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

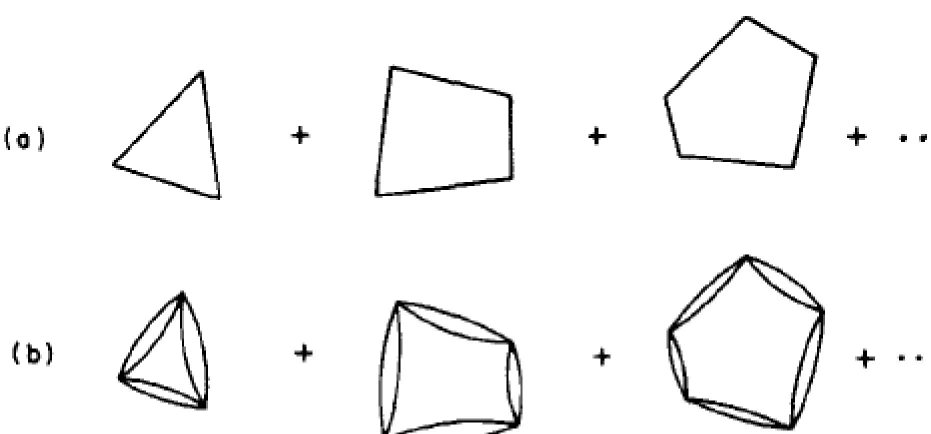
$$\exp(\beta J_{ij} S_i S_j) = \cosh \beta J_{ij} (1 + S_i S_j \tanh \beta J_{ij}). \tag{3}$$

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 $\langle J \rangle = 0$).



$$F = N f_0 + (N/Z) f_1 + \text{lower order},$$

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

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

We note that the divergent part f_1 is intrinsically 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

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

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

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

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

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

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:

$$\partial F/\partial \lambda_i = 0. \qquad (2.4.4)$$

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

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

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

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

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

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

Expansion over m_i near $T_c = J$

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

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

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 $\tilde{J}^2 \bar{\chi}$:

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

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

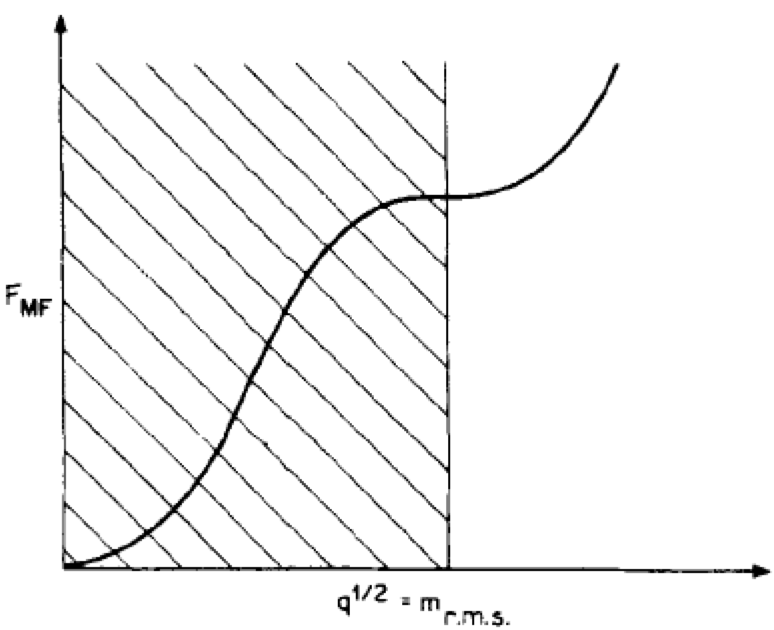
$$(2\tilde{J} - \beta \tilde{J}^2 - T) q = (T - \beta \tilde{J}^2) q^2 + 3Tq^3 + T \sum_i M_i{}^3 \delta m_i + 0(q^4).$$

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

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

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

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

$q = |\tau|$

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

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

Marginal stability condition

A J Bray and M A Moore

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

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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.

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

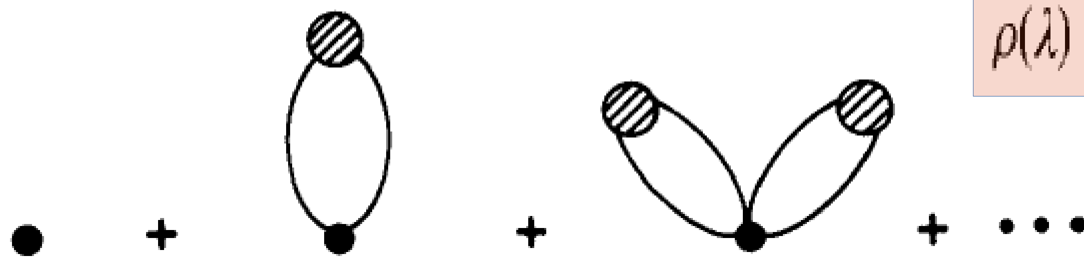


Figure 3. Graphs for the Green function G_{ii} in the thermodynamic limit. A dot connected to $2n$ lines carries a factor $(f_i)^{n+1}$. A shaded circle represents the average Green function $\bar{G}$. Each loop then carries a factor $\beta^2\tilde{J}^2\bar{G}$.

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

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

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

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)

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

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

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

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

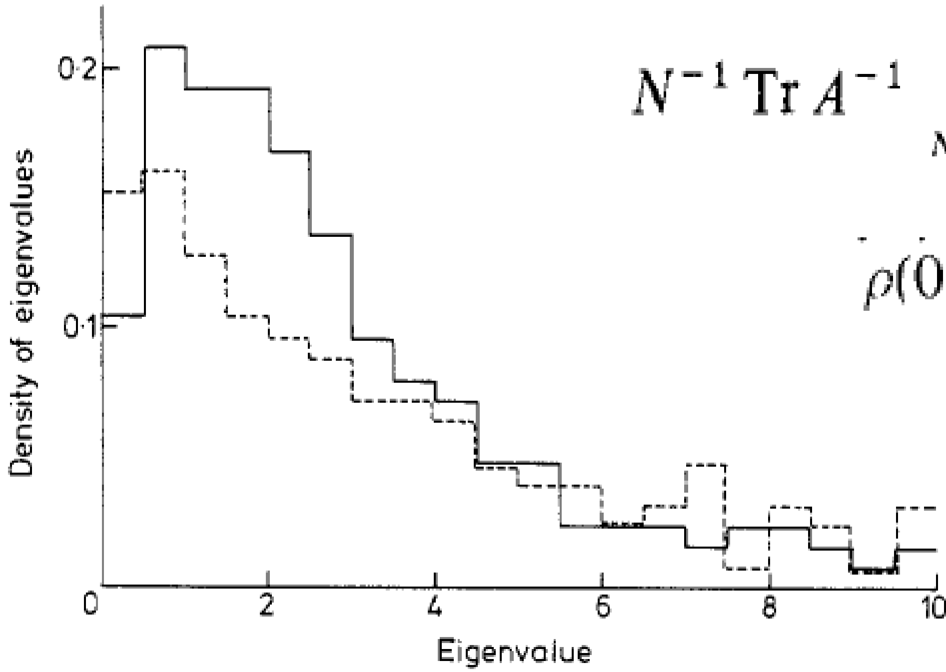


Figure 1. Full lines: histrogram of the density of eigenvalues of the matrix **A**, $\rho(\lambda)$, versus λ for a typical system with $N = 250$ for $T/T_c = 0{\cdot}6$ (eigenvalues $\lambda > 10$ not shown). Broken lines: historgram of $\tilde{\rho}(u) = (2/3)u^{-1/3}\rho(u^{2/3})$ versus u.

Marginal stability: basic feature of spin glass state

trace of the square of the susceptibility matrix

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

Diverges !

Low temperatures: P(h) distribution

At low temperatures, TAP have argued that $q \simeq 1 - \alpha(T/T_c)^2$

S(0) = 0

Local effective fields $h_i = \sum_j J_{ij} m_j$

Then TAP equations lead to

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

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.

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

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 $1 = \beta^2 J^2 \overline{(1 - m^2)^2}$ 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

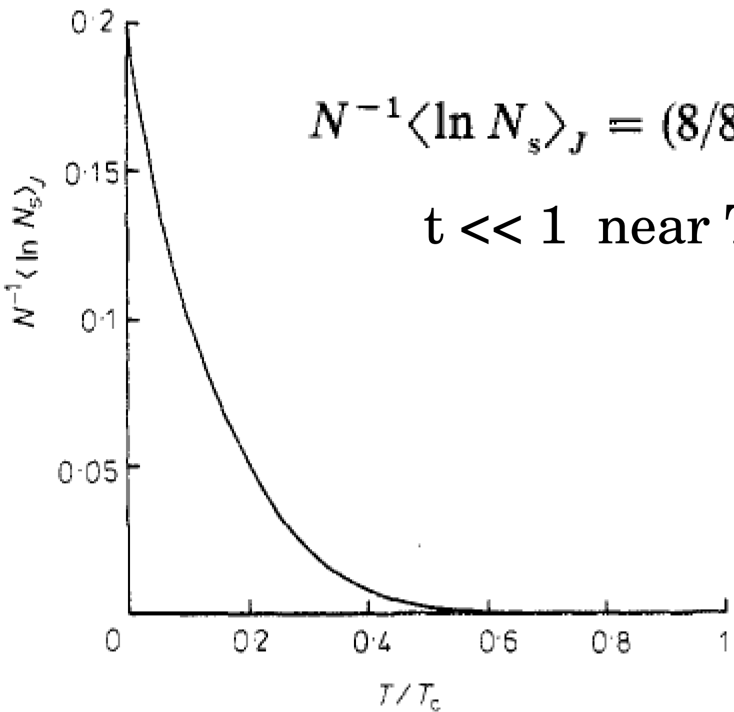
$$N_s(f) = N^2 \int_0^1 \mathrm{d}q \int_{-1}^{1} \prod_i (\mathrm{d}m_i)\, \delta\Big(Nq - \sum_i m_i^2\Big)\, \delta\Big(Nf - \sum_i f(m_i)\Big) \prod_i \delta(G_i) |\det \mathbf{A}|$$

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

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

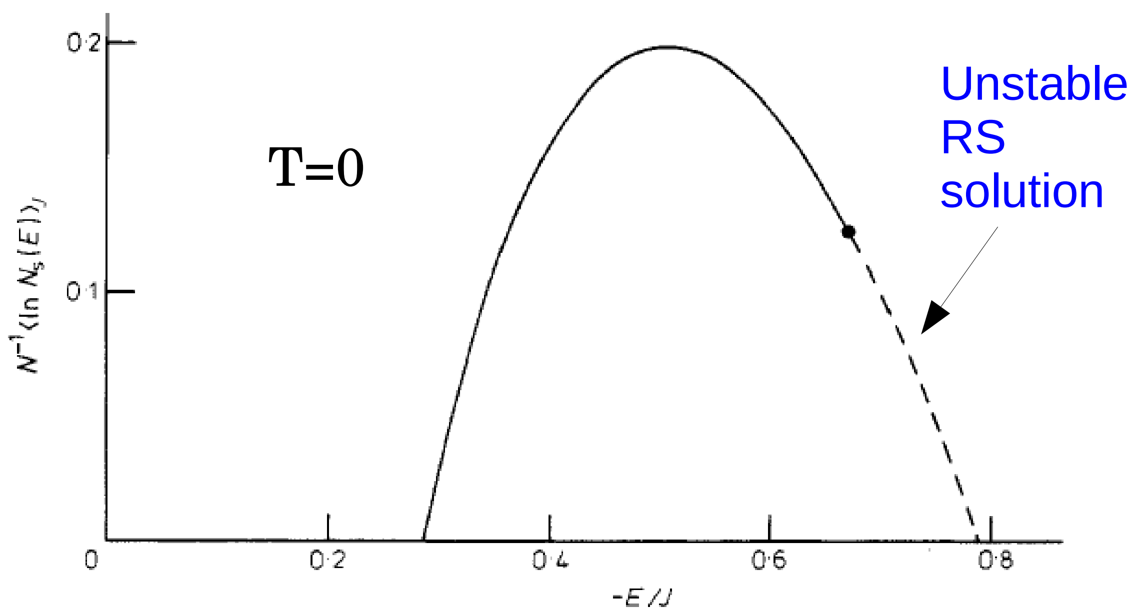
$$\langle N_s(f) \rangle_J = \int \prod_{(ij)} (\mathrm{d}J_{ij} P(J_{ij}))\, N_s(f).$$

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



$$N^{-1}\langle \ln N_s \rangle_J = (8/81) t^6$$

$t << 1$ near T_c



Major conclusions

- SG state is characterized (within infinite-range model) by an exponential (in N) number of metastable states – solutions of TAP equations.
- All these solutions are *marginally stable;* thus gapless 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

Few problems to solve

1. Derive TAP equations for XY and Heisenberg spin glass models, as well as for the “gauge glass” model. Notice crucial difference between XY spin glass with real random-sign couplings and gauge glass with complex random phases
2. Add weak transverse field to the Ising spin glass model, to make it “slightly quantum”. Derive then the corresponding TAP equations. Check for the marginal stability hypothesis: is it still correct ? Try to do it both near T_c and at $T=0$ limit.

3. Perform calculation of the number of TAP equation solutions as described in the paper by Bray and Moore (1980) and then generalized it for the case of gauge glass (solutions which are related by U(1) global rotation should be treated as identical).
4. Include weak uniform external magnetic field into Ising spin glass model, obtain the corresponding TAP equations and study density of states $\rho(\lambda)$ for the eigen-modes of fluctuations near TAP solution. Show that the edge of this spectrum is located at $\lambda = 0$ below some line on the (h,T) plane. Find location of this line at small h.