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LETTER TO THE EDITOR

$1/p$ expansion for a p-spin interaction spin-glass model in a transverse field

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Abstract. We develop systematic $1/p$ expansions for the p-spin interaction spin-glass model in a transverse field. This model can be solved using the static approximation (SA), which is expected to be valid in the limit $p\rightarrow\infty$. For large, but finite p, corrections to SA can be obtained, and the non-trivial time dependence of the imaginary time correlation function for quantum spins calculated. These corrections qualitatively change the low temperature behaviour for large p. In particular the corrections to the SA result in the entropy vanishing exponentially as the temperature tends to zero. We compute the finite p changes in the phase diagram, and discuss the emergence of a new critical point ending the transition line separating the two paramagnetic phases.

Several infinite range models exhibiting spin-glass behaviour have been solved [1]. However, the addition of quantum fluctuations precludes an exact solution even in this mean field limit. Numerous studies of quantum versions of Heisenberg and Ising spin glasses [2–12] show that the difficulties originate from the presence of an additional dynamical self-coupling induced by averaging over randomness. Specifically, this averaging induces an interaction coupling the quantum spin at different imaginary times. The coupling constant $\lambda(t, t')$ is determined self-consistently.

An approximate solution to the problem can be obtained by replacing $\lambda(t, t')$ by an appropriate time average. This method, which was originally proposed by Bray and Moore [5] and is referred to as the *static approximation* (SA), can be readily used to solve the mean field equations and the resulting phase diagram can be computed. Furthermore, Thirumalai, Li and Kirkpatrick (TLK) studied the stability of the replica-symmetric (RS) solution in the spin-glass (SG) phase [12]. The RS solution was shown to be stable in a region of the SG phase. However, TLK also pointed out the limitations of the SA by examining the low temperature properties of the theory. In particular, it is found [12] that the entropy does not vanish at zero temperature. Moreover, the theory also predicts a finite slope $\mathrm{d}T_q/\mathrm{d}\Gamma$ of the critical glass transition line as $T\rightarrow 0$. This is in apparent violation of thermodynamics which would require this slope to diverge at low temperatures [13]. It is interesting to note that although these features appear to be just artefacts of the theory, they have nevertheless been used to interpret [14] recent experiments [15, 16, 17] on proton glasses.

In order to gain a better understanding of quantum spin-glass problems, it would be helpful to examine the limits of the validity of the static approximation by applying it to an exactly solvable model. Very recently, it has been suggested [18] that the p-spin interaction model in a transverse field with $p=\infty$ is the appropriate choice since the

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quantum fluctuations can be exactly accounted for using the static approximation. In this model which is the quantum analogue of the 'simplest spin glass' [19], the interaction $\lambda(t, t')$ of spins at different imaginary times can either be infinite (suppressing quantum fluctuations) or zero. The static approximation is formally exact in this limit because $\lambda(t, t')$ does not have a non-trivial time dependence.

A more stringent test of the static approximation would be to examine its validity for large but *finite* p, where $\lambda(t, t')$ not only has a finite value but in principle can also have a complicated time dependence. For this model a systematic $1/p$ expansion is possible, and thus one can examine the differences between the exact solution and the predictions obtained using SA. Since the interesting differences occur in the paramagnetic phases, we confine our attention to this region of the phase diagram. In addition to assessing the limitations of SA, we also examine the changes in the structure of the phase diagram at large but finite p.

We consider the model with the Hamiltonian

$$\mathcal{H} = -\sum_{j_1\cdots j_p}{}' J_{j_1\cdots j_p}\hat{\sigma}^z_{j_1}\ldots\hat{\sigma}^z_{j_p} - \Gamma\sum_j \hat{\sigma}^x_j \tag{1}$$

where $\hat{\sigma}^z$ and $\hat{\sigma}^x$ are the Pauli matrices, the prime indicates summation over all distinct clusters of p spins and the random bond interaction elements $J_{j_1\cdots j_p}$ are distributed according to

$$P[J_{j_1\cdots j_p}] = (N^{p-1}/\pi p!)^{1/2}\exp\left[-\frac{(J_{j_1\cdots j_p})^2 N^{p-1}}{J^2 p!}\right]. \tag{2}$$

Using the Trotter–Suzuki discretised path integral formulation [20] and the replica trick [1], one can average [11, 12] Z^n where Z is the partition function, over random bond elements and the result is [18]

$$[Z^n] = \mathrm{Tr}\exp[-\beta\bar{\mathcal{H}}]$$

where

$$-\beta\bar{\mathcal{H}} = \frac{1}{4}(\beta J)^2\frac{p!}{N^{p-1}}\frac{1}{M^2}\sum_{t,t'}\sum_{j_1\cdots j_p}{}'\sum_{\alpha,\beta}(\mu^\alpha_{j_1}(t)\mu^\beta_{j_1}(t'))\ldots(\mu^\alpha_{j_p}(t)\mu^\beta_{j_p}(t')) - \beta\mathcal{H}_0[\mu] \tag{3}$$

with $\alpha = 1, \ldots, n$ $(n\to 0)$ are replica indices, $t = 1, \ldots, M$ $(M\to\infty)$ (imaginary) time indices, $\mu^\alpha_j(t) = \pm 1$, and the non-interacting spin Hamiltonian is

$$-\beta\mathcal{H}_0[\mu] = a\sum_j\sum_t \mu_j(t)\mu_j(t+1) + C \tag{4}$$

with

$$a = \tfrac{1}{2}\ln\cosh(\beta\Gamma/M) \qquad C = \tfrac{1}{2}NM\ln[\cosh(\beta\Gamma/M)\sinh(\beta\Gamma/M)].$$

For infinite-ranged interactions, it is possible to decouple the interactions between various sites by introducing appropriate Lagrange multipliers [18, 19] (in order to constrain the order parameters) and the resulting (replicated) partition becomes

$$[Z^n] = \int \mathrm{D}Q_{\alpha\beta}(t, t')\mathrm{D}\lambda_{\alpha\beta}(t, t')\exp\{-NG[Q, \lambda]\} \tag{5}$$

where the (reduced) free energy $G[Q, \lambda]$ is given by:

$$G[Q, \lambda] = -\frac{1}{4}(\beta J)^2\frac{1}{M^2}\sum_{t,t'}\sum_{\alpha\leqslant\beta}Q^p_{\alpha\beta}(t, t') + \frac{1}{2}\frac{1}{M^2}\sum_{t,t'}\sum_{\alpha\leqslant\beta}\lambda_{\alpha\beta}(t, t')Q^p_{\alpha\beta}(t, t')$$
$$-\ln\mathrm{Tr}_{(\mu)}\exp\{-\beta\mathcal{H}_{\mathrm{eff}}[\mu, \lambda]\} \tag{6}$$

with the effective Hamiltonian:

$$-\beta\mathscr{H}_{\text{eff}}[\mu,\lambda]=\frac{1}{2}\frac{1}{M^2}\sum_{t,t'}\sum_{\alpha\leqslant\beta}\lambda_{\alpha\beta}(t,t')\mu^{\alpha}(t)\mu^{\beta}(t')-\beta\mathscr{H}_0[\mu]. \tag{7}$$

In the thermodynamic limit the partition function is dominated by the saddle point of $G[Q,\lambda]$ and we obtain the following set of self-consistent equations:

$$\lambda_{\alpha\beta}(t,t')=\tfrac{1}{2}(\beta J)^2pQ_{\alpha\beta}^{p-1}(t,t') \qquad Q_{\alpha\beta}(t,t')=\langle\mu^{\alpha}(t)\mu^{\beta}(t')\rangle \tag{8}$$

where the averages are taken with respect to $-\beta\mathscr{H}_{\text{eff}}[\mu,\lambda]$.

These equations cannot, for arbitrary values of p, be solved exactly due to the complicated, time dependent form of the effective Hamiltonian $-\beta\mathscr{H}_{\text{eff}}[\mu,\lambda]$. However, for the special value $p=\infty$, $\lambda_{\alpha\beta}(t,t')$ becomes independent of time [18]. This is because $Q_{\alpha\beta}(t,t')\leqslant 1$ and it follows that $\lambda_{\alpha\beta}(t,t')$ can either be 0 or ∞. The order parameters $\chi(t,t')=Q_{\alpha\alpha}(t,t')$ and $q_{\alpha\beta}=Q_{\alpha\neq\beta}(t,t')$ ($q_{\alpha\beta}$ must be time independent) can be used to identify three possible phases [18] of the model. For $q_{\alpha\beta}=0$, $\chi(t,t')\leqslant 1$, all λs vanish and we are left with non-interacting quantum spins—a 'quantum paramagnetic' (QP) phase. Alternatively, when $\chi=1$, $\lambda_{\alpha\alpha}=\infty$ which suppresses all quantum fluctuations and the problem reduces to the classical limit. Consequently, two more phases emerge—the 'classical paramagnetic' (CP) phase and the (classical) spin-glass (SG) phase, having structures identical to the classical p-spin ($p=\infty$) interaction model. (Note that in the SG phase at least some of the $q_{\alpha\beta}$s are 1 (for $p=\infty$) so that the corresponding λs diverge, completely suppressing quantum fluctuations, so that we cannot have a 'quantum spin-glass phase' in this limit.) Thus, for $p=\infty$, our problem is reduced to either the classical limit, or to non-interacting quantum spins, and there are no non-trivial effects of quantum fluctuations.

In order to examine the finite p behaviour let us first set up the static approximation which amounts to retaining only the zero Martsubara frequency component of $\chi(t,t')$. The free energy of the paramagnetic phases is found to be $F=TG$ with

$$G(\chi,\lambda)=-\tfrac{1}{4}(\beta J)^2\chi^p+\tfrac{1}{2}\lambda\chi-\ln\int \mathrm{D}z\cosh[(\beta\Gamma)^2+\lambda z^2]^{1/2}-\ln 2 \tag{9}$$

where

$$\int \mathrm{D}z\equiv\int_{-\infty}^{+\infty}\frac{\mathrm{d}z}{\sqrt{2\pi}}\,\mathrm{e}^{-z^2/2}.$$

For large but finite values of p, we expect the solutions to be close to the ones at $p=\infty$, allowing us to perform systematic expansions because λ can assume either very large or very small values. In particular, in the CP phase, where $\lambda\sim p$ is large we can use steepest descent methods to perform the necessary computations giving

$$\chi_{\text{CP}}=1-\frac{1}{p^2}\frac{4(\Gamma/J)^2}{(\beta J)^2}+\ldots \tag{10}$$

and

$$G_{\text{CP}}=-\tfrac{1}{4}(\beta J)^2-\ln 2-\frac{1}{p}(\Gamma/J)^2+\ldots. \tag{11}$$

Just as in the classical case [19], the entropy of the CP phase becomes negative at low temperatures where the physical solution corresponds to either the QP or the SG phase (the CP solution is physically meaningful only in the region where its entropy is positive). For the QP phase, we can expand in λ which is small and get

$$\chi_{QP} = \frac{\tanh(\beta\Gamma)}{(\beta\Gamma)} + \frac{1}{4(\beta\Gamma)^2}\left(3 - 3\frac{\tanh(\beta\Gamma)}{(\beta\Gamma)} - \tanh^2(\beta\Gamma)\right)p \times \exp\{-p\ln[(\beta\Gamma)/\tanh(\beta\Gamma)]\} + \ldots \tag{12}$$

and

$$G_{QP} = -\ln\cosh(\beta\Gamma) - \ln 2 - \tfrac{1}{4}(\beta J)^2 p\exp\{-p\ln[(\beta\Gamma)/\tanh(\beta\Gamma)]\} + \ldots. \tag{13}$$

In this case there are only *exponentially small* finite p corrections within SA. It is instructive to examine the low temperature predictions for the QP phase since that is where the difficulties of SA for $p=2$ become transparent [12]. For the free energy $F = TG$ the above result yields a *power-law* dependence $F - F(T=0) \sim -T^{p-1}$ giving the entropy $S \sim T^{p-2}$. Although the entropy does vanish at $T=0$, we stress that SA still violates the third law of thermodynamics which requires not only the entropy, but *all the derivatives* of the free energy to vanish in this limit.

The CP-QP phase boundary is determined by equating the free energies of the two phase which, ignoring the exponentially small corrections, gives the equation

$$\frac{1}{4}(\beta J)^2 + \frac{1}{p}(\Gamma/J)^2 = \ln\cosh(\beta\Gamma). \tag{14}$$

At high temperatures this transition line diverges at $\Gamma/J = 1/\sqrt{2}$ for $p=\infty$, but for finite p we obtain:

$$\Gamma(T, p) = \frac{1}{\sqrt{2}}\left(1 + \frac{1}{p}\frac{T^2}{J} + \ldots\right).$$

The finite p corrections within SA thus seem to favour the CP phase at high temperatures.

It is important to determine the limitations of our large p results. By going back to (7), we can see that for fixed p, λ can be made arbitrarily small at sufficiently high temperatures and so the CP phase (λ large) cannot exist. In fact, by re-examining the above result we can see that the perturbation theory breaks down at temperatures $T/J \sim \sqrt{p}$. For fixed p, from (9) and (11) it follows that, as the temperature is increased, the CP value of χ decreases, while the QP value increases. At some point, we expect these two solutions to coalesce ending the phase transition line in a *critical point*. In order to examine this high temperature region in detail, let us return to (8) which is exact for any p as long as SA is valid. It is convenient to define the rescaled temperature $t = T/(J\sqrt{p})$ and write the order parameter as $\chi = 1 - \zeta/p$ in order to factor out the p dependence at $T \sim \sqrt{p}$. Expanding in $\beta\Gamma \sim 1/\sqrt{p}$, the reduced free energy can be written as $G = \tilde{G}/4pt$ with:

$$\tilde{G}(\zeta) = -(\zeta+1)\,e^{-\zeta} - 2(\Gamma/J)^2\Phi\left(\frac{1}{2t^2}e^{-\zeta}\right) + \text{constant} \tag{15}$$

where

$$\Phi(x) \equiv e^{-x/2}\int Dz\, x^{-1/2} z^{-1}\sinh(x^{1/2}z).$$

The minima of the free energy corresponding to the two phases cannot be obtained analytically, but having eliminated the p dependence it is now straightforward to numerically evaluate these solutions and calculate the corresponding phase boundary. The resulting high temperature phase diagram is presented in figure 1 where the first order phase transition line separating the CP and QP phases is indeed seen to end at a critical point at $t^* = 0.2593$ and $\Gamma^*/J = 0.7579$. Note that as p is increased, the critical temperature $T^* \sim t^*\sqrt{p}$ also grows, whereas the critical value of the transverse field Γ^* remains independent of p. As a consequence, the critical point is, for large p located deep in the semi-classical region justifying the above expansion in $\beta\Gamma$.

Having obtained the leading finite p corrections within SA, let us next try to perform analogous calculations by going beyond the SA. In the CP phase, although χ is time-dependent its value still has to be close to 1. Thus (see (7)) the Lagrange multiplier can be written in the form

$$\lambda(t, t') = \lambda_0 + \tilde{\lambda}(t, t') \tag{16}$$

where $\lambda_0 = \frac{1}{2}(\beta J)^2 p$ and $\tilde{\lambda}(t, t')$ is expected to be small. Our effective Hamiltonian, (6) can be broken in a large static part and a small perturbation

$$-\beta\mathscr{H}_{\rm eff} = -\beta\mathscr{H}_{\rm eff}^{\rm stat} + \tilde{V} \tag{17}$$

where

$$-\beta\mathscr{H}_{\rm eff}^{\rm stat} \equiv -\beta\mathscr{H}_{\rm eff}[\lambda = \lambda_0] \qquad \text{and} \qquad \tilde{V} \equiv -\beta\mathscr{H}_{\rm eff}[\lambda = \tilde{\lambda}].$$

We can now expand our free energy, (5) in $\tilde{V}$, and by taking a functional derivative with respect to $\tilde{\lambda}(t, t')$ we obtain an expression for the order parameter

$$\chi_{\rm CP}(t, t') = \frac{\int {\rm D}z\ {\rm Tr}[\mu(t)\mu(t')\exp\{(z\sqrt{\lambda/M})\ \Sigma_t\,\mu(t) - \beta\mathscr{H}_0[\mu]\}]}{\int {\rm D}z\ {\rm Tr}[\exp\{(z\sqrt{\lambda/M})\ \Sigma_t\,\mu(t) - \beta\mathscr{H}_0[\mu]\}]}. \tag{18}$$

The required computations reduce to finding correlation functions for a single quantum spin in a field [21] giving

$$\chi_{\rm CP}(\tau) = \frac{\int {\rm D}z[(z\sqrt{\lambda_0}/\beta\tilde{\Gamma})^2\cosh(\beta\tilde{\Gamma}) + (\beta\Gamma/\beta\tilde{\Gamma})^2\cosh[(\beta\tilde{\Gamma})(1-2\tau)]}{\int {\rm D}z\ \cosh(\beta\tilde{\Gamma})} \tag{19}$$

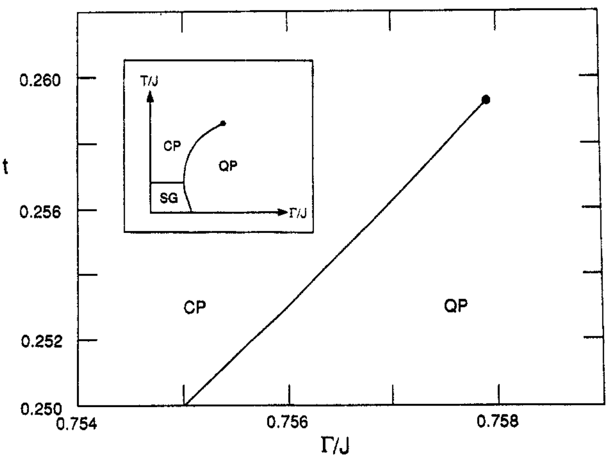

Figure 1. The high-temperature phase diagram in the large p limit. The first order phase transition line that separates the two paramagnetic phases is plotted in terms of the scaled temperature $t = T/J\sqrt{p}$ and the transverse field Γ/J. The dot at the end of this line represents the critical point located at $t^* = 0.2593$ and $\Gamma^*/J = 0.7579$. The inset depicts schematically the global structure of the phase diagram at large but finite p.

with

$$\beta\tilde{\Gamma} \equiv [\lambda_0 z^2 + (\beta\Gamma)^2]$$

and we have used a continuous time notation ($\tau \equiv t/M$, $M \to \infty$). In order to compare our result with SA, we can write the order parameter in the suggestive form

$$\chi_{\mathrm{CP}}(\tau) = 1 + \frac{1}{p^2} \frac{4(\Gamma/J)^2}{(\beta J)^2} f(\tau) \tag{20}$$

since $f(\tau) = -1$ in the static approximation (9). For fixed τ, it is possible to evaluate the integrals by steepest descents and show that the time dependence of $f(\tau)$ is exponentially weak for large p. As an illustration, we have plotted the numerically calculated $f(\tau)$ for various p values in figure 2. This figure shows the manner in which the time dependent corrections to the static approximation diminish for large p. Since the p dependence of $f(\tau)$ actually represents *subleading corrections*, we must conclude that to leading order in p the static approximation remains valid in the CP phase. It is not difficult to see that an analogous conclusion actually holds even for the spin-glass phase. The presence of a SG ordering introduces additional local (longitudinal) fields acting on a quantum spin, suppressing quantum fluctuations even further.

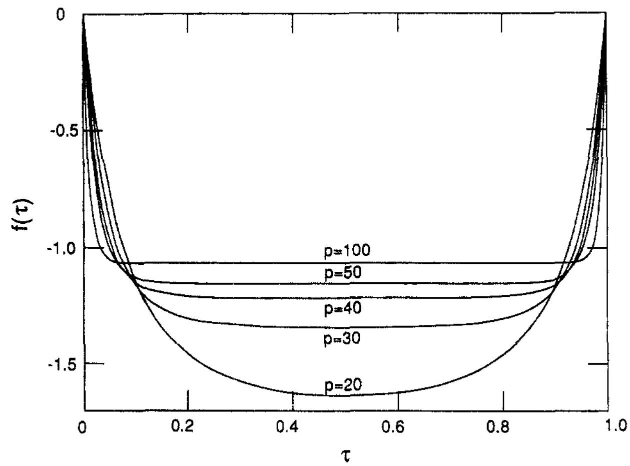

Figure 2. Time dependent corrections to the spin auto-correlation function $\chi(\tau)$ in the CP phase (see text). The function $f(\tau)$ is equal to -1 in the static approximation (SA). Since the p-dependence of $f(\tau)$ represents subleading corrections, SA is valid to leading order in $1/p$.

In the QP phase the Lagrange multiplier is expected to be small and we can expand the free energy (5) directly in $\lambda(t, t')$. To obtain the leading large p corrections it is necessary to go to second order in λ, and the resulting expression for the order parameter is

$$\chi_{\mathrm{QP}}(\tau, \tau') = \chi_0(\tau, \tau') + \tfrac{1}{2}(\beta J)^2 p \int_0^1 \mathrm{d}\tau_1 \int_0^1 \mathrm{d}\tau_2 [\chi_0^{(4)}(\tau, \tau', \tau_1, \tau_2) - \chi_0(\tau, \tau')\chi_0(\tau_1, \tau_2)] \chi_0^{p-1}(\tau_1, \tau_2) \tag{21}$$

where $\chi_0(\tau, \tau')$ and $\chi_0^{(4)}(\tau, \tau', \tau_1, \tau_2)$ are the well known two- and four-point time-correlation functions for a single quantum spin [11] calculated using the Hamiltonian

$\beta\mathcal{H}_0$. The required integrations although difficult in general, considerably simplify for large p, and after lengthy but straightforward algebra we get

$$\chi_{QP}(\tau)=\chi_0(\tau)+\frac{1}{p}[(\beta J)/[(2\beta\Gamma)\tanh(\beta\Gamma)]]^2$$
$$\times[(1-\chi_0(\tau))+2(\beta\Gamma)\chi_0(\tau)(\tanh(\beta\Gamma)-(1-2\tau)\tanh[(\beta\Gamma)(1-2\tau)])] \tag{22}$$

where

$$\chi_0(\tau)=\cosh[(\beta\Gamma)(1-2\tau)]/\cosh(\beta\Gamma). \tag{23}$$

From this result we can obtain the leading corrections for the reduced free energy

$$G_{QP}=-\ln\cosh(\beta\Gamma)-\ln 2-\frac{1}{p}(\beta J)[4(\Gamma/J)\tanh(\beta\Gamma)]^{-1}. \tag{24}$$

In contrast to the corresponding SA results, the low temperature corrections to the free energy $F=TG$ are now *exponentially* small: $F-F_0\sim-\exp\{-2\beta\Gamma\}/p$, in agreement with thermodynamics. Furthermore, we note that the large p convergence is also qualitatively changed: instead of exponential we now have *power-law* $\sim 1/p$ corrections to both the order parameter and the free energy.

In this letter we have investigated the role of quantum fluctuations and the relevance of the static approximation (SA) in quantum spin glasses. By performing a systematic large p expansion for the p-spin interaction quantum spin-glass model we have been able to explicitly calculate the leading (imaginary) time corrections to the dynamical self-coupling $\chi(\tau)$. In both the classical paramagnetic and the spin-glass phase we find to leading order $\chi(\tau)$ to be actually *time independent*, making SA valid in these instances. Our calculations also show that similar conclusions cannot be drawn in the quantum paramagnetic phase where we find a strong disagreement between SA and the exact, time-dependent results. Not only is the low temperature behaviour incorrectly predicted within SA, but including quantum fluctuations actually changes the large p convergence in the QP phase.

Interesting changes in the phase diagram have also been observed for finite p, where we find a new critical point ending the phase boundary between the classical-paramagnetic and the quantum-paramagnetic phase. Presently, the structure of this high temperature region has been investigated only within SA since the large p perturbative approaches which allowed accurate, time-dependent calculations, break down at $T/J\sim\sqrt{p}$. It would be interesting to try to extend time-dependent calculations to this region, but that would require a formally different approach than the one presented in this letter. It appears that a semi-classical calculation would be sufficient since our critical point is expected for large p to reside at $(\beta\Gamma)^*\ll 1$.

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