Method for replica symmetry breaking at and near $T=0$ with application to the Sherrington-Kirkpatrick model

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We describe a method which allows the treatment of high orders of replica symmetry breaking (RSB) at low temperatures as well as at $T=0$ directly, without a need for approximations or scaling assumptions. It yields the low-temperature order function $q(a,T)$ in the full range $0\leq a<\infty$ and is complete in the sense that all observables can be calculated from it. The behavior of some observables and the finite RSB theory itself is analyzed as the continuous RSB limit is approached. The validity and applicability of the traditional continuous formulation is then scrutinized and a continuous formulation for treating RSB in the Parisi gauge directly at $T=0$ is proposed.

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I. INTRODUCTION

The ordered phase of spin-glass models [1] has gained much attention over the past three decades, but still there are many open questions even in models which were designed to possess simple "mean-field-type" solutions. Typical for the difficulties encountered in the description of the ordered phase is the appearance of an ultrametric structure [2] in the mean-field theory of spin glasses, known as the Sherrington-Kirkpatrick (SK) model [3]. The correct treatment of the SK model involves a hierarchical scheme as introduced by Parisi [4], which only recently has been proven [5] to be exact in the limit of an infinite number of hierarchical steps of replica symmetry breaking (RSB). The rather formal RSB scenario has been connected to appealing pictures which reveal its physical content: there is a static interpretation by means of an ultrametric topology of the configuration space [2] and even a dynamical interpretation [6].

Though at temperatures right below the freezing transition T_C a small number κ of RSB steps is not a bad approximation, at temperatures $T\ll T_C$ the convergence of the results with respect to κ becomes worse. Traditionally, the $\kappa=\infty$ limit is formulated by a continuous theory in which the functional free energy $f[\tilde{q}(x)]$ is maximized with respect to the Parisi order function $\tilde{q}(x)$, $0\leq x\leq 1$ [1,4]. This was later expressed in a closed self-consistency form, involving a set of numerically solvable partial differential equations [7,8]. The treatment of Parisi RSB at finite temperatures is well established, meanwhile. Near T_C, even analytical solutions are available. At zero temperature, however, the proper form of the theory is still under discussion. The standard differential equations of the continuous formulation of Parisi RSB and their initial conditions become singular in the zero-temperature limit and the traditional formalism breaks down.[1]

In the literature, one finds two main directions of approaching the zero-temperature limit of Parisi RSB. Pankov proposed a beautifully simple scaling ansatz directly at infinite RSB, which becomes exact in a certain limit at zero temperature [10]. This limit, however, is far from being the only important region of the full zero-temperature solution, as we shall show later. On the other hand, our group has developed an exact finite RSB approach, which involves some advanced numerics when trying to reach orders of RSB high enough to obtain a confident extrapolation $\kappa\to\infty$. However, our approach allows for a numerically exact description of the *full* SK-model with all its difficulties and features at $T=0$. The numerical results can be used to construct and test analytical approximations or simpler alternative theories which capture the essential physics while being generalizable to more complex physical situations [11,12].

The low-temperature formulation that is developed in the present work directly identifies and analyzes the issues of the infinite RSB limit at zero temperature and resolves them by an appropriate rescaling of auxiliary quantities. It is based on the idea of rescaled Parisi block size parameters [4,13] $a_i=\beta m_i$ with $\beta=T^{-1}$. By this transformation, the nontrivial structure of the zero-temperature order function of the SK model can be resolved. In the traditional formalism, this structure is concentrated and hidden at the point $x=0$, where $\tilde{q}(x)$ becomes singular. Both Pankov's and our approach investigate this point, but while the scaling approach is incomplete in the sense, e.g., that it accounts only for the short-time observables or that it cannot describe the situation at finite external fields correctly, our approach yields the full zero-temperature solution.

The paper is organized as follows. In Sec. II, we give a short review of the issues encountered when performing the zero-temperature limit and show the connections between the two approaches mentioned above. In Sec. III, we derive the zero-temperature limit of the SK-model at finite orders of RSB. In Sec. IV, some results at low temperatures obtained with the finite RSB formalism are presented. In Sec. V, we discuss the $\kappa\to\infty$ limit of our theory.

II. THE $T=0$ LIMIT OF $\tilde{q}(x)$

The Parisi order function $\tilde{q}(x)$, $x\in[0,1]$ which is the central quantity of Parisi RSB at finite temperatures

[1]This statement is limited to Parisis RSB [4]. A more general RSB scheme [9] allows for a nonsingular continuous formulation at $T=0$ by exploiting the gauge invariance of the differential equations [8].

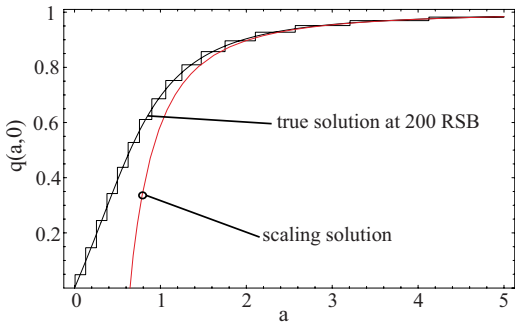

FIG. 1. (Color online) True $T=0$ order function $q(a,0)$ at order-200 RSB (black) and the step approximation at order-20 RSB. The lower (red) curve shows the result of Pankov scaling, i.e., $q(a,0)=1-\gamma a^{-2}$.

becomes a constant function at zero temperature $[\lim_{T\to 0} q(x)=1,\ x>0]$ with a singularity at $x=0$. Since typical observables like, e.g., the internal energy u involve integrals of the form $\beta\int_0^1 dx[1-\tilde{q}(x)]^2$, one is tempted to absorb the divergent factor β by a transformation $x\to a=\beta x$. The nontrivial zero-temperature structure which was concentrated at $x=0$ in the Parisi order function and created the singularity there is then "blown up" and resolved by the new order function $q(a)$. The transformation might remind the reader of Parisi-Toulouse (PAT) scaling [16]. The idea here is different, though, as we do not seek for a universal form of the order function (which is known to be nonexistent) but for a nonsingular zero-temperature theory.

The transformation $x\to a$ is not limited to $T=0$, of course, so that we can formulate a general low-temperature theory which allows a smooth transition from a treatment directly at $T=0$ to finite temperatures. The objective of our formalism is to find the function $q(a,T)$ with $a\in[0,\beta]$ from which one can obtain $\tilde{q}(x,T)=q(\beta x,T)$ at finite temperatures. At $\kappa<\infty$, $q(a,T)$ can be visualized as a step function with the number of steps equal to κ (see Fig. 1).

In this notation, the Pankov-scaling approach is equivalent to expanding $q(a,0)\simeq 1-\gamma a^{-2}$ near $a=\infty$ and calculating the coefficient γ. Knowledge of the a^{-2} term of this expansion is sufficient for short-time observables like the entropy or the nonequilibrium susceptibility. The full solution, however, must respect the functional dependence of $q(a,0)$ at all $a\in[0,\infty]$. Knowledge of the function $q(a,0)$ in its whole domain $[0,\infty]$ is needed to calculate, e.g., the ground state energy or the equilibrium susceptibility. Another point is that the effect of a finite external field is reflected by the small-a domain of $q(a,T)$ which is not resolved in [10]. In Fig. 1 the difference between the two solutions at small a is shown.

In order to obtain a well-defined zero-temperature limit, we start with a formulation of the theory at finite orders of RSB ($\kappa<\infty$), where $q(a,T)$ is a function with κ plateaus. The height of the ith plateau is given by the number $q_i\in[0,1]$ and the step positions are given by $a_i\in[0,\beta]$. If one aims at a continuous theory for $\kappa\to\infty$, one must first check that $\delta q_i=q_i-q_{i+1}$ and $\delta a_i=a_i-a_{i+1}$, i.e., the step heights and widths approach zero. For $T>0$, those requirements are satisfied and are the basis of the well-known Parisi differential equations [1,4,8]. At zero temperature and $\kappa\to\infty$, we still find $\delta q_i\to 0$, which is not surprising since q_i is always restricted to the interval $[0,1]$. However, some step widths δa_i grow indefinitely in this limit, so the assertion $\delta a_i\to 0$ which is needed to derive the Parisi differential equations fails at zero temperature. The nonvanishing δa_i correspond to those a_i that approach infinity for $\kappa\to\infty$, and so the derivation of the continuous theory fails at $a=\infty$, while for finite a a differential equation formulation is valid.

We want to stress the two different origins of the failure of a continuous theory. It is well known that the Parisi differential equation is formally invalid for $x>\bar{x}$, where $\bar{x}$ is the so-called break point [1]. This is because of the absence of block size parameters m_i in the interval $[\bar{x},1]$, even in the limit $\kappa\to\infty$. The largest m_i becomes equal to $\bar{x}$ in the continuous limit and all m_i fill the interval $[0,\bar{x}]$ where they get dense at finite temperatures. The validity domain of the differential equation can be extended *a posteriori* to the whole interval $[0,1]$ by defining $\tilde{q}(x)=\tilde{q}(\bar{x})$ and $\dot{\tilde{q}}(x)=0$ for $x>\bar{x}$.[2] In the zero-temperature limit, a new aspect appears: in addition to the absence of any parameters m_i beyond the break point $\bar{x}$, there is a domain where the parameters do not get dense for $\kappa\to\infty$, i.e., the interval $]0,\bar{x}]$. Instead, most of the parameters are exactly zero if the theory at $T=0$ is expressed in terms of m_i and not in terms of a_i.

As a result, at least the derivation of a differential equation in the regime $]0,\bar{x}]$ is questionable. Nevertheless, this regime has been investigated by means of a continuous theory [10]. We believe that the difference between the views of our work and [10] is a different order of limits: in the present work, we first take the zero-temperature limit and then let the order of RSB (κ) go to infinity, while in [10] the zero-temperature limit is taken after the $\kappa\to\infty$ limit.

In Sec. V of this paper, we show how the failure of a continuous theory at $a=\infty$ can be overcome by changing the initial condition of the partial differential equation which is valid for finite a only.

III. RECURSION TECHNIQUE FOR ARBITRARILY HIGH RSB ORDERS κ

We investigate the standard SK-model Hamiltonian [1,3] of N Ising spins $s_i=\pm 1$ with external field H,

$$\mathcal{H}_{\mathrm{SK}}=\sum_{i<j} J_{ij}s_i s_j - H\sum_i s_i. \tag{1}$$

The quenched random coupling constants J_{ij} are Gaussian-distributed random variables with zero mean and variance N^{-1}.[3] The model yields a freezing transition at $T_C=1$. Since the coupling constants' degrees of freedom are quenched, the free energy per spin of the system is given by $f=-T/N\langle\ln\langle\exp(-\beta\mathcal{H}_{\mathrm{SK}})\rangle_s\rangle_J$ where $\langle\cdot\rangle_s$ refers to an average

[2]Luckily, this convention is also useful for writing certain sums of parameters q_i and m_i as integrals over the domain $[0,1]$.

[3]The variance of the disorder distribution must scale as N^{-1} in order to obtain a meaningful thermodynamic limit. This choice also defines the energy and temperature scale of the system.

in the configuration space of Ising spins $s_i = \pm 1$ and $\langle \cdot \rangle_J$ refers to an average with respect to the coupling constants J_{ij}. In order to bypass the average of the logarithm we avail ourselves of the standard replica trick [17]. After transformation to a single-site model,[4] we introduce Parisi RSB for the replica coupling matrix, take the replica limit $n \to 0$ and the thermodynamic limit $N \to \infty$, and arrive at an expression for the free energy per spin (see also [1]),

$$f = -\frac{\beta}{2}(1 - 2q_1) + \frac{\beta}{4}\sum_{i=1}^{\kappa+1} q_i^2 (m_i - m_{i-1}) - \tilde{f} \tag{2}$$

with κ the order of RSB and q_i the values of the elements of the Parisi blocks with size m_i.[5] The nontrivial part $\tilde{f}$ of the free energy is given by the $(\kappa+1)$-fold nested integral

$$\begin{aligned}
\tilde{f} &= \frac{T}{m_\kappa}\int_{\kappa+1}^{G} \ln\left[\int_{\kappa}^{GE}\cdots\int_{2}^{GE}\int_{1}^{G}[2\cosh(\beta h_1)]^{m_1}\right] \\
&= \frac{T}{m_\kappa}\int \frac{dh_{\kappa+1}}{\sqrt{2\pi\Delta q_{\kappa+1}}} e^{-(H-h_{\kappa+1})^2/2\Delta q_{\kappa+1}} \\
&\quad \times \ln\left[\int \frac{dh_\kappa}{\sqrt{2\pi\Delta q_\kappa}} e^{-(h_{\kappa+1}-h_\kappa)^2/2\Delta q_\kappa}\right. \\
&\quad \times \left\{\cdots\left[\int \frac{dh_2}{\sqrt{2\pi\Delta q_2}} e^{-(h_3-h_2)^2/2\Delta q_2}\right.\right. \\
&\quad \times \left.\left.\left(\int \frac{dh_1}{\sqrt{2\pi\Delta q_1}} e^{-(h_2-h_1)^2/2\Delta q_1}\right.\right.\right. \\
&\quad \left.\left.\left. \times [2\cosh(\beta h_1)]^{m_1}\right)^{r_1}\right]^{r_2}\cdots\right\}^{r_{\kappa-1}}\Bigg].
\end{aligned} \tag{3}$$

For more clarity in the notation we have defined two types of Gaussian integral operators. The simple convolution operator, which convolves the function in its argument with a Gaussian distribution, is defined as

$$\int_i^G f(h_i) \equiv \int_{-\infty}^{\infty} \frac{dh_i}{\sqrt{2\pi\Delta q_i}} \exp\left(-\frac{(h_i - h_{i+1})^2}{2\Delta q_i}\right) f(h_i). \tag{4}$$

The widths of the Gaussian distributions are given in terms of the order parameters q_i as $\Delta q_i = q_i - q_{i+1}$, $\Delta q_{\kappa+1} = q_{\kappa+1}$. The second operator involves an additional exponentiation of the function the operator acts on, with a ratio r_{i-1} of block size parameters m_i,

$$\int_i^{GE} f(h_i) \equiv \int_i^G f(h_i)^{r_{i-1}}, \quad r_{i-1} = \frac{m_i}{m_{i-1}}. \tag{5}$$

The last Gaussian convolution (indexed by $\kappa+1$) in this sequence must be centered at the external field by defining $h_{\kappa+2} = H$. The Gaussian integral operators define "levels" $i = 1, \ldots, \kappa$. At each integration level i, i.e., after the application of $\int_i^{GE}$ in Eq. (3), one obtains a function of the single field variable h_{i+1}.

As explained above, it is convenient at low temperatures to transform to new block size variables $a_i = \beta m_i$. Since the block size ratios $r_i = \frac{m_{i+1}}{m_i} = \frac{a_{i+1}}{a_i}$ are not affected by the transformation $m \to a$, the definitions of the Gaussian integral operators also remain invariant.

$\tilde{f}$ depends on the temperature only at the innermost integrand of the sequence of integrations. This inner integrand, however, has a well-defined zero-temperature limit in the a formulation, namely,

$$[2\cosh(\beta h_1)]^{Ta_1} \overset{T\to 0}{\to} e^{a_1|h_1|}. \tag{6}$$

The utility of our formulation for low temperatures lies in the nonsingular limit of this inner integrand. It has been shown before [13] that the first integral can be performed analytically in the $T \to 0$ limit, but the integrals of the levels $i > 1$ cannot be solved exactly in general.

In an asymptotic regime, however, where $h_1 \to \pm\infty$, all integrals in (3) can be solved, even for finite temperatures. For large h_1 one finds for the inner integrand at arbitrary temperatures

$$[2\cosh(\beta h_1)]^{Ta_1} \overset{h_1\to\pm\infty}{\to} e^{a_1|h_1|}. \tag{7}$$

Further, it can be shown by completing the square in the argument of the exponential function of the integrand that the action of $\int_i^{GE}$ on a function of the form $\exp(a_{i-1}|h_i|)$ can be evaluated analytically in the limit $|h_{i+1}| \gg 1$. One finds

$$\int_i^{GE} e^{a_{i-1}|h_i|} \simeq \exp\left[a_i\left(|h_{i+1}| + \frac{1}{2}a_i\Delta q_i\right)\right]. \tag{8}$$

As a result, after the ith exponentiating Gaussian integral operation in (3) has been performed, one finds, up to a multiplicative constant, the same exponential asymptotic h behavior as of the inner integrand (6), but with $a_i|h|$ instead of $a_1|h|$.

The deviation of the integrals from their asymptotic forms at small h_i is incorporated in terms of auxiliary functions $\exp \mathcal{C}_i(h)$ which are defined by

$$\begin{aligned}
\int_i^{GE}\cdots\int_1^G [2\cosh(\beta h_1)]^{Ta_1} &= \exp\left[a_i\left(\frac{1}{2}\sum_{j=1}^{i} a_j\Delta q_j + |h_{i+1}|\right.\right. \\
&\quad \left.\left. + \exp \mathcal{C}_i(h_{i+1})\right)\right].
\end{aligned} \tag{9}$$

The functions $\exp \mathcal{C}_i$ are well defined and free of singularities at each level of integration and for all temperatures including $T = 0$. Furthermore, the domain in which $\exp \mathcal{C}_i(h) \neq 0$ is restricted to small h (see Fig. 2). The functions $\exp \mathcal{C}_i(h)$ are therefore the objects of our choice for the finite RSB numerics. At the zeroth level of integration the "initial condition"

[4] Due to the infinite-range coupling between the spins, the effective dimension of the problem is ∞ and so the mean-field theory is exact.

[5] We use the convention $q_i < q_{i-1}$ and $m_i < m_{i-1}$.

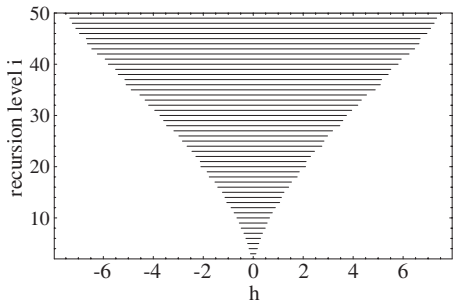

FIG. 2. Nontrivial domain of $\exp \mathcal{C}_i(h)$ for all levels i of the recursion sequence of a typical order-50 RSB calculation at $T=0$ and $H=0$ represented by the bars in the h direction. The nontrivial domain is defined as the interval where $\exp \mathcal{C}_i(h)$ is different from zero, i.e., $\exp \mathcal{C}_i(h) > 10^{-19}$.

$$\exp \mathcal{C}_0(h) = T \ln\left[1 + \exp\left(-\frac{2|h|}{T}\right)\right] \tag{10}$$

has a smooth transition from finite temperatures to $T=0$, i.e., $\lim_{T\to 0}\exp \mathcal{C}_0(h)=0$. Furthermore, all functions $\exp \mathcal{C}_i(h)$ obey an $h \to -h$ symmetry, irrespective of temperature T or external field H, and are continuous at $h=0$, though there is a kink at $h=0$ with $\partial_h \exp \mathcal{C}_i(h)|_{h=0^+}=-1$, $\forall\ i$. Therefore, it is sufficient to restrict ourselves to $h>0$ and introduce a boundary condition at $h=0$.

At finite κ, there are simple relations between successive auxiliary functions $\exp \mathcal{C}_i(h)$ and $\exp \mathcal{C}_{i-1}(h)$,

$$\exp \mathcal{C}_i(h) = \frac{1}{a_i}\ln\left\{\int_i^G \exp\left[a_i\left(|h'| - |h| + \exp \mathcal{C}_{i-1}(h') - \frac{1}{2}a_i\Delta q_i\right)\right]\right\}. \tag{11}$$

The integral levels are thus interpreted as levels of a recursive sequence of functions $\exp \mathcal{C}_i(h)$ that is defined by an initial condition (10) and a recursion relation (11) which depends on the order parameters. This recursive formulation is one of the central points of our finite-order RSB technique. It allows a systematic calculation of free energy derivatives with respect to the parameters q_i and a_i. These derivatives are again defined recursively and can be computed with high accuracy, as is required for high RSB orders.

The nontrivial part of the free energy can be expressed in terms of an integral of $\exp \mathcal{C}_\kappa$,

$$\tilde{f} = \int_{\kappa+1}^G [\exp \mathcal{C}_\kappa(h) + |h|] + \frac{1}{2}\sum_{k=1}^{\kappa} a_k \Delta q_k, \tag{12}$$

so that the free energy per spin can be written as

$$f = -\frac{T}{4}\chi_{\mathrm{ne}}^2 + \frac{1}{4}\sum_{i=1}^{\kappa} a_i[(q_i-1)^2 - (q_{i+1}-1)^2] - \int_{\kappa+1}^G [\exp \mathcal{C}_\kappa(h) + |h|] \tag{13}$$

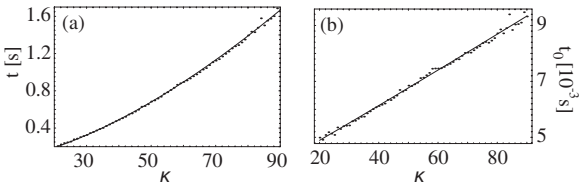

FIG. 3. Calculation times at $T=0$ in dependence on κ. (a) shows the calculation time $t \sim \kappa^{1.6}$ of the free energy with all derivatives and (b) the calculation time $t_0 \sim \kappa^{1.1}$ of a single derivative.

with the nonequilibrium susceptibility $\chi_{\mathrm{ne}}=\beta(1-q_1)$. For the continuous RSB limit, one can fix the domain boundaries of $q(a,T)$ by defining $a_{\kappa+1}\equiv 0$ and $a_0 \equiv \beta$. As a result, the first line of (13) becomes proportional to an integral $\int_0^\beta da[1-q(a)]^2$.

At finite κ, the free energy must be maximized with respect to $\{a_i, q_i\}$. This is done for $T=0$ (finite T) by a root search of the gradient of f in the 2κ-$((2\kappa+1)$-)dimensional parameter space.[6]

There are two main advantages of performing numerics in terms of $\exp \mathcal{C}$. The first is that the nontrivial domain of this function (i.e., where it is nonzero, see Fig. 2) is strongly restricted to the region of small h and so the numerical effort is reduced considerably. This is illustrated by Fig. 3 where the κ dependence of typical calculation times is shown. A single calculation involves the computation of the free energy and all its derivatives. Since the number of derivatives grows as $2\kappa+1$, the full calculation time grows more rapidly than linear. The calculation time normalized to the number of derivatives to calculate, however, grows nearly linearly with κ and therefore high orders of RSB may be obtained. The second advantage is that $\exp \mathcal{C}(h) \sim O(1)$ and no loss of numerical precision happens due to large numbers.

Figure 4 shows the functions $\exp \mathcal{C}_i$ at some recursion levels i. The initial condition is represented by the lowest curve, which is exactly zero for $T=0$ and remains finite for finite temperature, corresponding to the nonzero initial condition given in Eq. (10).

IV. RESULTS

In this section, we discuss some results of our extensive numerical computations according to the scheme described

[6]At zero temperature, $q_1=1$, because q_1 is the Edwards-Anderson order parameter.

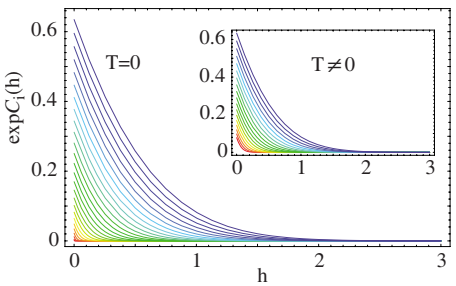

FIG. 4. (Color online) $\exp \mathcal{C}_i(h)$ at even recursion levels i for $T=0$ and $\kappa=50$. The lower curves (red) correspond to small i and the upper lines (blue) to large i. The inset shows a similar calculation at $T=0.1$ with $\kappa=30$.

in Sec. III. We have been able to perform calculations at extremely high orders of RSB (up to 200 at $T=0$ and up to 53 at finite temperatures) with unprecedented accuracy, allowing a deep insight into the subtleties that arise as κ approaches its physical limit $\kappa=\infty$.

In a previous publication we used order-42 RSB data to extrapolate the zero-temperature free energy to $\kappa=\infty$ by fitting f_κ to the function $f_\kappa=f_{\kappa=\infty}+\frac{\text{const}}{(\kappa+\kappa_0)^\alpha}$.[7] The extrapolation is now confirmed and extended in accuracy according to order-200 RSB high-precision numerics with the exp $\mathcal{C}$ formalism to $f_{\kappa=\infty}=-0.763\,166\,726\,566\,547$, $\alpha=4$. It is difficult to estimate the error of the extrapolated free energy. The fluctuations of the free energy of the finite-κ calculations are on an arbitrary small scale, due to the utilization of arbitrary-precision arithmetic. Thus, the accuracy of f_∞ depends only on the fit procedure. To give the reader an idea of the convergence level at order-200 RSB, let us state that $f_{200}-f_\infty\simeq 10^{-11}$. With standard fit methods, an accuracy of 10^{-13} is obtained, which represents the minimum accuracy of f_∞. With some technical tricks that are beyond the scope of this paper, however, it seems that the accuracy might be up to 10^{-15}. In any case, this is by far the most precise ground state energy ever obtained for the SK model and it provides a good test for all coming formalisms which work directly at $\kappa=\infty$ and $T=0$. In comparison with the literature, we find that the value is consistent with the estimate of Parisi [14] and also[8] with a more recent estimate [7].

At zero temperature the free energy f equals the internal energy u. At finite temperatures, they are still closely related by their Taylor expansions at $T=0$. We have checked numerically that the free energy can indeed be expanded in a Taylor series with regular exponents at $T=0$,

$$f(T)=f_0-s_0T+f_2T^2+f_3T^3+O(T^4), \tag{14}$$

where $s_0=-\chi_{\text{ne}}^2/4$ is the zero-temperature entropy, which can also be expressed in terms of the nonequilibrium or single-valley susceptibility χ_{ne}. The internal energy can be expressed by the same coefficients

$$u(T)=f-T\frac{df}{dT}=f_0-f_2T^2-2f_3T^3+O(T^4),$$

and also the temperature dependence of the entropy can be written as $s(T)=s_0-2f_2T-3f_3T^2+O(T^4)$. From our results we find $f_2\to 0$ and $f_3\to -0.24$, in agreement with the literature [7,10].

The zero-temperature entropy is directly related to the nonequilibrium susceptibility which can be written at finite-order RSB as[9]

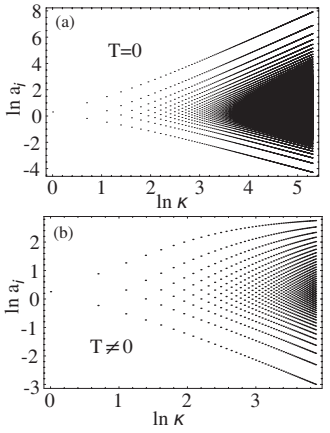

FIG. 5. ln a_i as a function of ln κ for $\kappa=1,\ldots,200$ at $T=0$ (a) and for $\kappa=1,\ldots,50$ for $T=0.03$ (b).

$$\chi_{\text{ne}}=-\frac{1}{2}\sum_{i=1}^{\kappa}a_i(q_i^2-q_{i+1}^2)-f. \tag{15}$$

We find that $\chi_{\text{ne}}\propto(\kappa+\kappa_0)^{-\gamma}$ with $\gamma=1.666\,664\pm 5\times 10^{-6}$. For an exponent, this numerical accuracy is sufficient to claim $\gamma=5/3$. As a result, both, the nonequilibrium susceptibility and the entropy vanish with irregular exponents 5/3 and 10/3, respectively, for $\kappa\to\infty$ at zero temperature. The implications of those irregular exponents will be discussed elsewhere [15].

As we have explained above, the natural formulation of the order function at low temperatures is the formulation in terms of a function $q(a,T)$ since it resolves the structure at the singular point $x=0$ of the original Parisi order function $\tilde{q}(x,T)$ at $T=0$. In order to better understand the critical properties of the zero-temperature order function, it is useful to discuss the finite-order RSB step approximation to $q(a,T)$. In Fig. 5 the logarithm of the parameters a_i are plotted as a function of ln κ. One can clearly see that for large a_i the spacing between successive a points does not vanish, while for moderate a_i, a continuum emerges. Also, at small a_i, a spacing appears on a ln a scale. This small ln a spacing, however, does not imply a discreteness on the a scale, on which the differential equations of a continuous theory are defined. At finite temperatures, the discreteness at large a disappears due to the restriction of a_i to the interval $[0,\beta]$, while the small-a discreteness remains. A finite external field would also destroy the small-a discreteness. The notion of nonzero plateau widths on a logarithmic scale is directly related to the discrete spectra of the r_i levels, which will be discussed more thoroughly elsewhere [15]. At this point, we want to stress the nonvanishing spacing between successive a_i parameters for small i.

At $T>0$, the identification of a break point $\bar{x}$ is important. One finds that

$$\bar{x}=\lim_{\kappa\to\infty}Ta_1. \tag{16}$$

From our computations at finite temperatures, we can extract a confident value for $\bar{x}$ at temperatures down to $T=0.015$. Below this temperature, calculations at $\kappa>50$ are needed.

[7] $\kappa_0\simeq 1.27$ is an offset which is used to improve the fit quality.

[8] The little deviation is due to a misprint in Ref. [7], as brought to our attention by one of the authors.

[9] Alternatively, it is also obtained by varying the free energy with respect to q_1. This has been checked and yields the same result.

We find $\bar{x}(T=0.015)=0.546\,83\pm10^{-5}$. An extrapolation of the finite-T break point to zero temperature yields $\bar{x}(T=0)=0.546\,86\pm5\times10^{-5}$, consistent with the literature values [7,10] but with accuracy extended by two orders of magnitude. At zero temperature, $\bar{x}$ is ill defined because $\tilde{q}(x,0)=1,\ \forall\ x>0$. As a consequence, one does not find $\bar{x}$ directly in the $T=0$ theory. In fact, there is a subtle noncommutativity of the $T\to0$ and $\kappa\to\infty$ limits for quantities like the break point [15].

At finite κ and $T=0$, all m_i are zero. From scaling arguments, however, one can see that there are finite m_i even at $T=0$ in the $\kappa=\infty$ limit. These are exactly the $m_i=Ta_i$ corresponding to the discrete a points (see Fig. 5) and so the finite m_i are also discrete.[10] In the continuous formulation of the infinite-order RSB limit, an initial condition of the partial differential equation is given at m_1.[11] There is, however, a region of discrete m_i where a continuous theory is invalid, so at $T=0$ the initial condition of the continuous theory is disconnected from the validity domain of the differential equation. This is why the traditional theory fails for $T=0$.

Two other important and closely related parameters are the T^2 coefficient of the T expansion of the Edwards-Anderson order parameter $q_{\mathrm{EA}}(T)=1-\alpha T^2+O(T^3)$ and the a^{-2} coefficient of the $1/a$ expansion of $q(a,0)=1-\gamma a^{-2}+O(a^{-3})$. At finite orders of RSB, there is also a linear term in the T expansion of q_{EA} with the coefficient equal to χ_{ne}, but this coefficient vanishes for $\kappa\to\infty$. From our numerical data, we can extract for the quadratic temperature coefficient of the Edwards-Anderson order parameter $\alpha=1.594\,10\pm0.000\,01$, exceeding the precision given in [10] by two orders of magnitude. The coefficient of the leading term in the $1/a$ expansion of $q(a)$ is estimated as $\gamma=0.4108\pm0.0001$, consistent with the high-precision calculation in [10].

In the following paragraph, we analyze our results from the viewpoint of PAT scaling [16]. In the original formulation, PAT scaling has been used to evaluate an (approximately) universal scaling function $\tilde{q}(x,T)\simeq f(x/T)$ for $x<\bar{x}$. It is known that this scaling does not hold exactly. If it held exactly, then $f(x/T)=q(x/T,0)$ at all temperatures and knowledge of the zero-temperature order function was sufficient to obtain the solution at all temperatures. In Fig. 6 we compare $q(a,0)$ to the result of the PAT hypothesis, which was obtained according to the description in [16].

In order to discuss the correction to PAT scaling near $T=0$, we rewrite the true order function $q(a,T)$ as

$$q(a,T)=\begin{cases}q(a,0)+\tilde{q}(a,T) & \text{for } a<\bar{a},\\ q(\bar{a},0)+\tilde{q}(\bar{a},T) & \text{for } a\geq\bar{a},\end{cases}\tag{17}$$

with $\bar{a}=\beta\bar{x}$, and $\tilde{q}(a,T)$ is the correction to PAT scaling near $T=0$. From the identity $1=\int_0^\beta da[1-q(a,T)]$ one can derive

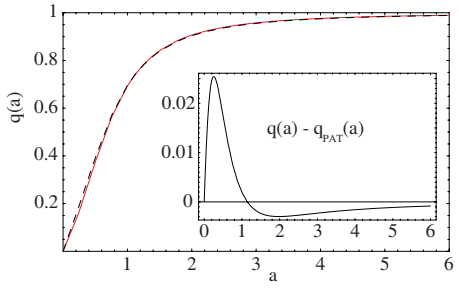

FIG. 6. (Color online) Comparison of the universal scaling function obtained by the PAT hypothesis (red, solid) and the zero-temperature order-200 RSB order function $q(a,0)$ (black, dashed). The inset shows the difference of the two curves.

the correction to the PAT-scaling break point at zero temperature,

$$\bar{x}(T=0)=\frac{1}{2}-\frac{1}{2\alpha}\lim_{T\to0}\int_0^{\bar{a}}da\frac{d}{dT}\tilde{q}(a,T)\tag{18}$$

with α the quadratic temperature coefficient of the Edwards-Anderson (EA) order parameter $q_{\mathrm{EA}}(T)\simeq1-\alpha T^2$. If we assume that $\tilde{q}(a,T)$ can be expanded in a Taylor series near $(a,T)=(\infty,0)$, i.e.,

$$\tilde{q}(a,T)=\sum_i T^i\tilde{q}_i(a)\quad\text{for } T\ll1\tag{19}$$

and

$$\tilde{q}_i(a)=\sum_j b_i^j a^{-j}\quad\text{for } a\gg1,\tag{20}$$

one can derive relations between the lowest coefficients of the $\tilde{q}(a,T)$ expansion, the quadratic temperature coefficient α of the EA order parameter, the break point, and the a^{-2} coefficient γ of the expansion of $q(a,0)$ at $a=\infty$:

$$b_1^0=b_1^1=0,\tag{21}$$

$$\alpha=\frac{\gamma}{\bar{x}^2}-b_2^0,\tag{22}$$

$$\int_0^\infty da\ \tilde{q}_1(a)=\frac{\gamma}{\bar{x}^2}(1-2\bar{x})-b_2^0.\tag{23}$$

The first relation states that $\tilde{q}_1(a)$ must approach zero faster than a^{-1} as $a\to\infty$. The parameters $\gamma,\alpha,\bar{x}$ are very well known from the literature and have been obtained from our numerical data, too. From the above relation, one can thus extract $b_2^0=-0.220\,35\pm0.000\,12$ and write the correction to PAT scaling near $(a,T)=(\infty,0)$ as

$$q(a,T)=q(a,0)-0.22T^2+O(T,a^{-1})^3.\tag{24}$$

Relation (23) can be used as a test for $\tilde{q}_1(a)$ extracted from numerics.

V. ∞-ORDER RSB LIMIT

As $\kappa\to\infty$, the number of parameters (q_i,a_i) goes to infinity as well and a smooth order function $q(a,T)$ defined on the

[10] This can also be seen from the discrete spectra, because of the definition of $r_{i-1}=a_i/a_{i-1}=m_i/m_{i-1}$.

[11] Sometimes in the literature one finds the initial condition at $x=1$, which is equivalent due to the triviality of the differential equations beyond the break point.

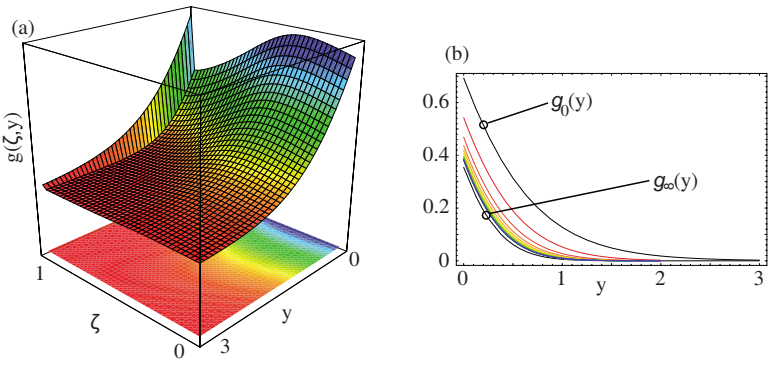

FIG. 7. (Color online) (a) Function $g(\zeta,y)$ with $\zeta=a/(1+a)$ at $T=0$ from an order-200 RSB calculation. (b) Initial condition $g_0(y)$ (top black line) at $x=1$, $a=\infty$ and the first ten integrations (red to blue). The bottom black line shows the initial condition $g_\infty(y)$ at $x=0$, $a=\infty$.

interval $[0,\beta]$ results for $T>0$. In this limit, the set of functions $\exp \mathcal{C}_i$ merges to one continuous function of two variables a and h defined as

$$\exp \mathcal{C}(a_i,h) = \lim_{\kappa\to\infty} \exp \mathcal{C}_i(h) \tag{25}$$

and the free energy for $H=0$ can be written as

$$f = -\frac{1}{4}\int_0^\beta da[q(a)-1]^2 - \exp \mathcal{C}(a=0,h=0). \tag{26}$$

$\exp \mathcal{C}(a,h)$ is the solution of the partial differential equation

$$\partial_a \exp \mathcal{C} = -\frac{\dot{q}(a)}{2}[\partial_h^2 \exp \mathcal{C} + 2a\partial_h \exp \mathcal{C} + a(\partial_h \exp \mathcal{C})^2] \tag{27}$$

with boundary and initial conditions

$$\partial_h \exp \mathcal{C}(a,h)|_{h=0^+} = -1, \quad \exp \mathcal{C}(a,\infty) = 0,$$

$$\exp \mathcal{C}(\beta,h) = T \ln[1+\exp(-2\beta h)] \tag{28}$$

for $h \geq 0$.

At finite temperatures, where the spacings between successive a_i and q_i approach zero as $\kappa\to\infty$, $\exp \mathcal{C}$ is well behaved, and the differential equation can be solved numerically. In this case Eqs. (27) and (28) are merely a reformulation of the Parisi theory [1,4], convenient at low temperatures. At exactly zero temperature, however, two problems arise which force us again to reformulate. First the discreteness in the large-a regime of $q(a)$ formally invalidates the differential equation at $a=\infty$, where the initial condition is given. Further, the second derivative of the initial condition has a divergence at $h=0$ as $T\to 0$.

The second issue can be resolved by a further rescaling $y=(a+1)h$ and introduction of the function $g(a,y)=(a+1)\exp \mathcal{C}[a,y/(a+1)]$. The initial condition at β for $\exp \mathcal{C}$ translates to $g(\beta,y)=\ln(1+e^{-2y})=g_0(y)$. Figure 7(a) shows the a and y dependence of $g(a,y)$ [for visualization purposes, the a axis has been mapped to the interval [0,1] by the introduction of the variable $\zeta=a/(1+a)$]. Obviously, for finite a (i.e., $\zeta<1$), $g(a,y)$ varies smoothly as a function of a and the description in terms of a partial differential equation is valid. In the large-a limit, however, a singularity appears. To understand the origin of this singularity and the method to handle it, we go back again to the finite-order RSB formulation. The investigation of the order-200 RSB calculations shows that at large a the difference between $g(a_i,y)$ and $g(a_{i+1},y)$ does not vanish with $\kappa\to\infty$ as it does for moderate $a \ll a_1$ [see Fig. 7(b)].[12] This means that the recursion relation (11) does not pass over to a differential equation at $a=\infty$. Instead, one can see that the recursion drives the function to a limiting function $g_\infty(y)$ from which the continuous part of $g(a,y)$ starts. In Fig. 7(b) the first ten functions $g_i(y)$ obtained by the recursion relation within a $\kappa=200$ calculation are shown together with $g_0(y)$ and the limiting function of the recursion $g_\infty(y)$. This limiting function has been obtained by numerically solving an ordinary differential equation, as explained below.

It is important at $T=0$ to distinguish different $a=\infty$ "points" by considering the corresponding position on an $x=aT$ scale. The initial condition of the function $g(a,y)$, for instance, is given at $a=\infty$ and $x=\bar{x}$—this is the function $g_0(y)$. The limiting function of the recursion sequence $g_\infty(y)$ is also given at $a=\infty$, but on an x scale the position is $x=0$. Thus, the recursion in Fig. 7(b) approaches the point $a=\infty$, $x=0$ from above.

To complete our discussion, we now approach the point $a=\infty$, $x=0$ from below. In the finite-a regime, the behavior of $g(a,y)$ is governed by a partial differential equation, instead of a recursion relation (the overdot refers to a derivative with respect to a, while the prime means a y differentiation):

$$\dot{g} = -\frac{\dot{q}}{2}(a+1)[(a+1)g'' + 2ag' + a(g')^2] + \frac{g-yg'}{a+1}. \tag{29}$$

In order to investigate this equation at zero temperature in the limit $a\to\infty$, where the initial condition is given, we expand the order function $q(a,0)=1-\gamma a^{-2}$ and Eq. (29) itself near $a=\infty$. To first order in a^{-1}, we find $\dot{g}=\frac{1}{a}F[g]$ with

$$F[g] = g - yg' - \gamma[g'' + 2g' + (g')^2]. \tag{30}$$

Obviously, an initial condition $g(\infty,y)$ of (29) with $F[g(\infty,y)]\neq 0$ would lead to a logarithmic singularity of $g(a,y)$ at $a=\infty$. The only nonsingular initial condition is therefore the solution to the ordinary differential equation $F[\tilde{g}(y)]=0$. Indeed, the solution $\tilde{g}(y)$ of this differential equation seems to be the limiting function $g_\infty(y)$ of the recursion at $a=\infty$ starting from $g_0(y)$, as discussed above. In

[12] a_1 is the largest a parameter in the finite RSB formulation.

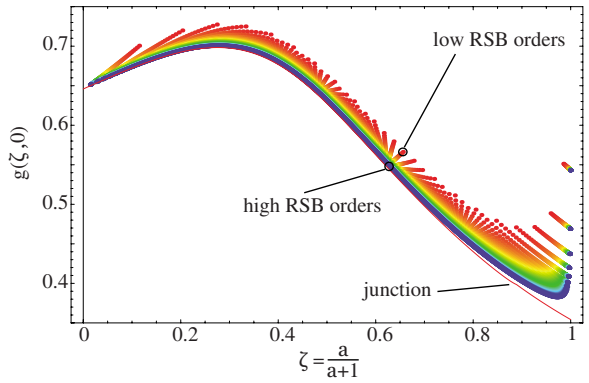

FIG. 8. (Color online) $g(\zeta,0)$ with $\zeta=a/(1+a)$ for up to 200 orders of RSB. The dots with the different colors refer to low (red) and high (blue) RSB orders. The solid line (red) is obtained by the ∞-order RSB formalism proposed in the text.

Fig. 7(b), the function $g_\infty(y)$ is the numerical solution of $F[g_\infty]=0$. In some sense, the partial differential equation governing the function $g(a,y)$ yields its own initial condition—it is the only initial condition that makes sense.

To further illustrate and confirm this line of reasoning and to better understand the transition $\kappa\to\infty$, we shall restrict our discussion of $g(a,y)$ to $y=0$ as representative for the a dependence of g. In Fig. 8 we plot $g(a_i,0)$ at $T=0$ for $\kappa<\infty$ varying from 10 to 200. Again, one can see the discreteness at $a=\infty$. For demonstration purposes, a calculation of $g(\zeta,y)$ directly at order-∞ RSB is plotted in Fig. 8. It has been calculated from Eq. (29). To obtain this solution at large a, Eq. (29) has been expanded up to order a^{-2} at $a=\infty$. The solution of this expansion around $a=\infty$ taken at $a=8$ ($\zeta\simeq 0.89$) was then used as an initial condition for the full partial differential equation (29) at $a=8$. By thoroughly looking at the line, one can see a small error near this junction point. With more effort, such as higher-order expansions at $a=\infty$ or advanced numerical methods for partial differential equations (e.g., pseudospectral methods [7]), the quality of the full continuous RSB solution at zero temperature can be greatly improved, but this is beyond the scope of this work.

VI. CONCLUSION

We have developed an RSB technique which allows calculations at extremely high orders of Parisi RSB near and at $T=0$. With the help of this technique, numerical calculations have been performed for up to 200 orders of RSB at $T=0$ and for up to 53 orders of RSB for finite temperatures. Several quantities have been extracted from these numerical calculations. In particular, their dependence on the order of RSB has been investigated. Further, we obtained, to our best knowledge, the most precise numerical value for the ground state energy of the SK model. The connection to PAT scaling has been analyzed and the first correction to the PAT-scaling assumption $q(x,T)=f(x/T)$ near zero temperature and $a=x/T=\infty$ has been discussed.

Furthermore, we have proposed an ansatz for a full treatment of the zero-temperature limit of Parisi RSB in the SK model directly at infinite order of RSB—in analogy to the continuous RSB formalism at finite temperatures [4]. It has been shown that the original initial condition of the partial differential equation [4]. must be replaced by a function which is defined as the solution of an ordinary differential equation.

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