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1999 J. Phys.: Condens. Matter 11 1537

(http://iopscience.iop.org/0953-8984/11/6/018)

J. Phys.: Condens. Matter **11** (1999) 1537–1544. Printed in the UK PII: S0953-8984(99)95907-6

Fermionic Thouless–Anderson–Palmer equations

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Received 10 July 1998, in final form 11 November 1998

Abstract. We derive the Thouless–Anderson–Palmer (TAP) equations for the fermionic Ising spin glass. It is found that, just as in the classical Sherrington–Kirkpatrick spin-glass model, the conditions for stability and for validity of the free energy are equivalent. We determine the breakdown of the paramagnetic phase. Numerical solutions of the fermionic TAP equations at $T = 0$ allowed us to localize a first-order transition between the spin-glass phase and the paramagnetic phase at $\mu \approx 0.8$. We computed at zero temperature the filling factor $\nu(\mu)$ and the distribution of the internal fields. The saddle-point equations resulting from the calculation of the number of solutions to the TAP equations were found to be much more complicated, as in the classical case.

1. Introduction

Fermionic Ising spin-glass models can be viewed as generalizations of the standard spin-space models, the Sherrington–Kirkpatrick model being the best known and analysed representative of the latter class. Spins of the fermionic spin-glass models are defined on Fock space, whence the fermionic spin glasses are naturally described by the grand canonical ensemble. The chemical potential controls the fermion filling and hence the effective spin density. Away from half-filling, these models must therefore be considered as partners of diluted classical spin models. A classical spin-1 model also offers a non-magnetic state, but it is defined in a three-state-per-site space, which differs from the four-state fermionic space. Moreover, the fermionic Sherrington–Kirkpatrick model has in addition a second life, which is its quantum dynamical one, to be found in all of the fermionic Green's functions for example.

An extension to complex chemical potentials allows us to realize that the fermionic models, which may appear more special at first sight, are indeed the more general models. All spin-space models are embedded.

Quantum dynamical effects are absent in spin correlations, but the fermionic Green's function showed interesting quantum dynamical effects, which moreover turn out to be strongly dependent on Parisi replica-symmetry breaking. In addition to other instabilities of the replicated theory, there was a clear indication of a first-order phase transition into the magnetically disordered phase at high enough chemical potential, i.e. low enough spin density. The thermodynamic transition line is not easy to find at any order of replica-symmetry breaking. The $T = 0$ endpoint of this transition line does not present a standard quantum phase transition point of the magnetic phase diagram, since the spin correlations remain static. Nevertheless, the low-temperature behaviour is hard to access numerically and, despite the discontinuity in the transition, infinitely many steps of replica-symmetry breaking are the minimum requirement for solving the infinite-range model completely. Recent analysis shows an additional random-field-like instability, which may require vector replica-symmetry breaking too.

0953-8984/99/061537+08$19.50

This renders the problem very hard within the replica method, and help from other techniques is searched for. We therefore considered the extension of the famous local mean-field equations for the random Ising model derived by Thouless, Anderson and Palmer [18]. We generalize these TAP equations to the four-state fermionic spin glass, including a chemical potential μ:

$$\mathcal{H} = -\frac{1}{2}\sum_{ij} J_{ij}\sigma_i\sigma_j - \mu\sum_i n_i - \sum_i h_i^{ext}\sigma_i. \tag{1}$$

n_i is the number operator for site i. The operators σ_i may be expressed in terms of creation and annihilation operators as $\sigma_i = a^+_{i,\uparrow}a_{i,\uparrow} - a^+_{i,\downarrow}a_{i,\downarrow}$. The matrix J_{ij} represents Gaussian-distributed random interactions with variance J^2/N.

It is believed [2, 15] that the complete set of solutions to the TAP equations is equivalent to the fully replica-symmetry-broken solution in the quantum-field theory [6–9], so far only known for half-filling. We were able to solve the fermionic TAP equations numerically on the $T = 0$ axis and to determine the first-order transition at $\mu_c \approx 0.8$ where the paramagnetic and spin-glass free energies become equal. The dependence of the filling factor on the chemical potential and the distribution of the internal fields are given below.

In the replicated theory, the fermion filling factor turned out to be something of an obstacle, since an instability was encountered at low enough temperatures and away from half-filling. The unresolved problem of discontinuous behaviour of the fermion filling factor $\nu(\mu)$ at any finite step of replica-symmetry breaking also called for an analysis in a replica-free technique, which is provided in this paper by means of the fermionic TAP equations.

The application of the numerical methods used here could also be extended to finite-dimensional systems, addressing for instance the currently interesting issue of short-range fluctuations in tricritical behaviour.

2. Fermionic TAP equations

The free energy corresponding to the classical TAP equations is

$$\mathcal{F} = -\sum_i h_i^{ext}m_i - \frac{1}{2}\sum_{ij} J_{ij}m_i m_j - \frac{\beta}{4}\sum_{ij} J_{ij}^2(1-m_i^2)(1-m_j^2) + \frac{1}{\beta}\sum_i\left\{(1+m_i)\ln\left(\frac{1+m_i}{2}\right) + (1-m_i)\ln\left(\frac{1-m_i}{2}\right)\right\}. \tag{2}$$

In order to calculate the corresponding expression for the generalized fermionic model, we extended the linked-cluster diagrammatic theory given by Horwitz and Callen [3]. For the sake of simplicity, this rigorous and lengthy derivation is replaced by shorter and more intuitive arguments.

The terms involving logarithms in equation (2) correspond to the entropy of an ensemble of spins in the classical Sherrington–Kirkpatrick spin-glass model with relative occupations $n_{i\uparrow}$ and $n_{i\downarrow}$, using $m_i = n_{i\uparrow} - n_{i\downarrow}$. Now we replace these terms with the entropy of the ensemble in the extended fermionic four-state model. The relative occupations are denoted by $n_{i\uparrow}, n_{i\downarrow}, n_{i0}$ and $n_{i\uparrow\downarrow}$, setting $m_i = n_{i\uparrow} - n_{i\downarrow}$, $n_i = n_{i\uparrow} + n_{i\downarrow} + 2n_{i\uparrow\downarrow}$ and $\tilde{q}_i = n_{i\uparrow} + n_{i\downarrow}$. Then we account for the non-trivial occupation number of the magnetic states by replacing $1 - m_i^2$ in the Onsager reaction field by $\tilde{q}_i - m_i^2$. After a final Legendre transformation, the fermionic

free energy reads, using $\mathbb{T} = \tanh(\beta\mu)$,

$$\begin{aligned}\mathcal{F} = -\frac{1}{2}\sum_{ij} J_{ij} m_i m_j - \frac{\beta}{4}\sum_{ij} J_{ij}(\tilde{q}_i - m_i^2)(\tilde{q}_j - m_j^2) - \sum_i \mu(1 + (1-\tilde{q}_i)\mathbb{T}) + \frac{N}{\beta}\ln 2 \\ e + \frac{1}{\beta}\sum_i \left[\left(\frac{\tilde{q}_i + m_i}{2}\right) \ln\left(\frac{\tilde{q}_i + m_i}{2}\right) + \left(\frac{\tilde{q}_i - m_i}{2}\right) \ln\left(\frac{\tilde{q}_i - m_i}{2}\right) \right. \\ + \left(\frac{(1-\tilde{q}_i)(1-\mathbb{T})}{2}\right) \ln\left(\frac{(1-\tilde{q}_i)(1-\mathbb{T})}{2}\right) \\ \left. + \left(\frac{(1-\tilde{q}_i)(1+\mathbb{T})}{2}\right) \ln\left(\frac{(1-\tilde{q}_i)(1+\mathbb{T})}{2}\right) \right]. \end{aligned} \tag{3}$$

The system is characterized by the following $2N$ coupled TAP equations:

$$\begin{aligned} m_i &= \frac{\sinh(\beta H_i)}{\cosh(\beta H_i) + \cosh(\beta\mu)\exp(-\beta X_i)} \\ \tilde{q}_i &= \frac{\cosh(\beta H_i)}{\cosh(\beta H_i) + \cosh(\beta\mu)\exp(-\beta X_i)} \end{aligned} \tag{4}$$

where

$$H_i = h_i^{ext} + \sum_j J_{ij} m_j - \beta m_i \sum_j J_{ij}^2(\tilde{q}_j - m_j^2)$$

and

$$X_i = \frac{\beta}{2}\sum_j J_{ij}^2(\tilde{q}_j - m_j^2).$$

A third equation for the local filling factors $\nu_i = 1 + (1-\tilde{q}_i)\tanh(\beta\mu)$ follows from $\nu = -\partial_\mu \mathcal{G}$. In the replicated quantum-field theory, the corresponding equation $\nu = 1 + (1-\tilde{q})\tanh(\beta\mu)$ turns out to be invariant under an arbitrary number of replica-symmetry-breaking steps.

3. Convergence and stability

Inspired by Plefka's work on the classical system [12] and adopting his replacement $J_{ij} \to \alpha J_{ij}$, we can rederive the fermionic free energy by means of a Taylor expansion as follows:

$$\begin{aligned}\mathcal{G}(\alpha) = -\frac{\alpha}{2}\sum_{ij} J_{ij} m_i m_j - \alpha^2 \frac{\beta}{4}\sum_{ij} J_{ij}^2(\tilde{q}_i - m_i^2)(\tilde{q}_j - m_j^2) \\ + \frac{1}{\beta}\sum_i \left[\left(\frac{\tilde{q}_i + m_i}{2}\right) \ln\left(\frac{\tilde{q}_i + m_i}{2}\right) + \left(\frac{\tilde{q}_i - m_i}{2}\right) \ln\left(\frac{\tilde{q}_i - m_i}{2}\right) \right. \\ + \left(\frac{(1-\tilde{q}_i)(1+\mathbb{T})}{2}\right) \ln\left(\frac{(1-\tilde{q}_i)(1+\mathbb{T})}{2}\right) \\ \left. + \left(\frac{(1-\tilde{q}_i)(1-\mathbb{T})}{2}\right) \ln\left(\frac{(1-\tilde{q}_i)(1-\mathbb{T})}{2}\right) \right] \\ - \mu\sum_i (1 + (1-\tilde{q}_i)\mathbb{T}) - \sum_i h_i^{ext} m_i + \frac{N}{\beta}\ln 2 + \mathrm{O}(\alpha^3). \end{aligned} \tag{5}$$

The correct free energy is given by $\mathcal{G}(\alpha = 1)$. The diagrammatic expansion has already shown that, provided the series actually converges, the terms of cubic or higher order are suppressed in the thermodynamic limit. We may now determine the radius of convergence

of $\mathcal{G}(\alpha)$, which, by a standard theorem of complex analysis, is equivalent to the radius of convergence of

$$\partial_\alpha \mathcal{G}(\alpha) = -\frac{1}{2}\left\langle \sum_{ij} J_{ij}\sigma_i\sigma_j \right\rangle_\alpha = -\frac{1}{2}\sum_{ij} J_{ij}m_i m_j - \frac{1}{2\beta}\sum_{ij} J_{ij}\chi_{ij}(\alpha).$$

There, the susceptibility matrix χ is defined as

$$\chi_{ij}(\alpha) = \beta(\langle\sigma_i\sigma_j\rangle_\alpha - m_i m_j) = \partial_{h_i}\partial_{h_j}\mathcal{F}(\underline{h}, \underline{\chi}).$$

The radius of convergence is given by $\min(|\alpha|)$, where the minimization is done over the values of α with eigenvalues 0 in the inverse susceptibility matrix χ^{-1}. In the classical case the equation $(\chi^{-1})_{ij} = ([\partial_{\underline{h}}\partial_{\underline{h}}\mathcal{F}(\underline{h})]^{-1})_{ij} = \partial_{m_i}\partial_{m_j}\mathcal{G}(\underline{m})$ signifies that, when taking into account the special properties of the spectra of these random matrices [5], the local stability of a TAP solution implies the validity of the free energy at this point. In the fermionic model we have to deal with two different matrices, to describe either the convergence of the linked-cluster expansion $(\chi^{-1})_{ij}$ or the local stability of a given TAP solution by

$$\begin{pmatrix} \partial_{m_i}\partial_{m_j}\mathcal{G} & \partial_{m_i}\partial_{\tilde{q}_j}\mathcal{G} \\ \partial_{\tilde{q}_i}\partial_{m_j}\mathcal{G} & \partial_{\tilde{q}_i}\partial_{\tilde{q}_j}\mathcal{G} \end{pmatrix} = \begin{pmatrix} \partial_{h_i}\partial_{h_j}\mathcal{F} & \partial_{h_i}\partial_{\chi_j}\mathcal{F} \\ \partial_{\chi_i}\partial_{h_j}\mathcal{F} & \partial_{\chi_i}\partial_{\chi_j}\mathcal{F} \end{pmatrix}^{-1}.$$

A theorem given by Pastur [10, 11] used heavily by Plefka [12] and resolvent calculus can be applied to both cases to determine the limits of the support of the spectra.

It is very interesting to note that at the end of quite lengthy calculations the two matrices lead to exactly the same set of conditions, generalizing Plefka's convergence and stability conditions as follows:

$$\langle(\tilde{q} - m^2)^2\rangle \leqslant T^2 \tag{6}$$

$$\frac{1}{2}\langle\tilde{q}(1-\tilde{q})\rangle + 2\langle m^2 - m^4\rangle \leqslant T^2. \tag{7}$$

The known classical limit is obtained by setting $\tilde{q}_i = 1$. We have thus linked the local stability of TAP solutions to the finite support of the spectrum of random matrices in the thermodynamic limit. This gives a hint as to why the numerical search for these solutions is so difficult [4, 16, 17]: for finite N the support of these spectra becomes unbounded; see e.g. [5] for the exponential corrections to the semi-circle law at finite N. This means that for every solution the probability of having *negative* eigenvalues in the stability matrix is finite. But even just one negative eigenvalue prevents one from finding this solution via minimization algorithms.

4. Breakdown of the homogeneous paramagnetic solution

The TAP equations are readily solved numerically in the homogeneous paramagnetic phase, where they reduce to one single equation for $\tilde{q} = \tilde{q}_i$ given for all i by

$$\tilde{q} = \frac{1}{1 + \cosh(\beta\mu)\exp(-[(\beta J)^2/2]\tilde{q})}. \tag{8}$$

This is exactly the equation found in [6, 9, 14] for $\tilde{q}$ with a replicated quantum-field-theory approach.

The second-order transitions between the paramagnetic and the spin-glass phase are given by the intersection of the paramagnetic solutions with the stability conditions (equations (6) and (7)). In the next section we find a first-order transition on the $T = 0$ axis at $\mu_c \approx 0.8$. We expect a line of first-order transitions linking this point with the tricritical point. The broken line in the phase diagram (figure 1) gives only a schematic behaviour of this line, as the exact path is currently unknown.

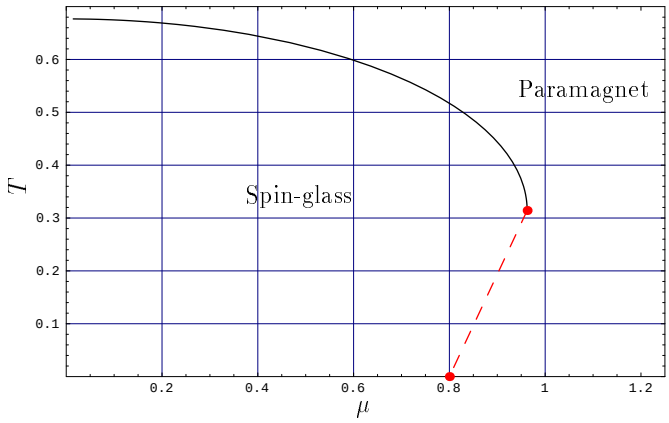

Figure 1. The phase diagram obtained from the fermionic TAP equations. The broken line is a linear approximation to the first-order transition line connecting the (calculated) tricritical point and the $T = 0$ critical point. The slope $\mathrm{d}T/\mathrm{d}\mu$ of the second-order transition line at the tricritical point is finite.

5. TAP equations at $T = 0$

At $T = 0$ the TAP equations reduce to

$$m_i = \Omega(h_i) \qquad \tilde{q}_i = m_i^2$$

where

$$h_i = \sum_i J_{ij} m_i$$

and $\Omega(x) = \Theta(x-\mu) - \Theta(\mu - x)$ denotes a modified sign function. The energy corresponding to these solutions is simply

$$f_{SG} = -\frac{1}{N} \sum_{(ij)} J_{ij} m_i m_j - \frac{\mu}{N} \sum_i n_i$$

which has to be compared with the free energy of the paramagnetic solution $f_{PM} = -2\mu$ to find the first-order transition. We were able to calculate numerically a huge number of spin-glass solutions. We first note the interesting dependence of the filling factor ν on the chemical potential (see figure 2). Unlike the discontinuous replica-symmetric and finite-step replica-symmetry-breaking solutions [7,8], the filling factor varies continuously with μ in the vicinity of $\mu = 0$. The numerical data for the increase of $\nu(\mu)$ near $\mu = 0$ are compatible with power-law fits, $|\delta\nu| \propto |\mu|^x$, $x > 1$, including exponential behaviour.

From the dependence of the energy difference between the spin-glass solutions and the paramagnetic solution (figure 3), we can deduce a first-order transition at $\mu = \mu_c \approx 0.8$. This critical value of μ can be viewed as a $T = 0$ analogue of T_c for the thermal first-order transitions.

Another very interesting feature shows up in the behaviour of the distribution of the local fields h_i. When applying a chemical potential, this probability density function is substantially modified. The 'soft gap' (see [13]) at $h_i = 0$ splits up into two soft gaps at $h_i = -\mu$ and $h_i = \mu$. Within the interval $[-\mu, \mu]$ another peak emerges (see figures 4 and 5).

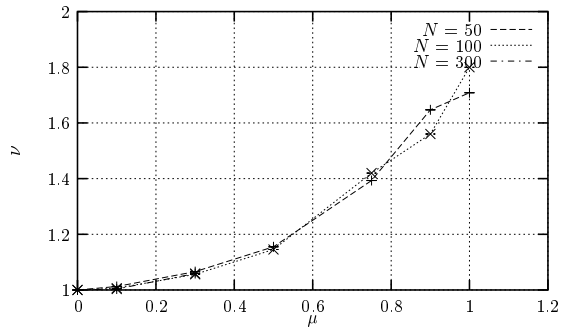

Figure 2. The filling factor $\nu(\mu)$ as a function of the chemical potential for systems of different sizes.

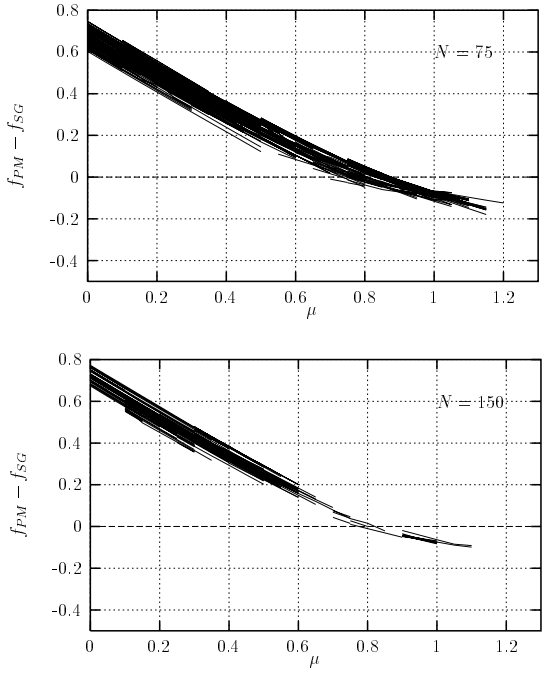

Figure 3. The energy gap between spin-glass solutions of the zero-temperature TAP equations and the corresponding paramagnetic solutions. We plot a large number of numerical solutions for systems of size $N = 75$ and $N = 150$ in order to show the effect of finite N on the fluctuation of the energy gap.

6. The number of solutions

The number of solutions of the TAP equations (related to the so-called complexity) can be calculated by adopting the procedure of Bray and Moore [1] for finite T or following Roberts [13] for $T = 0$. We were able to obtain in both cases fermionic generalizations of the saddle-point equations, which become extremely complicated due to the additional non-magnetic degrees of freedom. For example, in the finite-temperature case the number of TAP

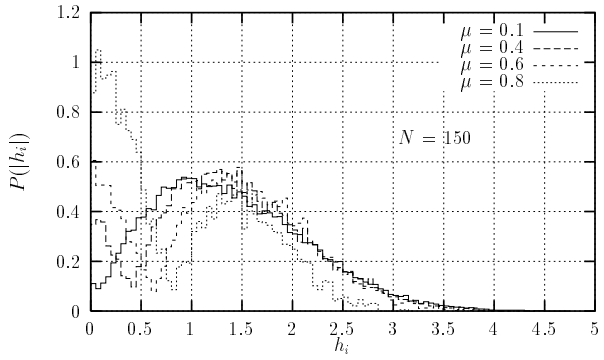

Figure 4. The internal field distribution $P(|h_i|)$ for $N = 150$ and different values of μ. The distribution $P(h_i)$ is symmetric. We used about 10 000 points for each histogram.

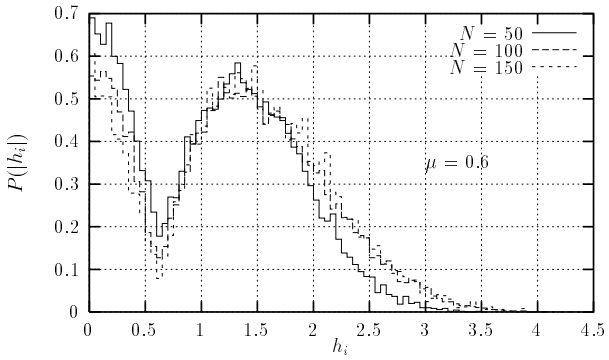

Figure 5. The scaling of $P(h_i)$ at $N = 50$, $N = 100$ and $N = 150$ for $\mu = 0.6$.

solutions is

$$\mathcal{N}(f) = \exp\left(N\left[-\frac{1}{2J^2}(\Delta^2 - B^2) - (\Delta + B)(\tilde{q} - q) - \eta q - uf - \varrho\tilde{q} + \ln I\right]\right) \tag{9}$$

where I is given below and the parameters $q, \tilde{q}, \eta, \varrho, \Delta$ and B are solutions to the corresponding saddle-point equations:

$$\begin{aligned}
&f = \langle \mathcal{F} \rangle_I \qquad q = \langle m^2 \rangle_I \qquad \tilde{q} = \langle \kappa \rangle_I \\
&0 = B\left\{1 - J^2 \langle \frac{(\kappa - (\kappa\lambda)^2)^2}{1 + B(\kappa - (\kappa\lambda)^2)} \rangle_I \right\} \\
&0 = \frac{1}{q}\langle \kappa\lambda(\tanh^{-1}(\lambda) - \kappa\lambda\Delta)\rangle_I - \Delta - J^2(\tilde{q} - q) \\
&\varrho = -(\Delta + B) - \frac{J^2}{2}\left\langle \Theta\sqrt{1 - \lambda^2}\kappa^2 \Xi \right\rangle \\
&\eta = \Delta + B + \frac{1}{2q}\left[1 - \frac{1}{J^2 q}\langle(\tanh^{-1}(\lambda) - \kappa\lambda\Delta)^2\rangle\right] + \frac{J^2}{2}\left\langle \Theta\sqrt{1 - \lambda^2}\kappa^2 \Xi \right\rangle
\end{aligned} \tag{10}$$

which can be viewed as an extension of the original equations given by Bray and Moore, but the average $\langle\cdot\rangle_I$ means averaging by use of the following kernel:

$$I = \int_0^1 \mathrm{d}\kappa \int_{-1}^1 \mathrm{d}\lambda \; g(\vec{x}, \kappa, \lambda)\delta(f(\vec{x}, \kappa, \lambda))$$

$$= \int_0^1 \mathrm{d}\kappa \int_{-1}^1 \mathrm{d}\lambda \, \frac{\kappa}{\sqrt{2\pi}\sqrt{q}J} \left[\frac{1 + B(\kappa - (\kappa\lambda)^2)}{(\kappa^2 - (\kappa\lambda)^2)} \right] (1-\kappa)^{u-1}$$
$$\times \exp\left(\eta(\kappa\lambda)^2 + \varrho\kappa + \frac{u\kappa\lambda}{2} \tanh^{-1}(\lambda) - \frac{1}{2J^2 q} (\tanh^{-1}(\lambda) - \kappa\lambda\Delta)^2 \right)$$
$$\times \delta\left(\ln\left(\frac{(\kappa^2 - (\kappa\lambda)^2)\cosh^2(\mu)}{(1-\kappa)^2} \right) - J^2(\tilde{q} - q) \right).$$

This kernel also gives the number of solutions. $\lambda = m/\kappa$ is the reduced magnetization. Ξ is an abbreviation for

$$\Xi = -\frac{u-2}{1-\kappa} + 2\eta\kappa\lambda^2 + \rho + \frac{u\kappa\lambda}{2} \tanh^{-1}(\lambda)$$
$$+ \frac{B(1 - 2\kappa\lambda^2)}{1 + B(\kappa - (\kappa\lambda)^2)} + \frac{\lambda\Delta}{J^2 q} (\tanh^{-1}(\lambda) - h^{ext} - \kappa\lambda\Delta).$$

These equations remain currently unsolved even numerically. The equations for $T = 0$ are equally hard to treat.

7. Forward look

The numerical work presented here should now be accompanied by exact analytic replica-symmetry-breaking calculations for arbitrary μ. In order to reproduce the behaviour of $\nu(\mu)$ and of $P(h_i, \mu)$, the generalizations of Roberts' saddle-point equations [13] should be solved. It would be desirable to have Parisi's solution (infinite-step replica-symmetry breaking) for $\mu \neq 0$. The answer to one of the open questions might reveal the exact path of the first-order transition line for $T \neq 0$. If this turns out to be impossible, one should find more refined numerical algorithms, which allow one to solve the fermionic TAP equations for $T \neq 0$.

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