Free-energy surface of spin-glasses: Thouless-Anderson-Palmer and Bethe-Peierls-Weiss models

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Previous numerical studies of the Thouless, Anderson, and Palmer (TAP) infinite-range Ising spin-glass equations have suggested that solutions were difficult to find and ill behaved in temperature. In order to test whether these results are a consequence of inadequate numerical schemes, we have devised and applied an improved approach. A search for minima of the TAP and (finite-range) Bethe-Peierls-Weiss (BPW) free-energy surfaces indicates that, in both cases, the well-behaved field-cooled minimum evolves with decreasing temperature T into a negative-entropy state. All other attempts to obtain minima led, at best, to piecewise continuous (in T) physical solutions. The inability to calculate well-behaved temperature-dependent magnetizations for the finite-size TAP and BPW theories appears to be a serious drawback for these approaches.

I. INTRODUCTION

The Thouless-Anderson-Palmer[1,2] (TAP) solution of the infinite-range Ising spin-glass model is more physical than alternative replica symmetry-breaking[3] approaches. However, it requires a considerable amount of numerical analysis in order to obtain physical results over a range of temperatures. Previous studies,[4–6] with the use of simple iterative techniques, have suggested that minima of the TAP free energy were difficult to find and, at best, only piecewise continuous[5] with changing temperature T. It is very possible that these results are a consequence of inadequate numerical schemes. Therefore, we have devised an improved approach to search for solutions of the TAP equations.

It is the purpose of this paper to apply this scheme in a more complete search than has previously been attempted for physical minima of the free-energy functional $F[\{m_i\}]$. Here m_i is the thermally averaged spin at the ith site. We use both the TAP and finite-range Bethe-Peierls-Weiss (BPW)[7] Ising models for F. TAP have argued, on the basis of a convergence criterion,[1,8] that all physical states on the free-energy surface must be higher-order stationary points; these are not easily found by numerical techniques. However, it is not likely that this is always the case for finite-size systems. Furthermore, the utility of the TAP approach depends on finding numerical solutions of their equations for finite N. It should be noted that our numerical scheme, which we will discuss in more detail below, is applicable over the entire free-energy surface, especially including the region where the TAP convergence criterion is satisfied.

It is widely thought[4,9–12] that the free-energy surface of a spin-glass contains a vast amount of information about the macroscopic properties of these systems. Recently, attention has focused on the nature of the energy barriers[13–15] in the infinite-range Ising model. Bray and Moore[4,11] have numerically searched for quadratic minima and analytically counted the stationary points of the TAP free-energy functional. A surprising result of their numerical calculations was that they were *unable* to find any solutions to the TAP equations (at a fixed T) for 90% of their bond configurations. While they did not attempt to follow a given solution with T, Nakanishi[5] and other investigators[6] (using iterative techniques) observed that the solutions quickly disappeared upon changing temperature. Furthermore there appeared to be no nearby minimum to which the system flowed. While Nakanishi attributed his results to errors associated with applying the TAP scheme to finite N, it appears likely that such unphysical behavior might, at least in part, be a consequence of inadequacies in the numerical schemes used. It can be shown (as will be discussed below) that simple iterative techniques generate only a subset of all minima. Frequently minima are "lost" with changing T due to numerical problems which are artifacts of the iteration scheme, and are not related to the disappearance of a solution.

The ultimate test of the TAP theory and other theories of spin-glasses is whether they lead to reasonable results for physically measurable properties. Ideally, we would wish to compute the various history-dependent magnetizations[9] obtained with field-cooled (FC) or zero-field-cooled (ZFC), or magnetic hysteresis procedures. Results derived from Monte Carlo simulations[16] and, more recently, from the use of simple mean-field theory[12] (in which the reaction term in $F[\{m_i\}]$ is dropped) lead to good qualitative agreement with experiment. It is important to ascertain whether the TAP theory yields equally physical results. Furthermore, it is clearly of interest to study the finite range or BPW analog of the TAP equations. Unphysical results that might be found in the infinite-range model may well be attributed to "pathologies" associated with this special case. It is generally believed[17] that the FC minimum of $F[\{m_i\}]$ is the thermodynamic equilibrium state. The lack of irreversibility[9] of the state suggests that it evolves continuously from the (single) high-temperature paramagnetic minimum. For this reason, we made a systematic study of this FC state.

As noted above, an exhaustive search for the minima of a free-energy functional of N variables requires a more powerful method than the iterative techniques which have previously been applied. The obvious choice, Newton's method, is unsuitable for the analysis of large systems, because of the inordinate amount of matrix algebra involved.

Therefore, we have devised a technique that combines an iterative search with an acceptable amount of matrix algebra. This method is guaranteed to converge to all quadratic minima, provided one makes a reasonable first guess for the solution. This scheme will not converge to higher-order stationary points. (Unless otherwise indicated, the word minimum will henceforth refer only to a quadratic minimum.) While we use more powerful methods than the simple iterative techniques used previously, we are, as a result, restricted to the treatment of somewhat smaller systems.

The results we obtain are rather discouraging. We discuss them here for the TAP case but they apply also to the finite-range model as well. The well-behaved high-temperature FC state is found to evolve continuously (with decreasing T) into a state of negative entropy S. The calculated FC magnetization has a maximum at roughly the temperature at which S becomes negative. Solutions of the TAP equations can be readily generated at $T=0$, since these are equivalent to solutions of simple mean-field theory. However, we have been unable to heat these minima up beyond very low temperatures; at some point they may become higher-order stationary points which cannot be studied numerically. Alternatively, they may disappear altogether. Random searches, along the lines pursued by Bray and Moore,[4] did not reveal many minima. In general, the system found its way back to the unphysical FC state. After the main body of this work was completed, it was pointed out[18] that Monte Carlo simulations occasionally generated TAP solutions. However, upon closer examination, we found that these also had unphysical properties. The picture of the TAP free-energy surface that emerges is that if there are physical minima of F, they are mostly, if not all, higher-order stationary points. So far, no physical numerical solution has been found which can be followed over the entire range of temperatures. While these results are not inconsistent with the TAP convergence criterion (derived in the thermodynamic limit), it is nevertheless unexpected that for finite-size systems, the only physical states are higher-order minima. Since the TAP equations require numerical solutions (except at special temperatures) it now appears unlikely that one can extract many physical results from this theory.

II. CONVERGENCE AND STABILITY OF ITERATIONS

Both the TAP equations and the BPW equations [derived from $(\partial F/\partial m_i)=0$] constitute a set of coupled, nonlinear, algebraic equations for which no closed-form solution exists. In the simplest iterative method of solution, an initial set of spin variables, $\{m_i\}$, is used to calculate a set of effective local fields, $\{h_i\}$, from which a new set of spin variables, $\{m_i'\}$, are generated[1,7]:

$$h_i^{\mathrm{TAP}}=\left[H+\sum_j J_{ij}m_j\right]_{\mathrm{MF}}-\beta m_i\sum_j J_{ij}^2(1-m_j^2)\ , \tag{2.1}$$

$$h_i^{\mathrm{BPW}}=\left[H+\sum_j J_{ij}m_j\right]_{\mathrm{MF}}+\sum_j\left[\beta^{-1}\tanh^{-1}\left(\frac{1-g_{ij}^2-r_{ij}}{2(m_i-g_{ij}m_j)}\right)-J_{ij}m_j\right], \tag{2.2}$$

$$g_{ij}\equiv\tanh(\beta J_{ij})\ , \tag{2.3a}$$

$$r_{ij}\equiv[(1-g_{ij}^2)^2-4g_{ij}(m_i-g_{ij}m_j)(m_j-g_{ij}m_i)]^{1/2}\ , \tag{2.3b}$$

$$m_i'=\tanh(\beta h_i)\ . \tag{2.4}$$

Here, H is the applied magnetic field and J_{ij} is the exchange interaction between spins on the ith and jth sites. The exchange interactions are distributed according to the probability distribution,

$$P(J_{ij})=\left[\frac{Z}{2\pi\tilde{J}^2}\right]^{1/2}\exp\left[-\frac{ZJ_{ij}^2}{2\tilde{J}^2}\right], \tag{2.5}$$

where Z is the number of interacting neighbors, and $\tilde{J}$ is a typical exchange interaction. In the TAP case, $Z=N$, and the sum over sites in Eq. (2.1) includes all sites. In the BPW case, the sum over sites in Eq. (2.2) includes only the Z nearest neighbors of the ith site. Equation (2.4) is iterated many times, until convergence is obtained and $m_i=\tanh(\beta h_i)$ is satisfied to the desired degree of accuracy. The terms in $(\ )_{\mathrm{MF}}$ in Eqs. (2.1) and (2.2) correspond to naive mean-field theory, while the remainder is called the "reaction field". The effective local field can be expressed generally as

$$h_i=-\frac{\partial F}{\partial m_i}+\frac{1}{\beta}\tanh^{-1}(m_i)\ , \tag{2.6a}$$

which allows [from Eq. (2.4)] the iteration scheme to be written directly in terms of the free energy

$$\tanh^{-1}(m_i')-\tanh^{-1}(m_i)=-\beta\frac{\partial F}{\partial m_i}[\{m_i\}]\ . \tag{2.6b}$$

A set of spin variables $\{m_i^*\}$ is a fixed point of this iteration scheme if, and only if, it is also a stationary point of the free energy.

Because the iteration scheme in Eq. (2.6b) is expressed in terms of F, the conditions for the stability of the fixed points (stationary points) under iteration can also be phrased in terms of the free energy. We will show below that in order for the iteration scheme in Eq. (2.6b) to converge to a fixed point, the fixed point must be a quadratic minimum of the free energy, as opposed to a quadratic maximum or saddle point, or a higher-order stationary point. Furthermore, the straightforward iteration scheme will *not* converge to *all* minima, only to a restricted subset. This makes it likely that solutions to the TAP equations have been missed or lost in previous numerical studies, and provides the motivation for formulating a more elaborate scheme.

In the remainder of this section, an improved iteration scheme is introduced, and its convergence and stability properties analyzed. We phrase the problem in rather general terms, and begin with a free-energy functional whose minima we seek. Consider an iterative scheme of the form

$$m_i'=g\left[-\alpha\frac{\partial F[\{m_i\}]}{\partial m_i}+g^{-1}(m_i)\right], \tag{2.7}$$

where $g(x)$ is a one-to-one monotonically increasing function of its argument, and α is a constant. The straightforward iteration scheme discussed above corresponds to

$g(x)=\tanh(\beta x)$ and $\alpha=1$. More generally, the parameter α controls how much of the previous iteration is retained, and will be chosen so as to expedite convergence. Equation (2.7) may be rewritten as

$$g^{-1}(m_i')-g^{-1}(m_i)=-\alpha\frac{\partial F}{\partial m_i}[\{m_i\}]\ , \tag{2.8}$$

which shows that a fixed point of the iteration scheme is a stationary point of the free energy, and vice versa.

We may relate the stability of this iterative scheme to the properties of the curvature matrix $(\partial^2 F/\partial m_i\,\partial m_j)$. Consider an initial spin configuration $m_i=m_i^*+\delta m_i$ infinitesimally close to the fixed point $\{m_i^*\}$, so that after one iteration,

$$m_i'=m_i^*+\delta m_i'\ . \tag{2.9}$$

It follows from Eq. (2.7) that

$$\frac{\delta m_i'}{d_i^*}=\sum_j[Q(\{m^*\})]_{ij}\frac{\delta m_j}{d_j^*}\ , \tag{2.10}$$

where $d_i^*\equiv[g'(g^{-1}(m_i^*))]^{1/2}$ and $Q(\{m^*\})$ is a real symmetric matrix whose matrix elements are

$$[Q(\{m^*\})]_{ij}=\delta_{ij}-\alpha d_i^*\frac{\partial^2 F[\{m^*\}]}{\partial m_i\partial m_j}d_j^*\ . \tag{2.11}$$

In order for repeated iteration of Eq. (2.10) to converge to the fixed point, the eigenvalues of $\underline{Q}$ (which are real) must all be less than one in magnitude ($Q_{\max}<1$ and $Q_{\min}>-1$). In terms of the positive-definite diagonal matrix, $D_{ij}\equiv\delta_{ij}d_i^*$, and the Hessian or curvature matrix for the free energy,

$$A_{ij}\equiv\frac{\partial^2 F[\{m^*\}]}{\partial m_i\partial m_j}\ ,$$

we may write $\underline{Q}=1-\alpha\underline{D}\,\underline{A}\,\underline{D}$. The condition that the maximum eigenvalue of $\underline{Q}$ be less than 1 implies

$$\alpha(\underline{D}\,\underline{A}\,\underline{D})_{\min}>0\ , \tag{2.12}$$

where $(\underline{D}\,\underline{A}\,\underline{D})_{\min}$ denotes the minimum eigenvalue of the matrix $\underline{D}\,\underline{A}\,\underline{D}$. For $\alpha>0$, Eq. (2.12) will be satisfied if the Hessian is positive definite, i.e., the fixed point is a minimum of the free energy. (If α was taken to be negative, $Q_{\max}<1$ would be satisfied for maxima of the free energy.) It follows from this that the straightforward iteration scheme discussed earlier and applied elsewhere[4,5,12] ($\alpha=1$) can only converge to minima. This point was made by Bray and Moore[4] for the TAP case, and is more generally valid for any free-energy functional. The requirement that the minimum eigenvalue of $\underline{Q}$ be greater than -1 implies

$$\alpha(\underline{D}\,\underline{A}\,\underline{D})_{\max}<2\ , \tag{2.13}$$

where $(\underline{D}\,\underline{A}\,\underline{D})_{\max}$ denotes the largest eigenvalue of the matrix $\underline{D}\,\underline{A}\,\underline{D}$. It is this criterion that the straightforward iteration scheme ($\alpha=1$) may fail to satisfy when the Hessian matrix becomes too large (corresponding to a minimum of the free energy that is too "deep").

For a given minimum of the free energy, the choice of α that leads to the most rapid convergence is the value for which $Q_{\max}=-Q_{\min}$,

$$\alpha_{\text{optimal}}=\frac{2}{(\underline{D}\,\underline{A}\,\underline{D})_{\max}+(\underline{D}\,\underline{A}\,\underline{D})_{\min}}\ . \tag{2.14}$$

Although α_{optimal} is not known until the fixed point is found, one can follow a solution by taking small steps in T and H, and beginning the search for the new solution with the value of α_{optimal} for the old solution. In Secs. III and IV this approach [with $g(x)=\tanh(\beta x)$ and α chosen as above] is applied to the TAP and BPW cases, respectively.

For the special case of naive mean-field theory solved by straightforward iteration[12] ($\alpha=1$), we make the following observations. It is not only true that when convergence occurs the extremum is a minimum, but also that failure of convergence is connected to the disappearance of the minimum. This follows from an empirical observation that the minimum and maximum eigenvalues of Q are equal and opposite to within 1%, so that Eqs. (2.12) and (2.13) are violated simultaneously. Therefore, when solving for the minima of the naive mean-field free energy, the straightforward iteration scheme is adequate.

While the discussion thus far relates only to Ising spins, we have also considered the vector spin case. In this case, we find that straightforward iteration will converge only to minima provided that the matrix $M_{\mu\nu}\equiv(\partial m_i^\mu)/(\partial h_i^\nu)$ (where μ,ν are Cartesian coordinate labels, and h_i is the Weiss field at site i) has eigenvalues whose magnitudes are less than 1.0. We have found that in "naive" mean-field theory this holds for any n-vector model, with or without anisotropy.[19]

III. NUMERICAL RESULTS FOR THE TAP MODEL

In this section we present the results of a numerical search for solutions to the infinite-range TAP equations. Two types of numerical calculations were performed. In the first, the TAP equations were solved for a small external magnetic field at a temperature considerably above the spin-glass transition temperature T_g. The solution at the highest T was obtained using the iteration scheme described in Sec. II, with the known high-temperature expansion providing an initial guess for the iteration procedure. This high-temperature solution was then followed as the temperature was lowered in small decrements to a value well below T_g. We refer to this as the field-cooled (FC) minimum. In the second type of calculation an initial spin configuration was generated at random, and used to start the iterative search for minima of F in a small magnetic field for temperatures below T_g. We refer to this as the random-search calculation. Both studies were performed for sample systems of 25, 30, 40, 50, 60, and 75 spins each. Convergence was assumed when $\sum_i(m_i'-m_i)^2/\sum_i m_i^2\le 10^{-10}$.

For all the sample systems considered,[20] the results of the FC calculations were qualitatively similar. The results for the FC state at $N=75$ are representative, and are shown in Fig. 1. In this figure, the magnetization $M\equiv N^{-1}\sum_i m_i$ and the Edwards-Anderson (EA) order parameter $q\equiv N^{-1}\sum_i m_i^2$ are plotted as functions of the reduced temperature T/T_g, for an external magnetic field $H=0.05T_g$. Both M and q have maxima near the transition temperature, indicating that the inverse susceptibility has a minimum in the vicinity of $T=T_g$. The inverse susceptibility does not vanish, however, and the high-

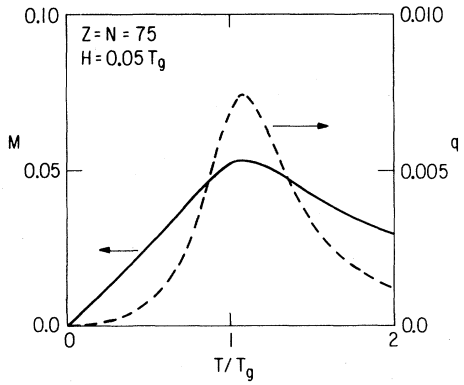

FIG. 1. The field-cooled (FC) TAP magnetization M (left axis, solid curve) and EA order parameter q (right axis, dashed curve) vs reduced temperature T/T_g for a number of spins $N=75$ in magnetic field $H=0.05T_g$.

temperature state remains stable down to zero temperature, where M and q vanish as T and T^2, respectively. This field-cooled state has negative entropy, and is therefore clearly unphysical, for $T<0.6T_g$; both the entropy and the free-energy approach minus infinity as the temperature goes to zero. This solution is the continuation to finite H of the trivial solution to the TAP equations in zero field: $\{m_i\}\equiv 0$, for all T. However, this state (which we call the nonmagnetic state) evolves continuously from the physical high-temperature state, and is not unstable at any intermediate temperature. This absence of instability at all T can occur only for finite systems, since the curvature or Hessian matrix is given by

$$A_{ij}=\delta_{ij}\left[1+\beta^2\sum_k J_{ik}^2\right]-\beta J_{ij}\ ,$$

and has, in the infinite-system limit, the minimum eigenvalue $(1-\beta\tilde{J})^2$, which vanishes quadratically at $T=T_g=\tilde{J}$. Presumably, in the thermodynamic limit, the high-temperature state will evolve continuously into a physical low-temperature state, yielding a well-behaved FC magnetization. For finite-size systems, this apparently occurs in naive mean-field theory,[12] but not in the TAP case. For finite N it is presumed that a new physical solution to the TAP equations is to be found near the nonmagnetic state, before it becomes unphysical, and that the system undergoes a discontinuous, or first-order, jump to this new state.

In an attempt to locate the expected nearby state, we undertook random-search calculations in which new spin configurations were generated at random with a uniform sampling of phase space. Once the new spin configuration was generated, the iteration scheme of Sec. II was applied with the iterations begun with $\alpha=\alpha_{\text{optimal}}$ for the nonmagnetic state. The value of α was updated to the local optimal value periodically throughout the iteration procedure. The iterations were continued until convergence was obtained; and then a new random starting configuration was generated and the procedure was repeated. Some twenty to thirty random initial configurations were considered at $T=0.1T_g$, $T=0.5T_g$, and $T=0.8T_g$, for each of the sample systems for which the field-cooled calculations were done. In every case, the iteration scheme eventually converged to the state obtained by cooling—no other solution to the TAP equations was ever found. Owing to the constraints of matrix algebra, the systems we considered were necessarily somewhat smaller than those considered by Bray and Moore,[4] who found an occasional solution (in 10% of their bond configurations.) The present approach, however, represents a considerably more thorough search for each bond configuration than has been done previously.

IV. NUMERICAL RESULTS FOR THE BPW MODEL

Calculations analogous to those described in the previous section were carried out for the Bethe-Peierls-Weiss free-energy functional,[7,21]

$$F_{\text{BPW}}[\{m_i\}]=\beta^{-1}\sum_i\left[\frac{1+m_i}{2}\ln\left[\frac{1+m_i}{2}\right]+\frac{1-m_i}{2}\ln\left[\frac{1-m_i}{2}\right]\right]-H\sum_i m_i$$
$$-\beta^{-1}\sum_{i,j}\left[m_i\tanh^{-1}\left[\frac{1-g_{ij}^2-r_{ij}}{2(m_j-g_{ij}m_j)}\right]+\tfrac{1}{4}\ln\left[\frac{r_{ij}+1+g_{ij}^2-2g_{ij}m_im_j}{2(1-g_{ij}^2)}\right]\right],\qquad(4.1)$$

where g_{ij} and r_{ij} are defined in Eqs. (2.3). In this section, we present the results of these calculations and compare them to the results for the TAP case. As in Sec. III, two types of studies were performed; field-cooled and random-search calculations. Because many more iterations were required to reach convergence than in the TAP case, the investigation of the BPW free-energy surface presented here is of a more limited nature than that presented in the preceding section. Five sample BPW spin glasses were studied: four different sample systems of two- dimensional (2D) spin-glasses (consisting of a 5×5 array of spins), and one 3D sample BPW spin-glass (consisting of a $5\times 5\times 5$ array of spins).

The results for the FC state are quite sensitive to the external field. Figure 2 shows the FC magnetization and EA order parameter as functions of the reduced temperature for a characteristic 2D BPW system at two different values of the external field: $H=0.04T_g$ and $0.08T_g$. These field-cooled solutions are fully reversible (as in the TAP case) for a fixed magnetic field. The lower-field results [Fig. 2(a)] are similar to those found for the TAP case: Both M and q have maxima in the vicinity of the glass temperature, and extrapolate to unphysically small values at low T. The lower-field state could be followed only down to $T=0.75T_g$ because of the large number of iterations (~ 8000) required for convergence; in this same

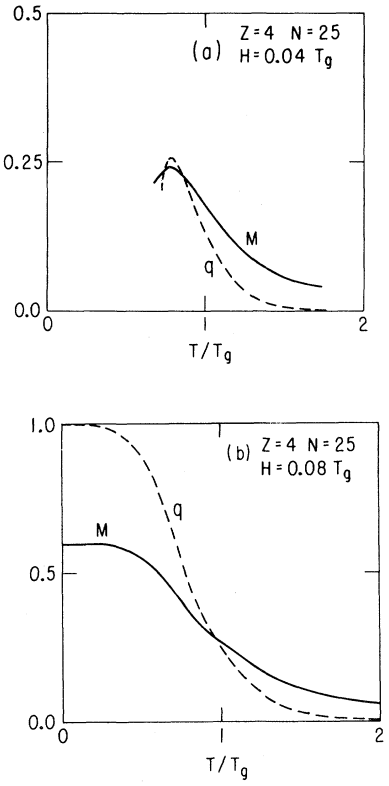

FIG. 2. The FC 2D BPW magnetization M (solid curve) and EA order parameter q (dashed curve) vs T/T_g for $N=25$ with (a) $H=0.04T_g$ and (b) $H=0.08T_g$.

range, the entropy of the lower-field state became negative. The higher-field state [Fig. 2(b)] could be followed all the way down to zero temperature, where, in contrast to the results obtained in Sec. III, M and q behave as expected on physical grounds: $q\rightarrow 1$ for $T\rightarrow 0$, and M is relatively constant for $T<T_g$. The zero-temperature limit of the higher-field FC solution satisfies the mean-field condition,

$$m_i=\mathrm{sgn}\left[H+\sum_j J_{ij}\,m_j\right], \tag{4.2}$$

and thus constitutes a simple mean-field ground state. (This is not necessarily the only zero-temperature solution of the BPW equations, as shown in the Appendix.) Unlike in the mean-field case, the BPW expression for the entropy becomes negative in the higher-field FC state for low-enough temperature. Thus, as in the TAP and low-field BPW cases, the FC state becomes unphysical at low temperatures.

Random-search calculations were performed for the 2D BPW system at the temperatures $T=0.51T_g$, $T=0.67T_g$, and $H=0.08T_g$. The calculations carried out at the higher temperature resulted, for all 30 attempts, in reconvergence to the field-cooled state. At the lower temperature, this procedure resulted, for all 36 attempts, in convergence to a new state, distinct from the FC state. The new state has lower entropy and free energy, and is much less magnetized than the field-cooled state. (Both states have negative entropy at this temperature.) Attempts to follow this new state to either higher or lower temperatures were not successful, despite the use of temperature increments as small as $\Delta T=0.005T_g$.

The results of the three-dimensional FC calculation are shown in Fig. 3 for $H=0.03T_g$. The magnetization and the EA order parameter are plotted as functions of reduced temperature. These results are qualitatively similar to those found for the 2D model at $H=0.04T_g$. The magnetization and EA order parameter have maxima for temperatures near T_g, where they take on unphysically small values. The extraordinarily large number of iterations and small temperature increments required for convergence prevented us from following the field-cooled solution all the way down to $T=0$. Random-search calculations were performed for the 3D BPW system at $T=0.55T_g$. In each of the six random-search calculations performed, the result was reconvergence to the field-cooled solution. No other solution to the 3D BPW equations was found.

V. OTHER SEARCH TECHNIQUES

In addition to the field-cooling and random-search techniques, we have also explored two other methods for generating solutions to the TAP equation. We have heated $T=0$ solutions, obtained from naive mean-field theory (which is equivalent to TAP in this limit). In addition, following a proposal by Dasgupta and Sompolinsky[18] which was made after the body of this work was completed, we have used Monte Carlo methods to find TAP solutions. Like the methods discussed in Secs. III and IV, these approaches lead to unphysical results.

We derived solutions to the $T=0$ TAP equations by field cooling within naive mean-field theory. This procedure always generates low-energy solutions, which are comparable in energy to those obtained in Monte Carlo simulations. Once the $T=0$ TAP solution is obtained, the reaction term is included and the temperature slowly raised. At temperatures in the range of $0.2T_g$ the solution becomes unstable; that is, the curvature vanishes in at least one direction, and the free-energy minimum disappears. We were therefore unable to heat such solutions above roughly $0.2T_g$.

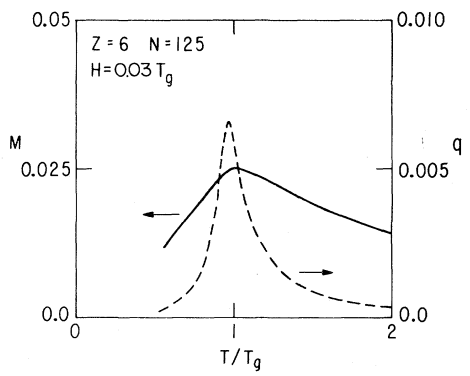

FIG. 3. The FC 3D BPW magnetization M (left axis) and EA order parameter q (right axis) vs T/T_g for $N=125$ and $H=0.03T_g$.

Recently, Dasgupta and Sompolinsky[18] have shown that that careful Monte Carlo annealing of the Sherrington-Kirkpatrick (SK) model (beginning at temperatures well above T_g, and cooling to $T \equiv 0.5T_g$) may sometimes be useful in obtaining solutions to the TAP equations. The set of spin averages $\{\langle \sigma_i \rangle\}$ resulting from this technique is used as the starting configuration $\{m_i\}$ in a search for a TAP solution. A root-finding method (asymptotically equivalent to Newton's method) is then applied to locate the TAP minimum. Dasgupta and Sompolinsky carefully screened their bond configurations to insure faithful representation of the infinite-system bond statistics, yet found convergence to a TAP solution for only 40% of the bond configurations.

We have heated and cooled TAP solutions generated from Monte Carlo using our numerical scheme. Our analysis of a representative set[18] of these TAP solutions indicates that they become unphysical upon cooling; the entropy becomes negative or anomalously small and the minimum disappears for $T \simeq 0.4T_g$. Moreover, the Edwards-Anderson q exhibits an unphysical maximum for $T \simeq 0.45 - 0.5T_g$. Upon heating, the solutions persist up to temperatures ranging from $0.8T_g$ to $1.2T_g$ (depending on the bonds) at which point the minimum disappears with $q \simeq 0.15$—0.35. We conclude, therefore, that there is a sizable first-order jump into a high-temperature state. Presumably the first-order jump is a finite-size effect. The temperature dependence of q just prior to this disappearance of the minimum is nonanalytic, and is hence inconsistent with the linear temperature dependence expected from analysis valid in the thermodynamic limit.[1,2] In summary there is, at best, a narrow window in temperature, extending roughly from $0.5T_g$ to $0.75T_g$, in which these Monte Carlo—generated solutions to the TAP equations can be physical. It is interesting to note that, since Monte Carlo simulations do not lead to these unphysical results, the TAP solutions cannot correspond to those obtained using Monte Carlo methods, except in a narrow range of temperatures. Presumably the discrepancy between the two approaches is due to the fact that the TAP equations are only approximate for finite N.

VI. CONCLUSIONS

Bray and Moore[11] and DeDominicis *et al.*[10] have argued that there are a large number of solutions to the TAP equations at low T (of order $e^{0.2N}$ for $T=0$). In view of our numerical results, and those of others,[4,5] we are forced to conclude that these solutions do *not* correspond to quadratic minima of the free energy, but must be quadratic maxima or saddle points, or higher-order stationary points. This view is consistent with the claim of[1] TAP that all physical states are higher-order saddle points; it is also somewhat stronger, for it addresses the global properties of the free-energy surface. There are very few positive entropy (quadratic) minima on the surface, even for finite-size systems. Moreover, these appear to be at best, piecewise continuous with varying temperature.

Our studies can shed some light on the effect of the range of the interaction on the free-energy surface. The fact that the TAP model yields unphysical results cannot be ascribed to mathematical pathologies associated with infinite-range interactions. We find the finite-range BPW case and that of TAP to be generally very similar. The main difference lies in the nature of the mean-field ground states [Eq. (4.2)]. At $T=0$ the mean-field equations are satisfied by the TAP and by some BPW ground states. In the latter case such states may be generated by field cooling at high fields, but not in the former. More importantly the BPW mean-field ground states found in this way have negative entropy S. In the TAP case (and presumably in the BPW case) there are mean-field ground states with $S > 0$, which evidently cannot be found by cooling at constant field.

In addition to providing information about the *unphysical* FC states, the present calculations present a scenario for the behavior of the *physical* field-cooled magnetization M^{FC} which has not yet been found numerically for the TAP and BPW theories. This magnetization is thought[17] to correspond to that obtained using thermodynamic arguments. According to Parisi,[3] M^{FC} is relatively constant at low T for the infinite-range Ising model. It is also reversible with respect to heating and cooling. These features have also been verified by Monte Carlo simulations on finite-size systems,[16] and appear to be true in naive mean-field theory[12] and experiment.[22] It is interesting to note that, in the TAP or BPW cases, the *physical* FC magnetization must necessarily exhibit a first-order jump at T_g, where the paramagnetic state becomes unphysical. This jump is not seen in naive mean-field theory, or in the limit $N \rightarrow \infty$, because in these cases the paramagnetic state has a divergent susceptibility that allows the system to move continuously from one state to another as the temperature is lowered. In our studies of the TAP and BPW cases, we have not been able to find the physical low-temperature state to which the system jumps discontinuously. Presumably, it corresponds to a higher-order stationary point to which our iteration procedure cannot converge.

It is discouraging to observe that the success which Soukoulis *et al.*[12] had (using naive mean-field theory) in reproducing the measured field and temperature dependence of the various history-dependent magnetizations cannot be duplicated in the (presumably better) TAP and BPW theories. The "problem" clearly lies with the reaction term in F, whose presence leads to (unphysical) negative entropy solutions. This situation is quite different from the case of nondisordered ferromagnets, for which the corrections to naive mean-field theory improve the accuracy of the solution.[23] There are, however, similarities between this aspect of the spin-glass problem and the problem of the electronic structure of disordered systems, where apparently reasonable corrections to mean-field theory (the coherent-potential approximation) yield negative state densities.[24] Substantial progress has been made recently in an effort to structure the corrections to the coherent-potential approximation so as to guarantee positive-definite state densities.[25] It may be speculated that to obtain physical results in the spin-glass case, the corrections to naive mean-field theory must be grouped in a manner that preserves the positivity of the entropy and generally leads to well-behaved thermodynamic properties.

It is quite probable that the TAP theory simply is inadequate when applied to finite size systems. That is, that physical results will be found only in the thermodynamic limit. The inapplicability of iterative techniques in solving the TAP equations necessitates the use of some matrix

analysis and, therefore, reduces the size of the systems which can be considered. At these small N the TAP equations are evidently significantly in error and correction terms appear to be important. Nakanishi[5] has demonstrated how complex these corrections are. Furthermore, he finds only a partial improvement in his numerical results when these higher-order terms are included. Presumably a large number of "cluster corrections" are needed in order to get well-behaved solutions to the TAP equations at finite N. In summary, it appears to be extremely difficult to generate a theory for the free energy $F[\{m_i\}]$ which goes beyond naive mean-field theory and which also leads to physical numerical results for finite-size systems.

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APPENDIX: BPW GROUND STATES

The self-consistent Bethe-Peierls-Weiss equations [Eqs. (2.2)–(2.4)] become indeterminate as $T\rightarrow 0$ when written in terms of the spin variables $\{m_i\}$. If, however, they are written in terms of the local fields, $\{h_i\}$, the zero-temperature limits can be extracted as follows:

$$h_i = H + \sum_{j\,[=\mathrm{nn}(i)]} h_{ij} \ , \tag{A1}$$

where

$$h_{ij} \equiv \begin{cases} h_j \mathrm{sgn}(J_{ij}) - J_{ij}\mathrm{sgn}(h_j), & \text{if } h_i h_j J_{ij} > 0 \text{ and } |h_i| > |h_j| \le 2|J_{ij}| \quad \text{(A2a)} \\ \frac{1}{2}h_i, & \text{if } h_i h_j J_{ij} > 0 \text{ and } |h_i| = |h_j| \le 2|J_{ij}| \quad \text{(A2b)} \\ |J_{ij}|\,\mathrm{sgn}(h_i), & \text{if } h_j = 0,\ h_i \neq 0, \text{ and } J_{ij} \neq 0 \quad \text{(A2c)} \\ 0, & \text{if } J_{ij} = 0 \text{ or } h_i = h_j = 0 \quad \text{(A2d)} \\ J_{ij}\mathrm{sgn}(h_j), & \text{if } h_j \neq 0,\ h_i = 0, \text{ and } J_{ij} \neq 0 \\ & \quad \text{or if } h_i h_j J_{ij} < 0 \\ & \quad \text{or if } h_i h_j J_{ij} > 0 \text{ and } |h_i| < |h_j| \\ & \quad \text{or if } h_i h_j J_{ij} > 0 \text{ and } |h_i| \ge |h_j| \ge 2|J_{ij}| \quad \text{(A2e)} \end{cases}$$

and

$$\mathrm{sgn}(x) \equiv \begin{cases} 1, & x > 0 \\ 0, & x = 0 \\ -1, & x < 0 \ . \end{cases}$$

The other thermodynamic quantities also have a similar discontinuous behavior in the zero-temperature limit. Although Eqs. (A1) and (A2) are not equivalent to the zero-temperature mean-field equation [Eq. (4.2)], it should be noted that in all cases where the field-cooled BPW solutions could be followed down to very low temperatures, the spin configuration $\{m_i\}$ was also found to satisfy Eq. (4.2).

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[1]D. J. Thouless, P. W. Anderson, and R. G. Palmer, Philos. Mag. 35, 593 (1977).
[2]D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. 35, 1792 (1975).
[3]G. Parisi, J. Phys. A 13, 1115 (1980).
[4]A. J. Bray and M. A. Moore, J. Phys. C 12, L441 (1979).
[5]K. Nakanishi, Phys. Rev. B 23, 3514 (1981).
[6]M. Nass, C. M. Soukoulis, and K. Levin (unpublished).
[7]D. R. Bowman and K. Levin, Phys. Rev. B 25, 3438 (1982).
[8]T. Plefka, J. Phys. A 15, 1971 (1982).
[9]P. V. Chamberlin, M. Hardiman, L. A. Turkevich, and R. Orbach, Phys. Rev. B 25, 6720 (1982).
[10]C. DeDominicis, M. Gabay, T. Garel, and H. Orland, J. Phys. (Paris) 41, 923 (1980).
[11]A. J. Bray and M. A. Moore, J. Phys. C 13, L469 (1980).
[12]C. M. Soukoulis, K. Levin, and G. S. Grest, Phys. Rev. Lett. 48, 1756 (1982).
[13]H. Sompolinsky, Phys. Rev. Lett. 47, 935 (1981).
[14]J. A. Hertz (unpublished).
[15]N. D. Mackenzie and A. P. Young, Phys. Rev. Lett. 49, 301 (1982).
[16]S. Kirkpatrick and D. Sherrington, Phys. Rev. B 17, 4384 (1978); W. Kinzel, Phys. Rev. B 15, 4594 (1979).
[17]See, for example, P. Monod and H. Bouchiat, J. Phys. Lett. 46, 1693 (1981).
[18]C. Dasgupta and H. Sompolinsky (unpublished).
[19]See, for example, P. M. Levy, C. Morgan Pond, and A. Fert, J. Appl. Phys. 53, 2168 (1982).
[20]The number of different bond configurations considered for each N were: $N=25(5)$, $N=30(1)$, $N=40(1)$, $N=50(2)$, $N=60(1)$, $N=75(1)$.
[21]The presence in Eqs. (2.2)–(2.4) and (4.1) of hyperbolic functions whose arguments are proportional to β make the BPW equations very unstable and nearly indeterminate at very low temperatures. [The Appendix lists the many zero-temperature limits of Eqs. (2.2)–(2.4) as an example of this difficulty.] Ex-

tensive precautions were therefore taken in the numerical analysis of the BPW equations to prevent subtraction errors, divisions by zero, etc. arising from the presence of certain algebraic combinations of exponentially large and small quantities. It was necessary, for example, to iterate on the local fields, $\{h_j\}$, rather than on the spins, $\{m_j\}$, at low temperature. The discussion of stability in Sec. II remains valid, however, with only minor modifications due to the change of variables.

[22]See, for example, Ref. 9.

[23]See, for example, R. K. Pathria, *Statistical Mechanics* (Pergamon, New York, 1972), p. 428.

[24]A. Bansil, L. Schwartz, and H. Ehrenreich, Phys. Rev. B 12, 2893 (1975); H. K. Peterson, A. Bansil, and L. Schwartz, in *Structure and Excitation of Amorphous Solids, Williamsburg, Virginia, 1976,* Proceedings of an International Conference on Structure and Excitation of Amorphous Solids, edited by G. Lucovsky and F. L. Galeener (AIP, New York, 1976), p. 378; J. Bethel and J. L. Beeby, J. Phys. F 7, 1193 (1977).

[25]R. Mills and P. Ratanavararaksa, Phys. Rev. B 18, 5291 (1978); L. Schwartz, Phys. Rev. B 21, 522 (1980); B 21, 535 (1980).