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LETTER TO THE EDITOR

Solving the Schrödinger equation for the Sherrington–Kirkpatrick model in a transverse field

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Abstract. By numerically solving the Schrödinger equation for small sizes we investigate the quantum critical point of the infinite-range Ising spin glass in a transverse field at zero temperature. Despite its simplicity the method yields accurate information on the value of the critical field and critical exponents. We obtain $\Gamma_c = 1.47 \pm 0.01$ and check that exponents are in agreement with analytical approaches.

There has recently been renewed interest in the study of quantum phase transitions in disordered systems [1]. In particular, Ising spin glass models in a transverse field are simple systems in which to study the effect of competition between randomness and quantum fluctuations. The case of infinite-range models is especially interesting because they show non-trivial quantum phase transitions yet are to some extent amenable to analytical computations. The canonical example in this family of models is the quantum Sherrington–Kirkpatrick (SK) model in a transverse field. At zero transverse field this reduces to the usual SK model which has a finite-temperature transition to low-temperature phase where replica symmetry is broken [2]. As the transverse field is turned on, spin-glass ordering occurs at lower temperatures and above a certain critical field the spin-glass order is completely suppressed at the expense of ordering in the transverse direction. Our understanding of this model was significantly extended by the non-perturbative analysis of Miller and Huse [3] and also by the different approach of Ye *et al* [4]. The critical behaviour is now well established, and values for exponents, predictions for logarithmic corrections and estimates of the value of the critical field are known. The model is therefore well adapted as a testing ground for numerical methods to investigate quantum phase transitions. From this point of view, the phase diagram of the quantum SK model in a transverse field and its zero-temperature critical behaviour have been studied using numerical techniques such as spin summation [5], perturbation expansions [6] and quantum Monte Carlo methods [7]. It is the purpose of this letter to introduce a new numerical approach based on the intuitive method of directly solving the Schrödinger equation for finite systems. Despite its simplicity, this method is able to give quantitative information on the value of the critical field and critical exponents even for the very small size systems we consider.

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The SK model in a transverse field is defined by the Hamiltonian,

$$\mathcal{H} = \mathcal{H}_0 - \Gamma \mathcal{M}_x = -\sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z - \Gamma \sum_i \sigma_i^x \tag{1}$$

where σ_i^z and σ_i^x are Pauli spin matrices and Γ is the the transverse field. The indices i, j run from 1 to N where N is the number of sites. The J_{ij} are Gaussian distributed random variables with zero mean and $1/N$ variance. $\mathcal{H}_0$ is the term we call the interaction energy, while $\mathcal{M}_x$ stands for the magnetization in the transverse direction.

We propose to study this model by the direct method of numerically solving the real time Schrödinger dynamics,

$$\mathrm{i}\frac{\partial|\psi\rangle}{\partial t} = \mathcal{H}|\psi\rangle. \tag{2}$$

The wavefunction, $|\psi(t)\rangle$, of the system at time t can be written as a linear combination of basis states,

$$|\psi(t)\rangle = \sum_{\nu=1}^{2^N} a_\nu(t)|\nu\rangle. \tag{3}$$

We have chosen the basis states, $\{|\nu\rangle;\, \nu = 1, \ldots, 2^N\}$ to be eigenstates of each of the spin operators $\{\sigma_z^i;\, i = 1, N\}$, $|\nu\rangle = |s_1, s_2, \ldots, s_N\rangle$. This choice gives a geometric meaning to equation (2) because these eigenstates can also be interpreted as the vertices of a unit hypercubic cell of dimension N. Each vertex of this hypercubic Hilbert space is assigned a label ν and a corresponding complex variable a_ν, which together define the state of the system. This geometric picture can also be used to understand the action of the Hamiltonian operator on the basis states $|\nu\rangle$. The action of the first term in equation (1) on the state $|\nu\rangle$ is diagonal with eigenvalue E_ν^0 which is precisely the energy of the classical SK model in that state ($E_\nu^0 = \langle\nu|\mathcal{H}_0|\nu\rangle$). The operator σ_x^i acting on a given eigenstate $|\nu\rangle$ changes the value of one spin which corresponds to an adjacent vertex of the hypercube. The dynamical equations for the a_ν become

$$\mathrm{i}\frac{\partial a_\nu(t)}{\partial t} = E_\nu^0 a_\nu(t) - \Gamma \sum_{\mu(\nu)} a_\mu(t) \tag{4}$$

where $\mu(\nu)$ are nearest neighbours to the vertex ν in the hypercubic cell. The geometric picture also facilitates efficient computer code for this problem.

We wish to calculate thermodynamic properties of the Hamiltonian (1) at zero temperature. Such information could be obtained by finding the static ground state of the Hamiltonian $\mathcal{H}$. However, because we want this ground state for a range of transverse fields, it is convenient to use a dynamical procedure. At large Γ the Hamiltonian can be diagonalized and the ground state is given by $a_\nu(t = 0) = 1/2^{N/2}$. Starting from this configuration we reduce the transverse field adiabatically slowly, thus ensuring that the system remains in its ground state. This procedure is recommended by its simple physical interpretation but is not the most efficient method that could be envisioned. For example the phase of the wavefunction is not of interest, and for large systems a gain in speed could be achieved by some less direct method.

We have numerically integrated equation (4) for different values of N in the range $N = 2$–13, using a simple Euler algorithm. The value of the time step can be fixed by testing the conservation of energy for some excited state at fixed Γ. For the ground state we can be less careful and we choose a time step $\mathrm{d}t = 0.01$. The transverse field is allowed to decrease linearly from $\Gamma = 3$ down to $\Gamma = 0$. We find that a total time of 100 units

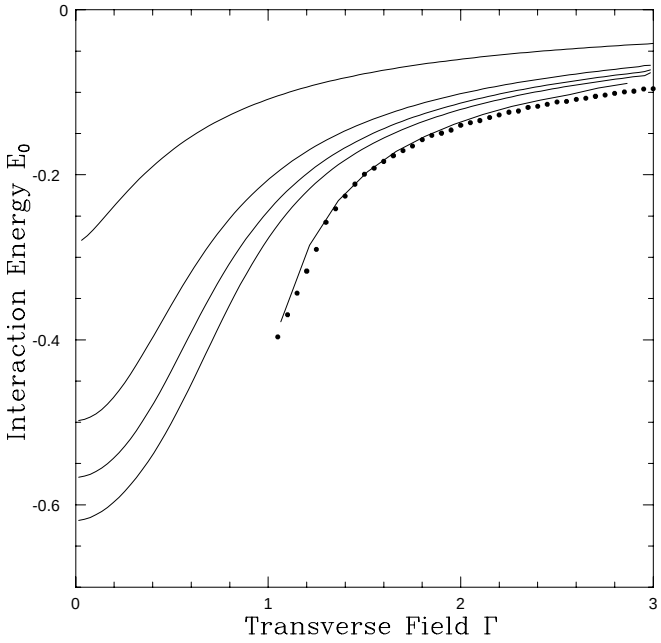

Figure 1. Interaction energy against tranverse field for (from top to bottom) $N = 2$ (analytic curve), $N = 5$ (50 000 samples), $N = 8$ (30 000 samples) and $N = 13$ (3000 samples). Errors are not shown, but are always less than 10^{-3}. The lowest continuous curve is the extrapolated data, $E_0(\infty)$, and the points have been obtained by quantum Monte Carlo methods [7].

(amounting to 10 000 integration steps) gives sufficiently slow variation of Γ for the adiabatic theorem to hold. The method has also been checked against the analytic solution of the model for $N = 2$. The errors from the discretization of the Schrödinger equation, from the adiabatic approximation and from the finite initial value of Γ are therefore well under control. The main source of error comes from sample-to-sample fluctuations. Data was averaged over many samples ranging from 50 000 for the smallest systems ($N = 3, 4, 5$) to 3000 for the largest sizes ($N = 10, 11, 13$). We have also considered 100 samples at $N = 17$ to confirm the tendency of the data, but have not used these points in our fits due to the large errors.

The simplest variable is the interaction energy, $E_0 = \langle 0|\mathcal{H}_0|0\rangle = \sum_\nu E_\nu a_\nu a_\nu^*$. It is plotted in figure 1 as a function of Γ for several different sizes. In figure 2 we show E_0 for three different values of Γ as a function of $1/N$. The different values of Γ are $\Gamma = 2.5$ in the quantum paramagnetic phase (QP) and $\Gamma = 1.45$ near the quantum critical (QC) point (see later). Data has been fitted with the least-squares method to a power law of the type $E_0(N) = E_0(\infty) + aN^{-b}$ [8, 9]. In the QP phase $b \simeq 0.93$, so corrections are essentially $1/N$ as expected. Close to the QC point we find $b = 0.73 \pm 0.02$ in agreement with the expected mean-field exponent

$$b = 1 + \frac{z}{d_u} + \frac{1}{\nu d_u} = \frac{3}{4}$$

where ν is the correlation length exponent ($\nu = \frac{1}{4}$), z is the dynamical exponent ($z = 2$)

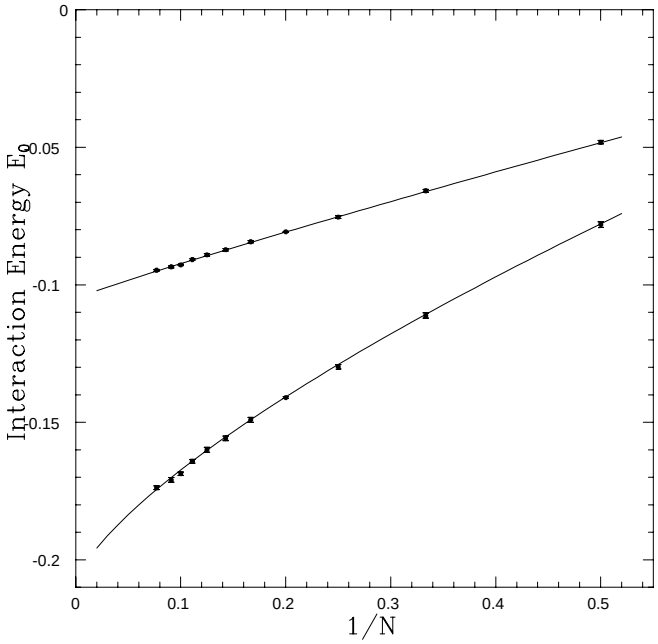

Figure 2. Interaction energy against $1/N$. At $\Gamma = 2.5$ in the QP phase (top) and $\Gamma = 1.45$ near the QC point (bottom). The points have error bars and the continuous curves show the power-law fits.

and d_{u} is the upper critical dimension ($d_{\mathrm{u}} = 8$). It is remarkable that even very small size systems fit on the curve. This data is summarized in figure 1 where we have also shown the best fit parameters $E_0(\infty)$ as a function of Γ in the region $\Gamma > 1.2$. The points are numerical data obtained by independent quantum Monte Carlo calculations [7] and show reasonable agreement with the extrapolated values. At smaller Γ, b decreases and it is no longer possible to ignore sub-leading corrections; nonetheless, at $\Gamma = 0$ we find $E_0(\infty) \simeq -0.763$ in agreement with the theory [2].

These results give us confidence in the method and encourage us to investigate the transition more closely. Because of the spin-glass nature of the transition, a clear signal does not appear in the more ordinary thermodynamic functions. A divergence will occur in the nonlinear susceptibility and we have also seen a peak in a Binder-like parameter for the kurtosis of the sample to sample distribution of the interaction energy. These observations suggest a transition in the region of $\Gamma \sim 1.5$ as expected, but are not the best way to obtain accurate information. To determine the critical field and critical exponents we consider the longitudinal susceptibility associated to the magnetization $\mathcal{M}_z = \sum_i \sigma_i^z$. It can be shown [10] that the longitudinal susceptibility (χ) for the SK model is precisely equal to 1 at the QP–QG boundary. To this end we have numerically computed χ. The usual quantum mechanical formula,

$$\chi = \sum_{n \neq 0} \frac{|\langle n|\mathcal{M}_z|0\rangle|^2}{E_n - E_0} \tag{5}$$

where $|n\rangle$ denotes the energy eigenstate with energy E_n, is not adapted to our needs

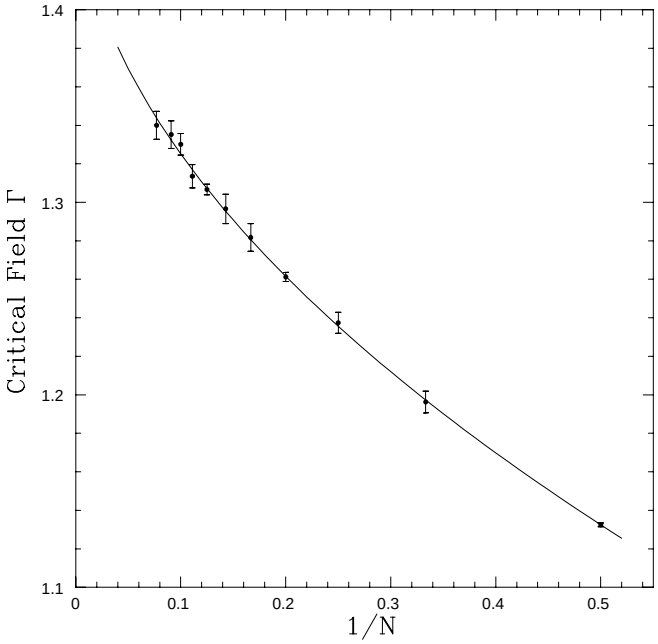

Figure 3. Critical transverse field plotted against $1/N$.

because it requires knowledge of the full spectrum. Instead, we solve the problem directly by applying a longitudinal magnetic field h small enough to be in the linear response regime. The susceptibility is computed as $\chi = \langle 0'|\mathcal{M}_z|0'\rangle/h$, where $|0'\rangle$ stands for the ground state in the presence of the field h. We need only solve the Schrödinger equation once for the perturbed Hamiltonian $\mathcal{H} + h\mathcal{M}_z$, since the magnetization of the unperturbed problem (without magnetic field) is strictly zero, as follows from a quantum mechanical symmetry. For zero transverse field this symmetry is the spin reversal symmetry of the classical SK model. In the thermodynamic limit $N \to \infty$ only one state is selected, but for our finite systems the wavefunction always contains a mixture of opposite magnetization states. In the perturbed case this symmetry is lost and at small transverse fields the action of the perturbation is to shift the wavefunction to a single magnetized state. This quantum tunnelling introduces a new time scale into the problem and the parameters we use in solving the Schrödinger equation should be re-examined. We have checked that the parameters we use give small errors (less than the errors from sample fluctuations) around the region of criticality.

The actual value of the perturbing field h can be taken in a wide range without affecting results, and we present data for h as small as 10^{-7}. Using the exact condition for criticality we define the critical transverse field by $\chi(\Gamma) = 1$, and in figure 3 we plot this Γ against $1/N$. Fitting the data to a power-law behaviour of the type $\Gamma = \Gamma_c + aN^{-b}$ we find $\Gamma_c = 1.47 \pm 0.02$, $a = -0.485 \pm 0.002$ and $b = 0.53 \pm 0.02$ in good agreement with the results obtained in perturbation theory by Ishii and Yamamoto [6] ($\Gamma_c = 1.506$) and with the result obtained by Miller and Huse [3] ($\Gamma_c = 1.46 \pm 0.01$). The coefficient b is very close to the expected value $b = 1/\nu d_u = 1/2$. If we consider the scaling at $\Gamma = 1.47$ we find that χ converges to 1 as N^{-c} with a value of the exponent $c \simeq 0.29$ compatible

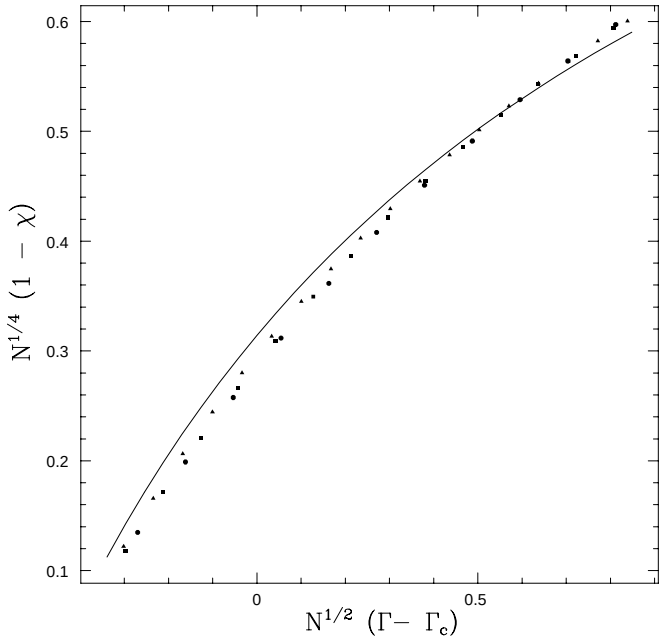

Figure 4. Data collapse for $N = 5$ (triangles), $N = 8$ (squares) and $N = 13$ (circles), shown for the range $1.2 < \Gamma < 2.0$ using our value of $\Gamma_c = 1.47$. The continuous curve is the analytical result for $N = 2$.

with $c = 2/d_u = 1/4$. The data collapse in the scaling region is shown in figure 4 where $(1-\chi)N^{2/d_u}$ is plotted as a function of $N^{1/\nu d_u}(\Gamma - \Gamma_c)$. The collapse is good and confirms the expected values $\nu = \frac{1}{4}$ and $d_u = 8$. Even the result for $N = 2$ lies close to the collapse line. Considering the simplicity of the method and the small sizes considered, the matching with data reported in the literature is impressive. This is particularly the case since logarithmic corrections are known to be present [3, 4].

In summary, a new and simple numerical method yielding good estimates of the critical field and confirming the critical exponents for the quantum phase transition of the SK model has been reported. The method consists in solving the Schrödinger equation for small sizes and computing expectation values in the ground state of the system. Quite remarkably, the system is within the scaling region even for very small sizes. The application of this method to other disordered systems such as the random orthogonal model [11] and the quantum Potts glass [12] would be very welcome.

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