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Parisi function $q(x)$ for spin glasses near T_c

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Résumé. — Nous calculons la fonction-paramètre d'ordre $q(x)$ pour un verre de spin de Sherrington-Kirkpatrick en champ nul, près de T_c . L'énergie libre est développée jusqu'à l'ordre $(T_c - T)^7$. La fonction de recouvrement dx/dq est parabolique au voisinage de $q = 0$. De manière générale, nous montrons que $q(x)$ ne contient que des puissances impaires de x en dessous de la région du plateau. En conséquence la distribution de recouvrement en champ nul est symétrique et possède des dérivées continues au point $q = 0$.

Abstract. — We compute the orderparameter function $q(x)$ for the Sherrington-Kirkpatrick spin-glass to high accuracy near $T = T_c$ in zero external field. The free energy is calculated to order $(T_c - T)^7$. The overlap function dx/dq is parabolic near $q = 0$. We show generally that $q(x)$ involves only odd powers of x below its plateau. Hence the overlap distribution in strictly zero field is symmetric with continuous derivatives at $q = 0$.

In the last few years there has been much progress in our understanding of the long-ranged random bond Ising model known as the Sherrington-Kirkpatrick (SK) spin-glass model [1]. By now Parisi's solution [2] obtained by the technique of replica symmetry breaking has passed all stability checks [3]. Sompolinsky has suggested a very stimulating interpretation of Parisi's orderparameter function $q(x)$, $0 \leq x \leq 1$, as local spin autocorrelation on long time scales τ_x ($\tau_1 \leq \tau_x \leq \tau_0$) [4]. The author has shown that, if one explicitly breaks the replica symmetry by an external field [5], one arrives at Sompolinsky's long time interpretation of $q(0)$. However, this interpretation seems to be inconsistent with statistical mechanics according to de Dominicis and Young [6]. The authors argue that one has to restore replica symmetry by summing over all degenerate saddle points. This concept has proven very fruitful. As a consequence Parisi [7] could prove that the inverse function of $q(x)$, $x(q)$, describes the bond averaged probability density for overlap between pure states of the system. The pure states cannot be isolated like in a ferromagnet and they can be associated [8] with certain solutions of the mean-field equations of Thouless, Anderson and Palmer [9].

In spite of its importance not much is known about the analytic behaviour of $q(x)$. $q(x)$ has a plateau q_1 for $x > x_1$ and is almost linear in x for $x < x_1$ near $T = T_c$ [10]. There is a second plateau q_0 for $x < x_0$ in an external field. In between $q(x)$ is monotonic [11]. Sommers and Dupont derived a closed set of equations to determine $q(x)$ and solved them numerically at $T = 0$ [12]. In this Letter we want to use these equations to determine $q(x)$ to higher order near

$T = T_c$. These equations involve a local magnetization $m(x, y)$ in a frozen field y on a time scale τ_x and a probability density $P(x, y)$ of frozen fields on a time scale τ_y . In a recent preprint Mezard and Virasoro [8] have analysed these functions in terms of the overlap of pure states and find that $P(x, y) dy$ describes the probability that pure states with mutual overlap $q(x)$ have local magnetization $m(x, y)$. Let us start with the equations determining $q(x)$ [12], which follow from Parisi's differential equation [2] and the stationarity of the free energy

$$q(x) = \int dy P(x, y) m^2(x, y) \quad (1)$$

$$\frac{\partial}{\partial x} m(x, y) = -\frac{\dot{q}(x)}{2} \left(\frac{\partial^2}{\partial y^2} m(x, y) + \frac{2x}{T} m(x, y) \frac{\partial}{\partial y} m(x, y) \right) \quad (2)$$

$$\frac{\partial}{\partial x} P(x, y) = \frac{\dot{q}(x)}{2} \left(\frac{\partial^2}{\partial y^2} P(x, y) - \frac{2x}{T} \frac{\partial}{\partial y} (P(x, y) m(x, y)) \right) \quad (3)$$

with initial conditions

$$m(1, y) = \tanh(y/T) \quad (4)$$

$$P(0, y) = \delta(y). \quad (5)$$

The external field is equal to zero. We have set $J = T_c = 1$, $k_B = 1$. A dot means the derivative with respect to x and in what follows a prime means the derivative with respect to y .

If we consider the x dependence of an integral $\int dy Pf$ we find by partial integration using (3)

$$\frac{d}{dx} \int dy P(x, y) f(x, y) = \int dy P(x, y) \left\{ \frac{\partial}{\partial x} + \frac{\dot{q}}{2} \left(\frac{\partial^2}{\partial y^2} + \frac{2x}{T} m \frac{\partial}{\partial y} \right) \right\} f(x, y). \quad (6)$$

Hence the averaged magnetization, $\bar{m}$, is independent of x . We denote the operator in wavy brackets on the rhs in (6) by Ω . We have

$$\Omega m = 0 \quad (7)$$

$$\left[\frac{\partial}{\partial y}, \Omega \right] = \frac{x}{T} \dot{q} m' \frac{\partial}{\partial y}. \quad (8)$$

The operator Ω acting on a product of functions yields

$$\Omega f \cdot g = (\Omega f) \cdot g + f \cdot \Omega g + \dot{q} f' g' \quad (9)$$

which can be generalized to multiple products. Using equations (6) to (9) we can easily rederive results of reference [11] by repeated differentiation of (1) with respect to x :

$$\dot{q} = \frac{d}{dx} \int dy P m^2 = \int dy P \Omega m^2 = \int dy P (2 m \Omega m + \dot{q} (m')^2) = \dot{q} \int dy P (m')^2. \quad (10)$$

For $\dot{q} \neq 0$ we find the marginal stability condition [11,13]

$$0 = 1 - \int dy P (m')^2. \quad (11)$$

By differentiating (11) we find

$$0 = \int dy P(2 m' \Omega m' + \dot{q}(m'')^2). \quad (12)$$

We here invoke the commutation relation (8) and have for $\dot{q} \neq 0$

$$0 = -\frac{2x}{T} \int dy P(m')^3 + \int dy P(m'')^2. \quad (13)$$

The latter equation determines e.g. the break point x_1 of Parisi's function above which $q(x) = q_1$. We differentiate (13) once again and obtain

$$\frac{2}{T} \int dy P(m')^3 = -\frac{6\dot{x}}{T} \int dy P(m'^2 \Omega m' + \dot{q} m'(m'')^2) + \int dy P(2 m'' \Omega m'' + \dot{q}(m''')^2). \quad (14)$$

By using

$$\left[\Omega, \left(\frac{\partial}{\partial y} \right)^2 \right] = -\frac{x\dot{q}}{T} m'' \frac{\partial}{\partial y} - \frac{2x\dot{q}}{T} m' \left(\frac{\partial}{\partial y} \right)^2 \quad (15)$$

we find

$$\frac{2}{T} \int dy P(m')^3 = \dot{q} \int P dy \left((m''')^2 - \frac{12x}{T} m'(m'')^2 + 6 \left(\frac{x}{T} \right)^2 (m')^4 \right). \quad (16)$$

This equation determines $\dot{q}(x)$. Higher derivatives yield equations for $\ddot{q}$, q [3], etc.

Let us evaluate equations (1), (11), (13), (16) at the break point x_1 ($x \rightarrow x_1$ from the left). From (4) we use the relation

$$m' = \frac{1}{T}(1 - m^2) \quad (17)$$

and have

$$q_1 = \overline{m^2} \quad (18)$$

$$T^2 = \overline{(1 - m^2)^2} = 1 - 2q_1 + \overline{m^4} \quad (19)$$

$$0 = -x_1 \overline{(1 - m^2)^3} + 2 \overline{m^2(1 - m^2)^2} \quad (20)$$

$$2 T^2 \overline{(1 - m^2)^3} = \dot{q}_1 (4(1 - 3m^2)^2 \overline{(1 - m^2)^2} - 48 x_1 \overline{(1 - m^2)^3 m^2} + 6 x_1^2 \overline{(1 - m^2)^4}). \quad (21)$$

The bar means $\int dy P \dots$. We consider these equations near T_c , and use $T = 1 - \tau$. It is easy to see that the moments $\overline{m^{2n}}$ are given, to lowest order in τ , by the SK solution

$$\overline{m^{2n}} = \tau^n \frac{(2n)!}{2^n n!} + \mathcal{O}(\tau^{n+1}). \quad (22)$$

Hence we immediately get from equations (18) to (21)

$$q_1 = \tau + \tau^2 + \mathcal{O}(\tau^3) \quad (23)$$

$$x_1 = 2\tau - 4\tau^2 + \mathcal{O}(\tau^3) \quad (24)$$

$$\dot{q}_1 = \frac{1}{2}(1 + 3\tau - 3\tau^2) + \mathcal{O}(\tau^3). \quad (25)$$

We may also evaluate the equations at $x = 0$. In appendix we show that $m(0, y)$ determines the distribution of the local equilibrium magnetization $\langle S \rangle$ so that generalized Fischer relations [14] are valid, similar to equation (17) and its derivatives

$$\left. \frac{\partial}{\partial y} m(0, y) \right|_{y=0} = \frac{1}{T} \overline{1 - \langle S \rangle^2} \quad (26)$$

$$\left. \left(\frac{\partial}{\partial y} \right)^3 m(0, y) \right|_{y=0} = - \frac{2}{T^3} \overline{(1 - 3 \langle S \rangle^2) (1 - \langle S \rangle^2)} \quad (27)$$

and so on. Here the bar means the configuration average (cf. appendix). From de Dominicis and Young [6] we know

$$\overline{\langle S \rangle^2} = \int_0^1 dx q(x) \quad (28)$$

and I provided a proof [11] of

$$\tau = \int_0^1 dx q(x) \quad (29)$$

for all $0 \leq \tau < 1$. Again to lowest order in τ , (22) is valid for the moments $\overline{\langle S \rangle^{2^n}}$. We find at $x = 0$

$$q_0 = \overline{\langle S \rangle^2} = 0 \quad (30)$$

$$T^2 = \overline{(1 - \langle S \rangle^2)^2} \quad (31)$$

$$2 T^2 \overline{(1 - \langle S \rangle^2)^3} = 4 \dot{q}_0 \overline{(1 - 3 \langle S \rangle^2) (1 - \langle S \rangle^2)^2}. \quad (32)$$

Hence we recover equation (29) and

$$\dot{q}_0 = \frac{1}{2} \frac{T^5}{(1 - 4\tau + 3 \overline{\langle S \rangle^4})^2} \quad (33)$$

which is an exact relation. Its power series approximation is determined by (22) as

$$\dot{q}_0 = \frac{1}{2} (1 + 3\tau) + \mathcal{O}(\tau^3). \quad (34)$$

Now we want to determine $q(x)$ for $0 < x < x_1$. The structure of equations (1) to (5) shows that we may expand in powers of x . From (30), (34) and (24) we have

$$q(x) = \frac{1}{2} (1 + 3\tau) x + ax^2 + bx^3 + \mathcal{O}(\tau^4). \quad (35)$$

With (25) we find $a = \mathcal{O}(\tau)$. We now use the exact relation (29) and obtain

$$\tau = \frac{1}{4} (1 + 3\tau) x_1^2 + a \frac{x_1^3}{3} + b \frac{x_1^4}{4} + (1 - x_1) q_1 + \mathcal{O}(\tau^5). \quad (36)$$

Equation (35) gives for $x = x_1$

$$x_1 = \frac{2 q_1}{1 + 3 \tau} + \mathcal{O}(\tau^3). \quad (37)$$

By inserting this into (36) and solving for q_1 we recover Sompolinsky's result [4]

$$q_1 = \tau + \tau^2 - \tau^3 + \mathcal{O}(\tau^4). \quad (38)$$

We can now employ (19), (20), (22) to construct x_1 to order τ^3 ,

$$x_1 = 2 \tau - 4 \tau^2 + 12 \tau^3 + \mathcal{O}(\tau^4). \quad (39)$$

With the help of (35), (39), (25) we determine a and b and obtain as our main result for $x < x_1$

$$q(x) = \frac{1}{2}(1 + 3 \tau) x - \frac{1}{8} x^3 + \mathcal{O}(\tau^4). \quad (40)$$

The coefficient $1/2$ in (40) improves Parisi's first calculation [2, 10]. By using again equation (36) we finally get

$$q_1 = \tau + \tau^2 - \tau^3 + \frac{5}{2} \tau^4 + \mathcal{O}(\tau^5). \quad (41)$$

An important remark should be made. It is obvious from the derivatives of equation (16) that $q(x)$ contains only odd powers of x . Hence $a = 0$ is an exact result. In zero external field $q(x)$ can be continued to an odd function with continuous derivatives at $x = 0$ corresponding to a symmetrized overlap function $\frac{dx}{dq}$. The regime of negative overlap corresponds to overlap between states in an infinitesimal external field and their time reversed counterparts. This is a natural consequence of the overlap interpretation [15]. From (40) we can calculate the overlap function $\frac{dx}{dq}$

$$\frac{dx}{dq} = \{ 2(1 - 3 \tau + 9 \tau^2) + 3 q^2 + \mathcal{O}(\tau^3) \} \theta(q) \theta(q_1 - q) + (1 - x_1) \delta(q - q_1) \quad (42)$$

where $\theta(y)$ is Heaviside's step function and $\delta(y)$ is Dirac's delta function. This is the overlap probability in an infinitesimal external field. For strictly zero external field it has to be symmetrized including a normalization factor $1/2$ [15].

It is not difficult to go one order beyond the calculation above. For this purpose it is useful to improve relation (22) for $x = 1$ with the help of (23) :

$$\overline{m^{2n}} = \tau^n \frac{(2n)!}{2^n \cdot n!} \left(1 + \frac{7n - 4n^2}{3} \tau + \mathcal{O}(\tau^2) \right) \quad (43)$$

which can most easily be seen by writing $\overline{m^{2n}}$ in Sompolinsky's form [4, 11].

We obtain

$$q(x) = \frac{1}{2}(1 + 3 \tau + 12 \tau^3) x - \frac{1}{8}(1 - \tau) x^3 + \mathcal{O}(\tau^5) \quad (44)$$

for $x < x_1$,

$$x_1 = 2\tau - 4\tau^2 + 12\tau^3 - 69\tau^4 + \mathcal{O}(\tau^5) \quad (45)$$

$$q_1 = \tau + \tau^2 - \tau^3 + \frac{5}{2}\tau^4 - \frac{39}{2}\tau^5 + \mathcal{O}(\tau^6). \quad (46)$$

The coefficients grow rapidly with order and it is rather likely that the expansion is asymptotic. The range of validity of an approximation decreases with order.

From the above expressions for $q(x)$ we deduce the thermodynamic properties of the SK model near $T = T_c$. We start from an expression for the internal energy per spin [2]

$$u = -\frac{1}{2T} \left(1 - \int_0^1 dx q(x)^2 \right). \quad (47)$$

The result is

$$\int_0^1 dx q(x)^2 = \tau^2 + \frac{2}{3}\tau^3 - \tau^4 + \frac{11}{5}\tau^5 - \frac{209}{15}\tau^6 + \mathcal{O}(\tau^7) \quad (48)$$

$$-2u = 1 + \tau - \frac{2}{3}\tau^3 + \frac{1}{3}\tau^4 - \frac{28}{15}\tau^5 + \frac{181}{15}\tau^6 + \mathcal{O}(\tau^7). \quad (49)$$

From (49) and the high temperature result we can calculate the free energy per spin

$$f = -(1 - \tau) \ln 2 - \frac{1}{4} \left(1 + \tau + \tau^2 + \frac{\tau^3}{3} - \frac{\tau^4}{6} + \frac{\tau^5}{30} - \frac{3}{5}\tau^6 + \frac{317}{105}\tau^7 \right) + \mathcal{O}(\tau^8). \quad (50)$$

One sees that the asymptotic expansion for f is good up to fifth order in τ . This is the first order where it differs from the SK solution [10]. From (49) and (50) one easily obtains the expansion for specific heat and entropy. x_1 is related to the dynamical critical index of Sompolinsky and Zippelius [16].

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Appendix.

We determine the relation between $m(0, y)$ and the distribution of local magnetizations $\langle S_i \rangle$. The key observation is the exact relation between the derivative of $\langle S_i \rangle$ with respect to the local external field b_i and $\langle S_i \rangle^2$ for an Ising system

$$\frac{\partial}{\partial b_i} \langle S_i \rangle = \frac{1}{T} (1 - \langle S_i \rangle^2). \quad (\text{A.1})$$

Obviously we can take higher derivatives

$$\left(\frac{\partial}{\partial b_i} \right)^2 \langle S_i \rangle = -\frac{2}{T^2} \langle S_i \rangle (1 - \langle S_i \rangle^2) \quad (\text{A.2})$$

and so on. In order to calculate the configuration average of these quantities with respect to the bonds $\mathcal{A}_{ij}$ in the limit of homogeneous external field $b_j \rightarrow b$, we consider a system with a localized external field $b_0 \neq b$, $b_j = b$ for $j \neq 0$. All information is then contained in $\langle S_0 \rangle$. $\langle S_0 \rangle$ can easily be calculated by the replica method. It turns out that $\langle S_0 \rangle$ is given by the usual expression for the averaged local magnetization with the explicit b dependence replaced by b_0 . Hence

$$\langle S_0 \rangle = \int \frac{dz}{\sqrt{2\pi}} e^{-z^2/2} m(0, b_0 + z\mathcal{A}\sqrt{q(0)}) . \quad (\text{A.3})$$

This is the only place where b_0 occurs. It does not modify the orderparameters. Taking the derivatives with respect to b_0 at $b_0 = b$ we can calculate all moments $\langle S_i \rangle^n$. In the limit $b \rightarrow 0$ we arrive at equations (26) and (27).

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