Thouless-Anderson-Palmer equations

Analog of the Ginzburg-Landau equations for spin glasses with locally random order parameter m_i

1) Original TAP derivation
2) Derivation by the Kirkwood free energy method
3) Solution of TAP equations near T_c :

expansion over small m_i and anomaly in the free energy

4) Marginal stability condition
5) Low-temperature behavior
6) Number of metastable solutions

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Solution of 'Solvable model of a spin glass'

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ABSTRACT

The Sherrington–Kirkpatrick model of a spin glass is solved by a mean field technique which is probably exact in the limit of infinite range interactions. At and above T_c the solution is identical to that obtained by Sherrington and Kirkpatrick (1975) using the $n \to 0$ replica method, but below T_c the new result exhibits several differences and remains physical down to $T = 0$.

The Sherrington–Kirkpatrick Hamiltonian

$$\mathscr{H} = -\sum_{(ij)} J_{ij} S_i S_j \qquad \text{Prob}\,(J_{ij}) \propto \exp\left(\frac{-Z J_{ij}^2}{2\tilde{J}^2}\right)$$

with a variance $\tilde{J}^2/Z$ where Z is the number of neighbours of each spin, presumed effectively infinite; we work in the limit $N \gtrsim Z \gg 1$.

§ 2. The high temperature region

For $T > T_c$ we make a high temperature series expansion for the free energy, using the standard identity

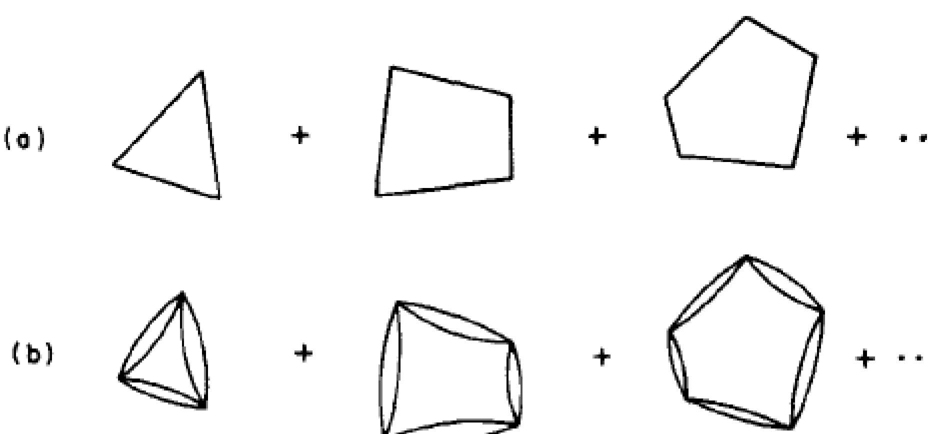
$$\exp(\beta J_{ij} S_i S_j) = \cosh \beta J_{ij}(1 + S_i S_j \tanh \beta J_{ij}). \tag{3}$$

Thus

$$\begin{aligned} -\beta F &= \langle \ln \operatorname{Tr} \exp(-\beta \mathscr{H}) \rangle_J \\ &= \langle \ln \prod_{(ij)} \cosh \beta J_{ij} \rangle_J + \langle \ln \operatorname{Tr} \prod_{(ij)} (1 + T_{ij} S_i S_j) \rangle_J \\ &= N\beta^2 \tilde{J}^2/4 + 0(N/Z) \\ &\quad + \langle \ln \operatorname{Tr} (1 + \sum_{(ij)} T_{ij} S_i S_j + \tfrac{1}{2} \sum_{(ij) \neq (kl)} T_{ij} T_{kl} S_i S_j S_k S_l \ldots) \rangle_J, \end{aligned} \tag{4}$$

where $T_{ij} = \tanh \beta J_{ij}$. The expansion may be analysed diagramatically (each line representing a T_{ij}), noting the following conditions for a non-vanishing diagram :

(*a*) There must be an even number of lines at each vertex.
(*b*) No line may be double *before* taking the logarithm.
(*c*) Every line must be double *after* taking the logarithm (because $\langle J \rangle = 0$).



$$F = Nf_0 + (N/Z)f_1 + \text{lower order},$$

$$f_0 = -T \ln 2 - \tilde{J}^2/4T,$$

$$f_1 = -\tfrac{1}{4} T \ln(1 - \beta^2 \tilde{J}^2) + \text{non-singular part}.$$

We note that the divergent part f_1 is intrii sically positive

the free energy below

T_c is *greater* than an analytic continuation of the high temperature result.

Below T_c we must introduce a mean field in order to reconverge the series for F. We employ the usual identity

$$\mathrm{Tr}\exp(-\beta\mathscr{H})=\mathrm{Tr}\exp(-\beta\mathscr{H}_0)\langle\exp(\beta\mathscr{H}_0-\beta\mathscr{H})\rangle_{\mathscr{H}_0}, \tag{6}$$

where $\mathscr{H}_0$ is a soluble mean field Hamiltonian which is to be used in evaluating the diagrams generated by $\exp(\beta\mathscr{H}_0-\beta\mathscr{H})$. An obvious ansatz is

$$(\mathscr{H}_0-\mathscr{H})_{ij}=J_{ij}(S_i-m_i)(S_j-m_j) \tag{7}$$

so that

$$(\mathscr{H}_0)_{ij}=J_{ij}(m_im_j-m_iS_j-m_jS_i)$$

where m_i is the mean spin on the ith site, to be determined self-consistently by the condition

$$\langle S_i\rangle_{\mathscr{H}_0}=m_i. \tag{8}$$

Ignoring the perturbation $\mathscr{H}-\mathscr{H}_0$ leads to the appealing (but incorrect) mean field equation

$$h_i=\sum_j J_{ij}m_j=T\tanh^{-1}m_i \tag{9}$$

In the Bethe method, we consider a 'cluster' of a central site 0 and all its neighbours j. On the neighbours j we assume mean fields h_j which, for a Cayley tree, are the only effect *their* neighbours can have on them. Using the smallness of J_{0j} ($\propto Z^{-1/2}$), it is easy to arrive at the following expressions for m_0 and m_j:

$$\left.\begin{aligned} m_0&=\tanh\beta\sum_j J_{0j}\tanh\beta h_j\\ m_j&=\tanh\beta h_j+m_0\beta J_{0j}(1-\tanh^2\beta h_j).\end{aligned}\right\} \tag{10}$$

$$
\left.\begin{aligned}
m_0 &= \tanh \beta \sum_j J_{0j} \tanh \beta h_j \\
m_j &= \tanh \beta h_j + m_0 \beta J_{0j}(1 - \tanh^2 \beta h_j).
\end{aligned}\right\} \tag{10}
$$

We may now eliminate the h_js (again using the smallness of J_{0j}), obtaining the fundamental equation

$$
\sum_j J_{0j} m_j - m_0 \beta \sum_j J_{0j}{}^2 (1 - m_j{}^2) = T \tanh^{-1} m_0 \tag{11}
$$

which supplants the incorrect eqn. (9), and must, of course, be valid for any choice of site 0. The correction term proportional to m_0 is more readily understood upon realizing that $\beta(1 - m_j{}^2)$ is the single-site susceptibility, χ_j, as may easily be proved. Equation (11) may thus be written

$$
m_0 = \tanh \beta \sum_j J_{0j}(m_j - m_0 J_{0j} \chi_j) \tag{12}
$$

and the second term on the right-hand side is seen as the response of site j to the mean spin on site 0; this must be *removed* from m_j when computing m_0.

$$
\begin{aligned}
F_{\mathrm{MF}} = &- \sum_{(ij)} J_{ij} m_i m_j - \tfrac{1}{2}\beta \sum_{(ij)} J_{ij}{}^2 (1 - m_i{}^2)(1 - m_j{}^2) \\
&+ \tfrac{1}{2} T \sum_i \left[(1 + m_i) \ln \tfrac{1}{2}(1 + m_i) + (1 - m_i) \ln \tfrac{1}{2}(1 - m_i)\right]
\end{aligned} \tag{13}
$$

As it must, direct differentiation of eqn. (13) gives eqn. (11). Additionally, eqn. (13) is quite physically transparent: the first term is the internal energy of a frozen lattice; the second term is the correlation energy of the fluctuations, and is just the $N\tilde{J}^2/4T$ term of eqn. (5), modified for the effective 'freedom', $1 - m_i{}^2$, of each spin; and the last term is the entropy of a set of Ising spins constrained to have means m_i.

Alternative derivation (Dotsenko,Feigelman & Ioffe 1990)

Instead of deriving the MF equations of state, we prefer to derive the free-energy functional of m_i that we shall use in subsequent Sections. The variation of this functional of m_i yields the equations of state (the TAP equations). To derive the effective functional of new variables m_i, we introduce a new term with Lagrange multiplier λ_i into the Hamiltonian (2.1.1), which ensures the condition $\langle \sigma_i \rangle = m_i$:

$$H_{\text{eff}} = H + H_{\text{L}}, \quad H_{\text{L}} = \sum_i (\sigma_i - m_i)\lambda_i. \tag{2.4.1}$$

We then expand the free-energy functional $F = -T \ln \{\Sigma_{\{\sigma\}} \exp(-H_{\text{eff}}/T)\}$ for the full interacting system as a series of cumulants in the interaction energy H:

$$\left.\begin{aligned} -\beta F &= -\beta F_0 + \sum_{n=1}^{\infty} \frac{1}{n!}(-\beta)^n c_n(H), \\ \beta F_0 &= \sum_i \lambda_i m_i - \ln \cosh \lambda_i. \end{aligned}\right\} \tag{2.4.2}$$

The first cumulants $c_n(H)$ are

$$\left.\begin{aligned} c_1(H) &= \langle H \rangle_{\text{L}}, \\ c_2(H) &= \langle H^2 \rangle_{\text{L}} - \langle H \rangle_{\text{L}}^2, \\ c_3(H) &= \langle (H - \langle H \rangle_{\text{L}})^3 \rangle_{\text{L}}, \end{aligned}\right\} \tag{2.4.3}$$

where $\langle \ldots \rangle_{\text{L}}$ denotes the average with respect to the reference Hamiltonian H_{L}. The expansion (2.4.2), (2.4.3) was introduced by Kirkwood [27] in 1938 as the expansion for the Ising model. The Lagrange parameter λ can be expressed through the condition:

$$\beta F = \sum_i \lambda_i m_i - \ln \cosh \lambda_i - \frac{1}{2} \sum_{i,j} J_{ij} \mu_i \mu_j - \frac{1}{2} \sum_{i \neq k, j} J_{ij} J_{jk} (1 - \mu_j^2) \mu_i \mu_k - \frac{1}{4} \sum_{i,j} J_{ij}^2 (1 - \mu_i^2 \mu_j^2),$$

where $\mu_i \equiv \tanh \lambda_i$.

$$\partial F/\partial \lambda_i = 0. \tag{2.4.4}$$

$$\beta F = \sum_i \lambda_i m_i - \ln\cosh\lambda_i - \frac{1}{2}\sum_{i,j} J_{ij}\mu_i\mu_j - \frac{1}{2}\sum_{i\neq k,j} J_{ij}J_{jk}(1-\mu_j^2)\mu_i\mu_k - \frac{1}{4}\sum_{i,j} J_{ij}^2(1-\mu_i^2\mu_j^2), \tag{2.4.5}$$

where $\mu_i \equiv \tanh\lambda_i$. Inserting (2.4.5) into (2.4.4), we get

$$m_i = \mu_i - \sum_j (1-\mu_i^2)J_{ij}\mu_j + O(J^2). \tag{2.4.6}$$

Finally excluding μ_i from (2.4.5) and (2.4.6), we obtain the TAP free-energy functional

$$F = -\frac{1}{2}\sum_{i,j} J_{ij}m_i m_j - \frac{1}{4T}\sum_{i,j} J_{ij}^2(1-m_i^2)(1-m_j^2) + \frac{T}{2}\sum_i \left[(1+m_i)\ln\frac{1+m_i}{2} + (1-m_i)\ln\frac{1-m_i}{2}\right] + \sum_i h_i m_i. \tag{2.4.7}$$

Sum over i,j
In TAP notations
it was sum over
pairs <i,j> thus
factor 2

Expansion over m_i near $T_c = J$

$m_i - \beta \sum_j J_{ij} m_j + J^2\beta^2 m_i = O(m_i^2)$, $\Sigma_j J_{ij}^2 = J^2$. $m_\lambda[1 - \beta J_\lambda + (\beta J)^2] = O(m_i^2)$.

$\rho(E) = (4-E^2)^{1/2}(2\pi)^{-1}\theta(4-E^2)$.

For T near T_c we expect m_i to be small and similar to the eigenvector M_i belonging to the largest eigenvalue $(J_\lambda)_{\max} = 2\tilde{J}$ of the matrix J_{ij} :

$$\sum_j J_{ij} M_j = 2\tilde{J} M_i \tag{15}$$

Slide 5

We first linearize eqn. (11), approximating $\sum_j J_{ij}{}^2 \chi_j$ by $\tilde{J}^2\bar{\chi}$:

$$\sum_j J_{ij} m_j = \beta\tilde{J}^2(1 - \overline{m^2})m_i + T(m_i + m_i{}^3/3 + m_i{}^5/5 + \ldots).$$

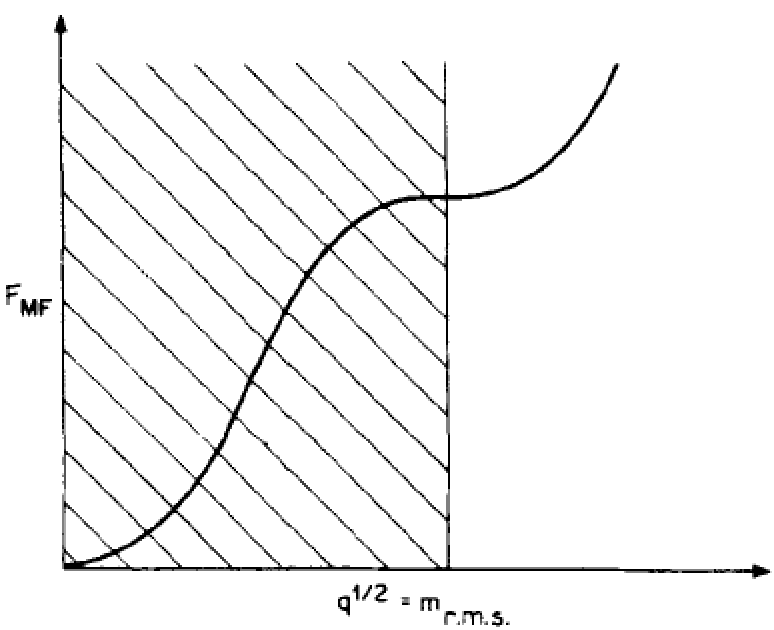
$m_i = M_i + \delta m_i$, $q = \overline{M_i{}^2}$ M_i is orthogonal to δm_i.

$$(2\tilde{J} - \beta\tilde{J}^2 - T)q = (T - \beta\tilde{J}^2)q^2 + 3Tq^3 + T\sum_i M_i{}^3\delta m_i + 0(q^4).$$

The term in δm_i is essential—there is no solution without it—but is difficult to estimate. Analysing the projection of eqn. (16) orthogonal to M_i by a combination of eigenvector expansions and numerical estimates, we find finally

$$(2\tilde{J} - \tilde{J}^2/T - T)q - (T - \tilde{J}^2/T)q^2 + (2T^2/\tilde{J} - 3T)q^3 \simeq 0. \tag{20}$$

Near $T_c = \tilde{J}$ this equation has a double zero at $q = \overline{m^2} = 1 - T/T_c$



$$F\{a_0\} = \frac{1}{6}(\tau + q)^3 - \frac{1}{6}\tau^3,$$

Alternative derivation (Dotsenko,Feigelman & Ioffe 1990)

$$m_i = a_0\psi_0(i) + \delta m_i = a_0\psi_0(i) + \sum_{\alpha\neq 0} a_\alpha \psi_\alpha(i), \qquad (4.1.6)$$

where ψ_0 corresponds to the largest $E_0 > E_\lambda$, and we restrict ourselves to Ising spins ($n=1$). Substitution of (4.1.6) into (4.1.3) yields

$$F = \frac{1}{2}\tau^2 q + \frac{1}{2}\tau q^2 + \frac{1}{2}q^3 + \frac{1}{3}\sum_i a_0^3\psi_0^3(i)\left[\sum_{\alpha\neq 0} a_\alpha\psi_\alpha(i)\right] + \frac{1}{2}\sum_{\alpha\neq 0}(\tau^2+2-E_\alpha)a_\alpha^2,$$

where $\tau = T - T_0 = T - 1$ and $q = a_0^2/N$.

Minimization over a_α leads to

$$a_\alpha = -\frac{1}{3}\frac{1}{2+\tau^2-E_\alpha}\sum_j a_0^3\psi_0^3(j)\psi_\alpha(j),$$

$$F\{a_0\} = \frac{1}{2}\tau^2 q + \frac{1}{2}\tau q^2 + \frac{1}{2}q^3 - \frac{1}{18}\sum_{i,j} a_0^3\psi_0^3(i)g(i,j)a_0^3\psi_0^3(j),$$

$q = |\tau|$

$$g_{ij} = \delta_{ij}\int \frac{\rho(E)\,\mathrm{d}E}{2-E+\tau^2} = \delta_{ij} + O(\tau).$$

$$F\{a_0\} = \frac{1}{6}(\tau+q)^3 - \frac{1}{6}\tau^3,$$

Marginal stability condition

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Evidence for massless modes in the 'solvable model' of a spin glass

For stable states eigenvalues of the matrix **A** are positive.

$$A_{ij} = \partial^2(\beta F)/\partial m_i \partial m_j$$

$$= -\beta J_{ij} + \left(\beta^2 \sum J_{ik}^2(1 - m_k^2) + (1 - m_i^2)^{-1}\right)\delta_{ij} - 2\beta^2 J_{ij}^2 m_i m_j$$

replacing $\sum_k J_{ik}^2(1 - m_k^2)$ by $\tilde{J}^2(1 - q)$

susceptibility matrix $\chi_{ij} = \partial m_i/\partial h_j$

$$(A^{-1})_{ij} = \beta^{-1}\chi_{ij} = \langle S_i S_j \rangle_c$$

the matrix Green function is $\mathbf{G}(\lambda) = (\lambda \mathbf{I} - \mathbf{A})^{-1}$

$$\rho(\lambda) = (N\pi)^{-1} \operatorname{Im} \operatorname{Tr} \mathbf{G}(\lambda - i\delta)$$

$$G_{ii} = f_i - f_i(\beta J_{ii}) f_i + f_i(\beta J_{ij}) f_j(\beta J_{ji}) f_i + \ldots$$

$$f_i = [\lambda - \beta^2 \tilde{J}^2(1 - q) - (1 - m_i^2)^{-1}]^{-1}$$

is the 'locator'.

$$G_{ii} = f_i + \beta^2 \tilde{J}^2 \bar{G} f_i^2 + \beta^4 \tilde{J}^4 \bar{G}^2 f_i^3 + \ldots = \{f_i^{-1} - \beta^2 \tilde{J}^2 \bar{G}\}^{-1} \qquad (10)$$

where $\bar{G} = N^{-1}\sum_i G_{ii}$ is the averaged Green function.

$$\rho(\lambda) = (1/\pi)(k_B T/\tilde{J})^3[\overline{(1 - m^2)^3}]^{-1/2}\lambda^{1/2}.$$

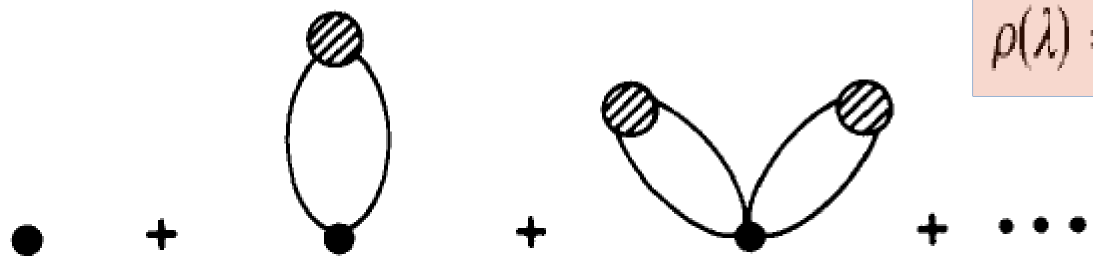


Figure 3. Graphs for the Green function G_{ii} in the thermodynamic limit. A dot connected to $2n$ lines carries a factor $(f_i)^{n+1}$. A shaded circle represents the average Green function $\bar{G}$. Each loop then carries a factor $\beta^2\tilde{J}^2\bar{G}$.

a self-consistency equation for $\bar{G}$: $\bar{G}(\lambda) = \overline{(f_i^{-1}(\lambda) - \beta^2\tilde{J}^2\bar{G}(\lambda))^{-1}}.$

For $\lambda = 0$, equation (10) becomes an identity. $G_{ii} = \{f_i^{-1} - \beta^2\tilde{J}^2\bar{G}\}^{-1}$

LHS: $G_{ii}(0) = -(A^{-1})_{ii} = -(1 - m_i^2)$

RHS: $[-\beta^2\tilde{J}^2(1 - q) - (1 - m_i^2)^{-1} - \beta^2\tilde{J}^2\bar{G}(0)]^{-1} = -(1 - m_i^2)$

For general λ we write $f_i^{-1} = \lambda + \beta^2\tilde{J}^2\bar{G}(0) - G_{ii}^{-1}(0)$, **For small λ**

$\bar{G}(\lambda) = \bar{G}(0) - \overline{G^2(0)}[\lambda + \beta^2\tilde{J}^2(\bar{G}(0) - \bar{G}(\lambda))]$ → $\bar{G}(0) - \bar{G}(\lambda) = \lambda\overline{G^2(0)}(1 - \beta^2\tilde{J}^2\overline{G^2(0)})^{-1}.$

and $\rho(\lambda) = (1/\pi)\,\mathrm{Im}\,\bar{G}(\lambda - i\delta) = 0$ at small λ unless $1 = \beta^2\tilde{J}^2\overline{G^2(0)}$ (*)

(*) is actually fulfilled (in the main order) for $q = |\tau|$!

Next orders in τ (lower T's)

$$1 = \beta^2 \tilde{J}^2 \overline{G^2(0)} = \beta^2 \tilde{J}^2 \overline{(1-m^2)^2} = \beta^2 \tilde{J}^2 (1 - 2q + r)$$

$$r = N^{-1} \sum_i m_i^4.$$

$$N^{-1} \operatorname{Tr} A^{-1} \underset{N\to\infty}{=} \int_0^\infty \mathrm{d}\lambda (\rho(\lambda)/\lambda) = \frac{1}{N} \sum_i (1 - m_i^2) = 1 - q$$

$$\rho(0) = 0.$$

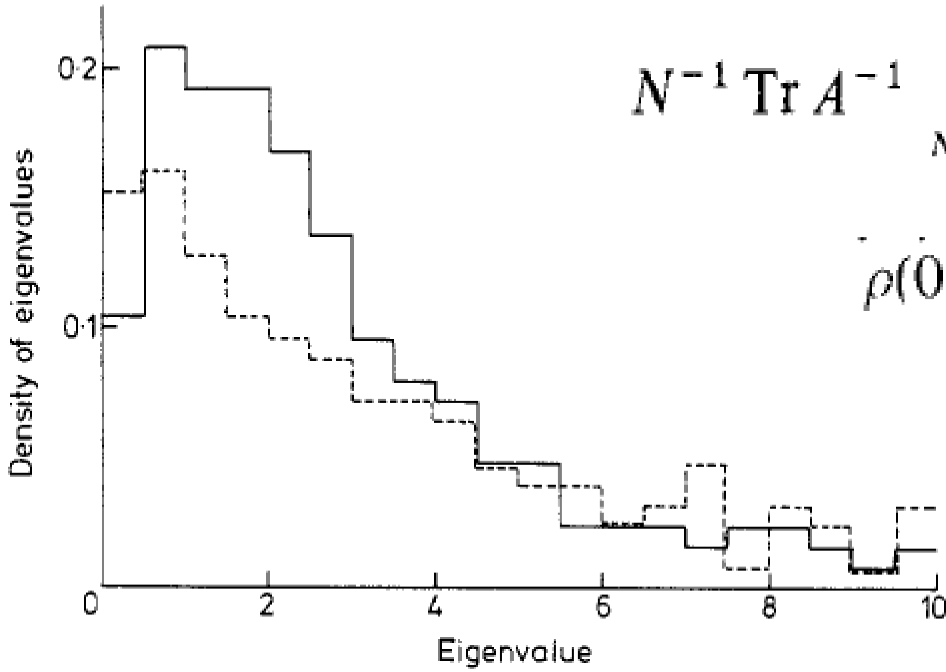


Figure 1. Full lines: histrogram of the density of eigenvalues of the matrix **A**, $\rho(\lambda)$, versus λ for a typical system with $N = 250$ for $T/T_c = 0{\cdot}6$ (eigenvalues $\lambda > 10$ not shown). Broken lines: historgram of $\tilde{\rho}(u) = (2/3)u^{-1/3}\rho(u^{2/3})$ versus u.

Marginal stability: basic feature of spin glass state

trace of the square of the susceptibility matrix

$$\chi_R = N^{-1} \sum_{i,j} \chi_{ij}\chi_{ji} = (\beta^2/N) \operatorname{Tr}(A^{-2}). \underset{N\to\infty}{=} \beta^2 \int \mathrm{d}\lambda (\rho(\lambda)/\lambda^2)$$

Diverges !

Low temperatures: P(h) distribution

At $T=0$ the mean field equation obviously selects a self-consistent lowest energy solution of

$$m_i = \text{sign}\,(h_i), \qquad h_i = \sum_j \tilde{J}_{ij} m_j$$

To derive the low temperature thermodynamics we assume

$$\lim_{h\to 0} p(h) = h/H^2 \qquad q = \overline{m^2} = 1 - \alpha(T/\tilde{J})^2 \quad (T \ll T_c),$$

The low temperature susceptibility

$$\chi = \bar{\chi}_j = 1{\cdot}665\, T/\tilde{J}$$

where H and α are parameters to be determined later.

$$h_i = \alpha T m_i + T \tanh^{-1} m_i$$

$$\overline{m^2} = \int_0^\infty m^2(h) p(h)\, dh \;\longrightarrow\; H^2/\tilde{J}^2 = \tfrac{1}{4}\alpha + (2\ln 2 + 1)/3 + \ln 2/\alpha,$$

TAP hypothesis: H is smallest possible → $\alpha = 2\sqrt{(\ln 2)} \simeq 1{\cdot}665$ and $H/\tilde{J} \simeq 1{\cdot}276.$

However, marginality condition $1 = \beta^2 \tilde{J}^2 \overline{(1-m^2)^2}$ leads to $\alpha \simeq 1{\cdot}810$ and $H/\tilde{J} \simeq 1{\cdot}277$

$S/Nk_B \simeq 0{\cdot}770(T/T_c)^2$ versus $0{\cdot}765(T/T_c)^2$

Metastable states in spin glasses

A J Bray and M A Moore J. Phys. C: Solid St. Phys., 13 (1980) L469–76. Printed in Great Britain

The density of solutions associated with a particular free energy f is

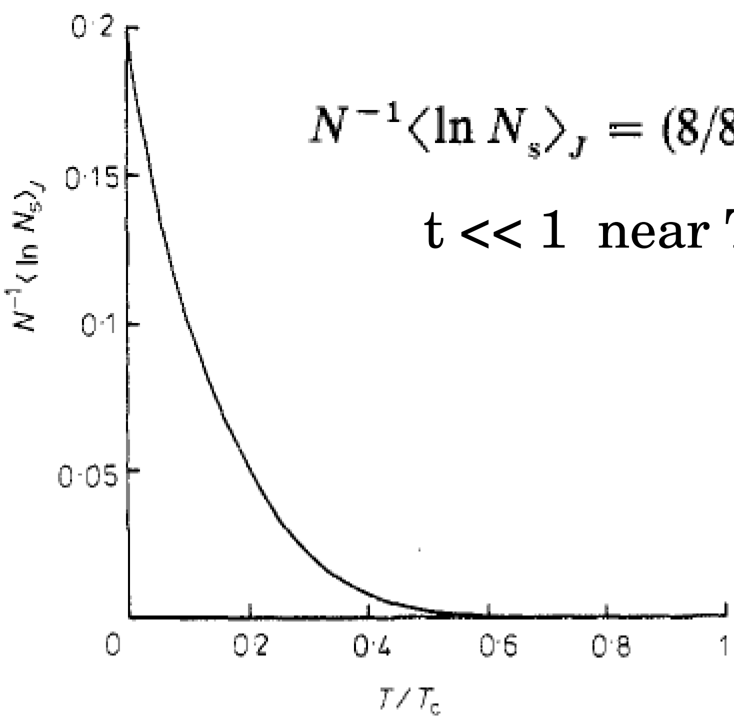
$$N_s(f) = N^2 \int_0^1 \mathrm{d}q \int_{-1}^{1} \prod_i (\mathrm{d}m_i)\, \delta\Big(Nq - \sum_i m_i^2\Big)\, \delta\Big(Nf - \sum_i f(m_i)\Big) \prod_i \delta(G_i) |\det \mathbf{A}|$$

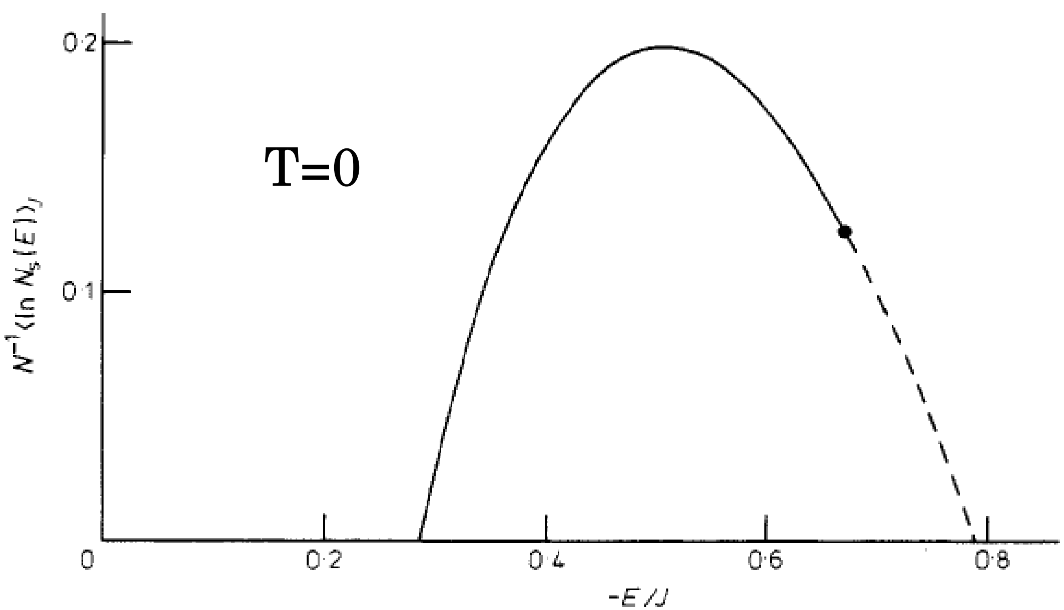
$$f = N^{-1} \sum_i f(m_i) = N^{-1} \sum_i [-\ln 2 - \tfrac{1}{4}\beta^2 J^2 (1 - q^2) + \tfrac{1}{2} m_i \tanh^{-1} m_i + \tfrac{1}{2} \ln(1 - m_i^2)].$$

$$G_i \equiv \tanh^{-1} m_i + \beta^2 J^2 (1 - q) m_i - \beta \sum_j J_{ij} m_j = 0$$

$$\langle N_s(f) \rangle_J = \int \prod_{(ij)} (\mathrm{d}J_{ij} P(J_{ij}))\, N_s(f).$$

$$A_{ij} = \partial G_i / \partial m_j = [(1 - m_i^2)^{-1} + \beta^2 J^2 (1 - q)]\, \delta_{ij} - \beta J_{ij} \equiv a_i \delta_{ij} - \beta J_{ij}.$$





Major conclusions

- SG state is characterized (within infinite-range model) by an exponential (in N) number of metastable states – solution of TAP equations.
- All these solutions are *marginally stable;* thus gap-less modes exist in the *absence of any continuous symmetry* of the Hamiltonian.
- Square of susceptibility matrix $\langle Tr [\chi^2_{ik}] \rangle$ diverges anywhere in the SG phase
- Free energy of SG state is not *a minimum but a saddle-point* as function of the macroscopic order parameter q