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LETTER TO THE EDITOR

Metastable states in the solvable spin glass model

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Abstract. The solutions of the equations of Thouless, Anderson and Palmer represent metastable states of the Sherrington–Kirkpatrick model of an Ising spin glass. A replica symmetry breaking scheme of the Parisi kind is employed to enumerate their distribution with free energy.

The characteristic non-ergodic behaviour of spin glasses arises from their large number of metastable states. For the Sherrington–Kirkpatrick (1975) (SK) infinite-range model of an Ising spin glass the metastable states are described by the solutions of the Thouless–Anderson–Palmer equations (1977, referred to as TAP). We have previously shown that there are a large number of these solutions (of order $\exp \alpha N$), where N is the number of spins in the system, and that these solutions fall into two classes (Bray and Moore 1980a, referred to as I). The first class contains those whose free energies $k_B Tf$ exceed a critical value $k_B Tf_c(T)$. Their properties and distribution with free energy are readily evaluated (see I, also de Dominicis *et al* 1980, Tanaka and Edwards 1980). The average number $\langle N_s(f)\rangle$ of these metastable states of free energy $k_B Tf$ is equal to the extremum with respect to n of $\exp(nfN)\langle Z^n\rangle$ where $\langle Z^n\rangle$ is the bond-averaged nth power of the partition function calculated within the two-group replica symmetry breaking scheme (Bray and Moore 1980b). These metastable states are 'uncorrelated'. The second class of metastable states have free energies $f<f_c(T)$ and are correlated, with the Edwards–Anderson order parameter a measure of the correlation between them. It is the purpose of this note to show how such states can be handled by the means of an extension of the Parisi symmetry breaking scheme (Parisi 1979).

The N TAP equations for the magnetisation m_i of the ith spin are

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

with their associated free energy (divided by $Nk_B T$)

$$f\{m_i\} = -\frac{\beta}{N}\sum_{(ij)} J_{ij} m_i m_j - \tfrac{1}{4}\beta^2(1-q)^2 + \frac{1}{2N}\sum_i \{(1+m_i)\ln[\tfrac{1}{2}(1+m_i)] + (1-m_i)\ln[\tfrac{1}{2}(1-m_i)]\} \tag{2}$$

where $\Sigma_{(ij)}$ means a sum over all distinct pairs, $q = N^{-1}\Sigma_i m_i^2$ and J_{ij} is a random exchange interaction with probability distribution

$$P(J_{ij}) = (N/2\pi)^{1/2}\exp(-NJ_{ij}^2/2). \tag{3}$$

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The metastable states are the local minima of the free-energy functional $f\{m_i\}$, which is stationary for the $\{m_i\}$ that satisfy the TAP equations. These equations are thought to be exact in the limit $N \to \infty$. The fact that many solutions of the TAP equations exist for temperatures T less than T_c ($T_c = 1$ in the units of equations (1)–(3)) suggests that the free energy barriers which separate the various minima of $f\{m_i\}$ become infinite in the thermodynamic limit, otherwise thermal fluctuations would mix and so destroy the metastable states. The existence of such infinite barriers emerges clearly in the dynamic calculations of Sompolinsky and Zippelius (1981). Because of these barriers the system remains trapped forever in a particular metastable state. Hence, if one is interested in constructing a theory to explain experiments (which for the SK model means Monte Carlo simulations!) it is not always appropriate to evaluate equilibrium properties derived in the usual way from the partition function Z. Such calculations invoke an unrestricted trace over the spins S_i and do not allow for the fact that the system is stuck in a particular metastable state. The history of the system determines that metastable state into which it settles. A particularly graphic example of the difference between the equilibrium value of a quantity and its value for a given metastable state is provided by the susceptibility χ. The Monte Carlo work of Kirkpatrick and Sherrington (1978) shows that χ apparently vanishes as $T \to 0$, whereas the equilibrium calculation of Parisi gives $\chi = 1$ for all $T < T_c$. The susceptibility determined in the Monte Carlo experiment is essentially just the induced magnetisation of a *given* metastable state divided by the small applied field h. In the equilibrium calculation, application of the field h, no matter how small, induces a hop to the new distinct state of lowest free energy, which has a magnetisation larger than that of the original state (Bray and Moore 1980c).

For a finite-range model of a spin glass, such as the Edwards–Anderson (1975) model, we speculate that metastable states still exist at finite temperatures provided the dimensionality of the system is greater than the lower critical dimension (LCD), which is generally supposed to be four (Fisch and Harris 1977, Reed *et al* 1978). Below the LCD, metastable states really only exist at $T = 0$, where they correspond to the various minima of the Hamiltonian $\mathcal{H} = -\sum_{(ij)} J_{ij}S_iS_j$. We suspect that the infinite barriers separating the minima melt away below the LCD, thereby preventing the existence of finite temperature metastable states. The numerical work of Morgenstern and Binder (1980) suggests that for two- and three-dimensional systems only uncorrelated metastable states exist and so the critical energy coincides with the ground-state energy.

It is convenient to substitute for $\sum_j J_{ij}m_j$ from equation (1) in equation (2) to express f as a sum of single-site terms:

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

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

$$N_s(f) = N^2 \int_0^1 dq \int_{-1}^1 \prod_i dm_i \delta\Big(Nq - \sum_i m_i^2\Big)\delta\Big(Nf - \sum_i f(m_i)\Big)\prod_i \delta(G_i)|\det \mathsf{A}| \tag{5}$$

where $|\det \mathsf{A}|$ is the Jacobian normalising the delta functions:

$$A_{ij} = \frac{\partial G_i}{\partial m_j} = [(1-m_i^2)^{-1} + \beta^2(1-q)]\delta_{ij} - \beta J_{ij} + O(N^{-1}). \tag{6}$$

We want to calculate $\langle \ln N_s(f)\rangle$ where the angular brackets denote an average over the $\{J_{ij}\}$. This is because $\ln N_s(f)$ is extensive, i.e. proportional to N, and so its average should give results pertinent to a *typical* system (see I, also Bray and Moore 1981). To compute $\langle \ln N_s(f)\rangle$ we shall use the replica method (Edwards and Anderson 1975), by writing

$$\langle \ln N_s(f)\rangle = \lim_{n\to 0} n^{-1} \ln\langle N_s^n(f)\rangle. \tag{7}$$

Introducing in equation (5) integral representations of the delta functions gives

$$N_s^n(f) = N^{2n}\int_0^1 \prod_\alpha \mathrm{d}q_\alpha \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \prod_\alpha \frac{\mathrm{d}\lambda_\alpha}{2\pi \mathrm{i}} \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \prod_\alpha \frac{\mathrm{d}u_\alpha}{2\pi \mathrm{i}} \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \prod_{i,\alpha} \frac{\mathrm{d}x_{i\alpha}}{2\pi \mathrm{i}} \int_{-1}^{1} \prod_{i,\alpha} \mathrm{d}m_{i\alpha}$$

$$\exp\Big(-N\sum_\alpha (\lambda_\alpha q_\alpha + u_\alpha f) + \sum_{i,\alpha} [\lambda_\alpha m_{i\alpha}^2 + u_\alpha f(m_{i\alpha}) + x_{i\alpha} g(m_{i\alpha})]$$

$$-\beta \sum_{(ij)\alpha} J_{ij}(x_{i\alpha} m_{j\alpha} + x_{j\alpha} m_{i\alpha})\Big) \prod_\alpha |\det \mathsf{A}\{J_{ij}, m_{i\alpha}\}| \tag{8}$$

where $g(m) = th^{-1}m + \beta^2(1-q)m$. Because of the factor N the integrals over q_α, λ_α and u_α will eventually be performed by steepest descents with the result that $q_\alpha = q$, $\lambda_\alpha = \lambda$ and $u_\alpha = u$. Therefore we shall drop the replica indices on these variables from the outset. In I it was shown that the error involved in bond-averaging the determinant of A separately was negligible as $N\to\infty$ which allows the following replacement in equation (8):

$$\prod_\alpha \det \mathsf{A}\{J_{ij}, m_{i\alpha}\} \to \exp\{\tfrac{1}{2}nN\beta^2(1-q)^2\} \prod_{i,\alpha} (1-m_{i\alpha}^2)^{-1}. \tag{9}$$

Performing the averages over the J_{ij} results in

$$\langle N_s^n(f)\rangle = \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \prod_{i,\alpha} \frac{\mathrm{d}x_{i\alpha}}{2\pi \mathrm{i}} \int_{-1}^{1} \prod_{i,\alpha} \frac{\mathrm{d}m_{i\alpha}}{1-m_{i\alpha}^2} \exp\Big(\tfrac{1}{2}nN\beta^2(1-q)^2$$

$$-nN(\lambda q + uf) + \sum_{i,\alpha} [\lambda m_{i\alpha}^2 + uf(m_{i\alpha}) + x_{i\alpha} g(m_{i\alpha})]$$

$$+\tfrac{1}{2}\beta^2 q \sum_{i,\alpha} x_{i\alpha}^2 + \frac{1}{2}\frac{\beta^2}{N}\sum_\alpha \Big(\sum_i x_{i\alpha} m_{i\alpha}\Big)^2$$

$$+\frac{1}{2}\frac{\beta^2}{N}\sum_{\alpha\neq\beta}\Big(\sum_i x_{i\alpha}x_{i\beta}\Big)\Big(\sum_j m_{j\alpha}m_{j\beta}\Big) + \frac{1}{2}\frac{\beta^2}{N}\sum_{\alpha\neq\beta}\Big(\sum_i x_{i\alpha}m_{i\beta}\Big)\Big(\sum_j m_{j\alpha}x_{j\beta}\Big)\Big). \tag{10}$$

We now introduce Hubbard–Statonovich variables V_α to decouple the $(\Sigma_i x_{i\alpha} m_{i\alpha})^2$ term, $\eta_{\alpha\beta}$ and $\eta_{\alpha\beta}^*$ to decouple the $(\Sigma_i x_{i\alpha} x_{i\beta})(\Sigma_j m_{j\alpha} m_{j\beta})$ terms and finally $\rho_{\alpha\beta}$ and $\rho_{\alpha\beta}^*$ to decouple the $(\Sigma_i x_{i\alpha} m_{i\beta})(\Sigma_j m_{j\alpha} x_{j\beta})$ terms, using variations on the identity

$$\exp\Big(\frac{1}{2}\frac{\beta^2}{N}a^2\Big) = \Big(\frac{N}{2\pi}\Big)^{1/2}\frac{1}{\beta}\int_{-\infty}^{\infty} \mathrm{d}V \exp\Big(-\frac{1}{2}\frac{NV^2}{\beta^2} + aV\Big).$$

The sites are decoupled after making these transformations which allows the integrals over $x_{i\alpha}$ and $m_{i\alpha}$ to be done separately, site by site. Then

$$\langle N_s^n(f)\rangle = \mathrm{Ext}\Big\{\exp\Big[nN(-\lambda q - uf - \Delta(1-q) - \Delta^2/2\beta^2)$$

$$-\frac{N}{2\beta^2}\sum_{\alpha\neq\beta}(\eta_{\alpha\beta}^*\eta_{\alpha\beta} + \rho_{\alpha\beta}^2) + N\ln I\Big]\Big\} \tag{11}$$

where

$$I=\int_{-\mathrm{i}\infty}^{\mathrm{i}\infty}\prod_\alpha\frac{\mathrm{d}x_\alpha}{2\pi\mathrm{i}}\int_{-1}^{1}\prod_\alpha\frac{\mathrm{d}m_\alpha}{1-m_\alpha^2}\exp\Big\{\sum_\alpha(\lambda m_\alpha^2+uf(m_\alpha)+x_\alpha(th^{-1}m_\alpha-\Delta m_\alpha)$$
$$+\tfrac{1}{2}\beta^2qx_\alpha^2)+\tfrac{1}{2}\sum_{\alpha\neq\beta}(\eta_{\alpha\beta}x_\alpha x_\beta+\eta^*_{\alpha\beta}m_\alpha m_\beta+2\rho_{\alpha\beta}m_\alpha x_\beta)\Big\}$$

and $V=-\beta^2(1-q)-\Delta$. Ext indicates that an extremum is sought with respect to Δ, λ, q, u, $\eta_{\alpha\beta}$, $\eta^*_{\alpha\beta}$ and $\rho_{\alpha\beta}$, in other words the integrals over these variables have been performed by steepest descents. (We have assumed that at the extremum $\rho_{\alpha\beta}=\rho_{\beta\alpha}$ and $V_\alpha=V$.)

Provided $f>f_c(T)$ the off-diagonal terms $\eta_{\alpha\beta}$, $\eta^*_{\alpha\beta}$ and $\rho_{\alpha\beta}$ are zero at the stable extremum (see I, Bray and Moore 1981). These terms, which are a measure of the degree of correlation between different metastable states of the same free energy f acquire non-zero values only for $f<f_c(T)$. If one assumes that $\eta_{\alpha\beta}$, $\eta^*_{\alpha\beta}$ and $\rho_{\alpha\beta}$ do not depend on the labels α and β, then one recovers the 'innocent replica' treatment of de Dominicis *et al* (1980), I and Roberts (1981). We suspect, however, that this replica symmetric ansatz is unstable like the Sherrington–Kirkpatrick solution of the SK model (de Almeida and Thouless 1978). In this note we explore the consequences of making a Parisi replica symmetry breaking ansatz for the off-diagonal matrices.

We start by considering the perturbative calculation of $\langle\ln N_s(f)\rangle$ near T_c. Set $t=1-T/T_c$ and assume u, q, $\eta_{\alpha\beta}=\mathrm{O}(t)$; λ, Δ, $\rho_{\alpha\beta}=\mathrm{O}(t^2)$ and $\eta^*_{\alpha\beta}=\mathrm{O}(t^3)$. Then

$$N^{-1}\langle\ln N_s(f)\rangle=\lim_{n\to0}(nN)^{-1}\ln\langle N_s^n(f)\rangle=D+OD$$

where

$$D=-\alpha Q/\beta^2-\Delta^2/2\beta^2-u(f+\ln2+\tfrac{1}{4}\beta^2-Q^2/4\beta^2)+\alpha Q-\tfrac{1}{4}uQ^2+\tfrac{1}{2}\Delta^2-2\alpha Q^2$$
$$+\tfrac{2}{3}uQ^3+\tfrac{17}{3}\alpha Q^3+2\alpha\Delta Q-\tfrac{17}{8}uQ^4-u\Delta Q^2-\Delta^2Q+\tfrac{1}{3}\Delta^3-\tfrac{62}{3}\alpha Q^4$$
$$-10\alpha\Delta Q^2+\tfrac{124}{15}uQ^5+\tfrac{17}{3}u\Delta Q^3+\tfrac{7}{2}\Delta^2Q^2+\alpha^2Q^2-\alpha uQ^3+\tfrac{1}{3}u^2Q^4+\mathrm{O}(t^7)\qquad(12)$$

and

$$OD=\frac{1}{2n}(1-\beta^{-2}-2Q+2\Delta+5Q^2)\Sigma'(\eta^*_{\alpha\beta}\eta_{\alpha\beta}+\rho^2_{\alpha\beta})$$
$$-\frac{1}{n}(2\alpha-uQ)(1-4Q)\Sigma'\eta_{\alpha\beta}\rho_{\alpha\beta}-\frac{1}{n}Q\Sigma'\eta^*_{\alpha\beta}\rho_{\alpha\beta}$$
$$-\frac{1}{3n}\Sigma'(\rho_{\alpha\beta}\rho_{\beta\gamma}\rho_{\gamma\alpha}+3\eta^*_{\alpha\beta}\eta_{\beta\gamma}\rho_{\gamma\alpha})$$
$$+\frac{1}{12n}\Sigma'(u^2\eta^4_{\alpha\beta}-8u\eta^3_{\alpha\beta}\rho_{\alpha\beta}+4\eta^3_{\alpha\beta}\eta^*_{\alpha\beta}+12\eta^2_{\alpha\beta}\rho^2_{\alpha\beta})+\mathrm{O}(t^7).\qquad(13)$$

Here $\alpha=\lambda-\Delta$ and $Q=\beta^2q$. The prime in the summation indicates a free sum over the replica labels with the diagonal terms excluded. We next parametrise each of the matrices $\eta_{\alpha\beta}$, $\eta^*_{\alpha\beta}$ and $\rho_{\alpha\beta}$ according to the Parisi scheme (Parisi 1979), when the 'off-diagonal term' OD becomes as $n\to 0$

$$OD = -\tfrac{1}{2}(1-\beta^{-2}-2Q+2\Delta+5Q^2)\int_0^1 \mathrm{d}x\,(\eta^*(x)\eta(x)+\rho^2(x))$$
$$+(2\alpha-uQ)(1-4Q)\int_0^1 \mathrm{d}x\,\eta(x)\rho(x)$$
$$+Q\int_0^1 \mathrm{d}x\,\eta^*(x)\rho(x)-\tfrac{1}{3}\int_0^1 \mathrm{d}x\left(x\rho^3(x)+3\rho(x)\int_0^x \mathrm{d}y\,\rho^2(y)\right)$$
$$-\int_0^1 \mathrm{d}x\left(x\eta^*(x)\eta(x)\rho(x)+\rho(x)\int_0^x \mathrm{d}y\,\eta^*(y)\eta(y)\right.$$
$$\left.+\eta(x)\int_0^x \mathrm{d}y\,\eta^*(y)\rho(y)+\eta^*(x)\int_0^x \mathrm{d}y\,\eta(y)\rho(y)\right)$$
$$-\frac{u^2}{12}\int_0^1 \mathrm{d}x\,\eta^4(x)+\tfrac{2}{3}u\int_0^1 \mathrm{d}x\,\eta^3(x)\rho(x)-\tfrac{1}{3}\int_0^1 \mathrm{d}x\,\eta^3(x)\eta^*(x)$$
$$-\int_0^1 \mathrm{d}x\,\eta^2(x)\rho^2(x). \qquad (14)$$

We now find the extremum of $N^{-1}\langle\ln N_s(f)\rangle$. This involves differentiating with respect to α, Q, Δ, u and functionally differentiating with respect to $\eta(x)$, $\eta^*(x)$ and $\rho(x)$. It proved impossible to solve analytically the resulting seven coupled nonlinear integral equations, except for one special value of the free energy $f(=f_{\min})$, which turns out to be that value of the free energy at which $\langle\ln N_s(f)\rangle=0$, i.e. the lower 'band-edge'. Then, to the order in t to which the calculation is valid,

$$q=t+t^2, \qquad \Delta=2t^2, \qquad u=-4t, \qquad 2\alpha-uQ=4t^3$$
$$\eta(x)=\eta(1)f(x), \qquad \eta^*(x)=\eta^*(1)f(x), \qquad \rho(x)=\rho(1)f(x)$$

where

$$f(x)=2x, \qquad x\leqslant x_1=\tfrac{1}{2}; \qquad f(x)=1,\ x>x_1$$

and $\eta(1)=t$, $\eta^*(1)=4t^3$ and $\rho(1)=-2t^2$. At the band-edge there exists only one metastable state—the state of lowest free energy. Consequently, one would expect then that $Q=\eta(1)$, since the meaning of these quantities is

$$Q=\beta\langle\langle m_i^2\rangle_s\rangle \qquad \text{and} \qquad \eta(1)=\beta^2\langle\langle m_i\rangle_s^2\rangle$$

where $\langle\ \rangle_s$ means an average over solutions at the given free energy. Hence, if there is a value of f for which there is only one metastable state, Q should then equal $\eta(1)$ (which in turn should be β^2 times the Edwards–Anderson order parameter $\langle\langle S_i\rangle_T^2\rangle$ and $\langle\ \rangle_T$ denotes the usual thermal average). To the order to which the above calculations are valid this expectation is borne out. This should be contrasted with the result obtained at the band-edge in the innocent replica approximation, namely $\eta(1)=0.3471t+O(t^2)$, $Q=t+O(t^2)$ (I). That Parisi symmetry breaking apparently gives $Q=\eta(1)$ at the band-edge finally convinced us of its essential correctness.

We believe that x_1 decreases from its value of $\tfrac{1}{2}$ at $f=f_{\min}$ down to zero at $f=f_c(T)$ (whose value is specified in I). Indeed, for values of f close to $f_c(T)$ the off-diagonal terms are small and a perturbation analysis of the equations becomes possible. One finds $x_1 \propto (f_c(T) - f)$. An interesting question is whether $f_{\min}$ coincides with the free energy given by the direct Parisi approach to calculating the partition function Z. To the order to which we have gone the answer seems to be yes, even though the value of x_1 is quite different (x_1 in Parisi's work only reaches $\frac{1}{2}$ at $T = 0$, (Vannimenus *et al* 1981)). Our value for q also apparently coincides with his $q(1)$. We conclude from this that the Parisi calculation gives the properties of the metastable state of lowest free energy at any value of the temperature and it is only this metastable state which evolves all the way down from T_c to absolute zero.

The perturbative calculation can be readily extended to include the effects of a uniform magnetic field h. Its effect is to modify the function $f(x)$ below a value x_0 to a constant $f(x) = f_0$, where $f_0 = 2x_0$ and $x_0^3 = 3(\beta h)^2/32t^3$. The new value of $f_{\min}$ is consistent with Parisi's solution as is the susceptibility ($\chi = 1$). This susceptibility is the equilibrium susceptibility and should not be confused with the susceptibility of a given state which is given by the relation $\chi = \beta(1-q)$.

It is possible, following Parisi (1979), to write down a differential equation whose solution would permit the calculation of $\langle \ln N_s(f) \rangle$ for arbitrary temperature T. We only give the result, which was obtained by the method of Duplantier (1981)

$$N^{-1}\langle \ln N_s(f)\rangle = -\lambda q - uf - \tilde{\Delta}(1-q) + \rho(1)(1-q) - \tilde{\Delta}^2/2\beta^2 + \tilde{\Delta}\rho(1)/\beta^2 - \rho(1)^2/2\beta^2 + \frac{1}{2\beta^2}\int_0^1 \mathrm{d}x\, (\eta^*(x)\eta(x) + \rho^2(x)) + f(0,0,0)$$

where $f(x, h_1, h_2)$ satisfies the differential equation

$$\frac{\partial f}{\partial x} = -\frac{1}{2}\frac{\mathrm{d}\eta}{\mathrm{d}x}\left[\frac{\partial^2 f}{\partial h_1^2} + x\left(\frac{\partial f}{\partial h_1}\right)^2\right] - \frac{1}{2}\frac{\mathrm{d}\eta^*}{\mathrm{d}x}\left[\frac{\partial^2 f}{\partial h_2^2} + x\left(\frac{\partial f}{\partial h_2}\right)^2\right] - \frac{\mathrm{d}\rho}{\mathrm{d}x}\left[\frac{\partial^2 f}{\partial h_1 \partial h_2} + x\frac{\partial f}{\partial h_1}\frac{\partial f}{\partial h_2}\right]$$

subject to the boundary condition

$$f(1, h_1, h_2) = \ln Z(h_1, h_2)$$

and

$$Z = [2\pi(Q - \eta(1))]^{-1/2}\int_{-1}^{1}\frac{\mathrm{d}m}{1-m^2}\exp\left(-\frac{(th^{-1}m - \tilde{\Delta}m + h_1)^2}{2(Q-\eta(1))} + (\lambda - \tfrac{1}{2}\eta^*(1))m^2 + uf(m) + mh_2\right).$$

The parameters λ, q, u, $\tilde{\Delta}$ and the functions $\eta(x)$, $\eta^*(x)$ and $\rho(x)$ are varied to make $\langle \ln N_s(f)\rangle$ an extremum. These equations look intractable but it might be possible to show that they coincide with the much simpler equations of Parisi when $f = f_{\min}$, where we expect $Q = \eta(1)$.

While there remain many interesting and unsolved topics in connection with the SK model it does now seem valid to refer to it as the solvable model for the spin glass transition.

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