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

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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 Read \[4\]. The critical behavior 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 behavior have been studied using numerical techniques such as spin summation \[3\], perturbation expansions \[4\] and quantum Monte Carlo methods \[5\]. 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.

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

$$\mathcal{H} = \mathcal{H}_0 - \Gamma M_x = - \sum_{i < j} J_{ij} \sigma_i^x \sigma_j^x - \Gamma \sum_i \sigma_i^x$$ \hspace{1cm} (1)

where $\sigma_i^x, \sigma_i^z$ are Pauli spin matrices and $\Gamma$ is 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 $M_x$ stands for the magnetisation in the transverse direction.

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

$$i \frac{\partial |\psi\rangle}{\partial t} = \mathcal{H} |\psi\rangle$$ \hspace{1cm} (2)

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

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

We have chosen the basis states, $\{ |\nu\rangle; \nu = 1, \ldots, 2^N \}$ to be eigenstates of each of the spin operators $\{ \sigma_i^z; i = 1, N \}$, $|\nu\rangle = |s_1, s_2, \ldots s_N\rangle$. 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 $\nu$ and a corresponding complex variable $a_\nu$, 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 $E^0_\nu$, which is precisely the energy of the classical SK model in that state ($E^0_\nu = \langle\nu|\mathcal{H}_0|\nu\rangle$). The operator $\sigma^x_i$ 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 $a_\nu$ become,

$$
\frac{i}{\hbar} \frac{\partial a_\nu(t)}{\partial t} = E^0_\nu a_\nu(t) - \Gamma \sum_{\mu(\nu)} a_\mu(t)
$$

(4)

where $\mu(\nu)$ are nearest neighbours to the vertex $\nu$ 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 $\Gamma$ the Hamiltonian can be diagonalised and the ground state is given by: $a_\nu(t=0) = 1/2^N$. 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 eq. (4) for different values of $N$ ranging from $N = 2$ to $N = 13$, 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 $\Gamma$. For the ground state we can be less careful and we choose a time step $dt = 0.01$. The transverse field is allowed to decrease linearly from $\Gamma = 3$ down to $\Gamma = 0$. We find that a total time of 100 units (amounting to 10000 integration steps) gives sufficiently slow variation of $\Gamma$ 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 discretisation of the Schrödinger equation, from the adiabatic approximation and from the finite initial value of $\Gamma$ are therefore well under control. The main source of error comes from sample to sample fluctuations. Data was averaged over many samples; ranging from 50000 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 $\Gamma$ for several different sizes. In figure 2 we show FIG. 1. Interaction energy against transverse field for (from top to bottom) $N = 2$ (analytic curve), $N = 5$ (50000 samples), $N = 8$ (30000 samples) and $N = 13$ (3000 samples). Errors are not shown, but are always less than $10^{-3}$. The lowest continuous line is the extrapolated data, $E_0(\infty)$, and the points have been obtained by quantum Monte Carlo methods.

FIG. 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.

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$E_0$ for three different values of $\Gamma$ as a function of $1/N$. The different values of $\Gamma$ are $\Gamma = 2.5$ in the quantum paramagnetic phase (QP) and $\Gamma = 1.45$ near the quantum critical (QC) point (see below). Data has been fitted with the least squares method to a power law of the type $E_0(N) = E_0(\infty) + aN^{-b}$ and $b = 3/4$. 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 $b = 1 + \frac{\nu}{\nu_d} = 3/4$ where $\nu$ is the correlation length exponent ($\nu = 1/4$), $z$ is the dynamical exponent ($z = 2$) and $\nu_d$ is the upper critical dimension ($\nu_d = 8$). 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 for $E_0(\infty)$ as a function of $\Gamma$ in the region $\Gamma > 1.2$. The points are numerical data obtained by independent Quantum Monte Carlo calculations and show reasonable agreement with the extrapolated values. At smaller $\Gamma$, $b$ 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.

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 the thermodynamic limit $N \to \infty$ only one state is selected, but for our finite systems the wavefunction always contains a mixture of opposite magnetisation 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 magnetised state. This quantum tunneling 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.

![FIG. 3. Critical Transverse field against 1/N.](image)

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 $\Gamma$ against $1/N$. Fitting the data to a power law behavior of the type $\Gamma = \Gamma_c + aN^{-b}$ we find $\Gamma_c = 1.47 \pm 0.02$, $a = -0.485 \pm 0.002$, $b = 0.53 \pm 0.02$ in good agreement with the results obtained in perturbation theory by Ishii and Yamamoto ($\Gamma_c = 1.506$) and with the result obtained by Miller and Huse ($\Gamma_c = 1.46 \pm 0.01$). The coefficient $b$ is very close to the expected value $b = \frac{\nu}{\nu_d} = 1/4$. If we consider the scaling at $\Gamma = 1.47$ we find that $\chi$ converges to 1 as $N^{-c}$ with a value of the exponent $c \simeq 0.29$ compatible with $c = \frac{1}{\nu_d} = 1/4$. The data collapse in the scaling region is shown in figure 4 where $(1 - \chi)N^\frac{1}{\nu_d}$ is plotted as a function of $N^\frac{\nu}{\nu_d}$. The collapse is good and confirms the expected values $\nu = 1/4$ and $\nu_d = 8$. 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].

![Image of a graph showing data collapse for different sizes.](image)

**FIG. 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 line is the analytical result for $N = 2$.

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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