model.[4] We shall see that (in the thermodynamic limit $N\rightarrow\infty$) this system displays long-range order at the same critical temperature $T_c=0$ for all spin dimensionalities ν.

The main point of our calculation is that for all ν the two-spin correlation function $\rho_N^{(\nu)}(r)$ can be expressed in terms of the ratio of the largest to the next-largest eigenvalue of a certain linear operator,

$$\rho_N^{(\nu)}(r)\sim(\lambda_1^{(\nu)}/\lambda_0^{(\nu)})^r, \qquad [N\rightarrow\infty], \tag{4}$$

where $\lambda_0^{(\nu)}$ and $\lambda_1^{(\nu)}$ are, respectively, the largest and next-largest eigenvalues of a certain linear operator. The eigenvalue spectrum $\lambda_n^{(\nu)}$ is found to be discrete for all $T>T_c$, whereas when $T\rightarrow T_c$, the entire discrete spectrum "collapses" into a single value. Thus the spontaneous magnetization $M_N^{(\nu)}$ which is given in terms of the two-spin correlation function as

$$M_N^{(\nu)}\equiv\lim_{r\rightarrow\infty}\rho_N^{(\nu)}(r), \tag{5}$$

has the value zero for $T>T_c$ but suddenly acquires a nonzero value as the eigenvalue spectrum collapses at $T=T_c$.

Our goal, then, is to calculate for general ν the two-spin correlation function

$$\rho_N(r)\equiv\langle\mathbf{S}_i\cdot\mathbf{S}_{i+r}\rangle = Q_N^{-1}\,\mathrm{tr}[\mathbf{S}_i\cdot\mathbf{S}_{i+r}\exp(-\beta\mathcal{H})], \tag{6}$$

where $Q_N\equiv\mathrm{tr}[\exp(-\beta\mathcal{H})]$ is the partition function for the system, and where the notation "tr" denotes an integration over the entire phase space of the N ν-dimensional unit vectors. Note that in Eq. (6), and henceforth, we omit writing the superscript ν on most symbols. We begin by writing out an expression for the integrand of the numerator of Eq. (6),

$$\begin{aligned}\mathrm{tr}[\mathbf{S}_i\cdot\mathbf{S}_{i+r}\exp(-\beta\mathcal{H})]&=A^{-N}\\ &\times\int\cdots\int \mathbf{S}_1\cdot\mathbf{S}_{1+r}\exp(K\mathbf{S}_1\cdot\mathbf{S}_2)\cdots\exp(K\mathbf{S}_r\cdot\mathbf{S}_{r+1})\\ &\times\exp(K\mathbf{S}_{r+1}\cdot\mathbf{S}_{r+2})\cdots\exp(K\mathbf{S}_N\cdot\mathbf{S}_1)\\ &\times d\Omega_1 d\Omega_2\cdots d\Omega_N,\end{aligned} \tag{7}$$

where $K\equiv\beta J$, $d\Omega_i$ denotes an element of "solid angle" in the ν-dimensional phase space of spin $\mathbf{S}_i$, and $A\equiv 2\pi^{\nu/2}/\Gamma(\nu/2)$ is the "area" of a ν-dimensional unit sphere. For example, if $\nu=2$, $d\Omega_i=d\theta$ and $A=2\pi$. Note that the translational periodicity allows us to choose $i=1$ in the integrand of Eq. (7). Consider now the integral equation

$$A^{-1}\int\exp(K\mathbf{S}_i\cdot\mathbf{S}_j)\Psi_n(\mathbf{S}_j)d\Omega_j=\lambda_n\Psi_n(\mathbf{S}_i) \tag{8}$$

the kernel of which can be represented in the form

$$A^{-1}\exp(K\mathbf{S}_i\cdot\mathbf{S}_j)=\sum_{k=0}^{\infty}\lambda_k\Psi_k^*(\mathbf{S}_i)\Psi_k(\mathbf{S}_j), \tag{9}$$

where the eigenfunctions Ψ_k are orthonormal and the largest eigenvalue, which we denote by λ_0, is nondegenerate. Use of Eq. (9) N times in Eq. (7) and doing the integrations over the entire phase space of all but spins $\mathbf{S}_1$ and $\mathbf{S}_{1+r}$ leads to the expression

$$\mathrm{tr}[\mathbf{S}_i\cdot\mathbf{S}_{i+r}\exp(-\beta\mathcal{H})]=\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\lambda_n^{N-r}\lambda_m^r I(n,m), \tag{10}$$

where

$$I(n,m)\equiv\iint \mathbf{S}_1\cdot\mathbf{S}_{1+r}\Psi_m^*(\mathbf{S}_1)\Psi_n(\mathbf{S}_1)\Psi_m(\mathbf{S}_{1+r})\times\Psi_n^*(\mathbf{S}_{1+r})d\Omega_1 d\Omega_{1+r}. \tag{11}$$

For the partition function $Q_N\equiv\mathrm{tr}[\exp(-\beta\mathcal{H})]$ we obtain, by exactly the same procedure,

$$Q_N=\sum_{k=0}^{\infty}\lambda_k^N. \tag{12}$$

We remark that the explicit form of the eigenvalues

λ_k and the eigenfunctions Ψ_k of the integral equation (8) have been calculated for $\nu=2$ and 3 by Joyce.[7] For general ν, the eigenfunctions are the hyperspherical harmonics in ν dimensions. The eigenvalues are obtained with the aid of the Funk–Hecke theorem,[8] with the result that

$$\lambda_n(K)=A^{-1}(2\pi)^{\nu/2}K^{-\nu/2+1}I_{n+\nu/2-1}(K). \qquad (13)$$

Next consider the limit of large N, whereupon $Q_N \sim \lambda_0{}^N$ and

$$\rho_N(r)=\lambda_0{}^{-N}\sum_{m=0}^{\infty}\lambda_0{}^{N-r}\lambda_m{}^r I(0,m). \qquad (14)$$

Observe that only the $m=1$ term in (14) survives and Eq. (14) reduces to Eq. (4). Thus we have proved that there is no long-range order so long as the maximum eigenvalue λ_0 is nondegenerate, but that when $\lambda_1 \to \lambda_0$, long-range order sets in as described by Eq. (5).

It is worth noting that the above argument can easily be generalized to treat a more general interaction of the form

$$\mathcal{H}_\nu=-\sum_{i=1}^{N} J_{i,i+1}\mathbf{S}_i{}^{(\nu)}\cdot\mathbf{S}_{i+1}{}^{(\nu)} \qquad (15)$$

in which the exchange parameters $J_{i,i+1}$ are arbitrary numbers.

One particular feature of our solution for a $d=1$ lattice which is valid for lattices of higher dimensionality is that as $\nu\to\infty$, the free energy approaches the free energy of the Berlin–Kac spherical model.[5] Another property which is true for $d=1$, but which we can advance only as a plausible conjecture for general d, is the inequality

$$\langle \mathbf{S}_i{}^{(\nu)}\cdot\mathbf{S}_j{}^{(\nu)}\rangle \geq \langle \mathbf{S}_i{}^{(\nu+1)}\cdot\mathbf{S}_j{}^{(\nu+1)}\rangle \qquad (16)$$

Eq. (16) says that the spin correlation function (for a given temperature and a given pair of sites i and j) decreases with increasing spin dimensionality; this is at least intuitively plausible, since the higher the spin dimensionality, the "floppier" are the spins. The conjectured relation (16) is supported for $d\geq 1$ by extrapolations from exact high-temperature series expansions, which suggest that not only the correlation function varies monotonically with ν, but also so do the other critical properties such as critical temperature and critical indices.[9]

In summary, then, we have seen that the onset of long-range order corresponds to a mathematical degeneracy of the maximum eigenvalue λ_0 of a certain linear integral equation for the case of nearest-neighbor interactions among isotropically interacting classical spins of arbitrary spin dimensionality situated on a linear chain lattice.[10] The generalization to interactions of arbitrary range is under investigation at the present time. Whether the quantum mechanical case can be explained in terms of eigenvalue degeneracy remains an open question.

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[1] J. Ashkin and W. E. Lamb, Jr., Phys. Rev. **64,** 159 (1943).

[2] M. Kac and C. J. Tompson, Proc. Nat. Acad. Sci. **55,** 676 (1966). An excellent review of the Kac model is M. Kac in *Statistical Physics, Phase Transitions, and Superfluidity*, M. Chrétien, E. Gross, and S. Deser, Eds. (Gordon and Breach, Science Publishers, Inc., New York, 1968), Vol. I. p. 241.

[3] C. J. Thompson, J. Math. Phys. **4,** 1059 (1968). We wish to thank the referee for calling this work to our attention.

[4] T. H. Berlin and M. Kac, Phys. Rev. **86,** 821 (1952).

[5] H. E. Stanley, Phys. Rev. **176,** 718 (1968).

[6] This generalized Hamiltonian was first introduced, to the best of our knowledge, in H. E. Stanley, Phys. Rev. Lett. **20,** 589 (1968). It was solved exactly for an open-ended linear chain ($d=1$) lattice in H. E. Stanley, Phys. Rev. **179,** 570 (1969). For $d>1$, it has thus far yielded to exact solution for $\nu=1$ (Ising spins), and even then only in the case of zero external magnetic field ($H=0$).

[7] G. S. Joyce, Phys. Rev. **155,** 478 (1968).

[8] See, e.g., *Higher Transcendental Functions* (McGraw-Hill Book Co., New York, 1953), Bateman Manuscript Project Vol. II, p. 247.

[9] H. E. Stanley, J. Appl. Phys. **40,** 1272 (1969).

[10] The relation of eigenvalue degeneracy to the surface tension and the correlation length of the Ising model for [2]-dimensional lattices has recently deen discussed by M. E. Fisher, J. Phys. Soc. Japan **26,** 87 (1969). We wish to thank Professor Fisher for calling this work to our attention.