Stability of the quantum Sherrington-Kirkpatrick spin glass model

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We study in detail the quantum Sherrington-Kirkpatrick (SK) model, i.e. the infinite-range Ising spin glass in a transverse field, by solving numerically the effective one-dimensional model that the quantum SK model can be mapped to in the thermodynamic limit. We find that the replica symmetric (RS) solution is unstable down to zero temperature, in contrast to some previous claims, and so there is not only a line of transitions in the (longitudinal) field-temperature plane (the de Almeida-Thouless, AT line) where replica symmetry is broken, but also a quantum de Almeida-Thouless (QuAT) line in the transverse field-longitudinal field plane at $T = 0$. If the QuAT line also occurs in models with short-range interactions its presence might affect the performance of quantum annealers when solving spin glass-type problems with a bias (i.e. magnetic field).

I. INTRODUCTION

Recently there has been a resurgence of interest in quantum spin glasses. This is motivated by the possibility that quantum annealing (QA) might be an effective way to solve optimization problems. There have been both experiments on real hardware made by D-Wave with up to around 2000 qubits and simulations both on special models and on problems which have can be embedded naturally onto the D-Wave machine.

Bottlenecks in QA occur where the gap between the ground state and the first excited state becomes very small. One situation where this occurs is at a quantum phase transition, so it is useful to locate and characterize quantum phase transitions in models that are commonly used for QA, which are generally spin glasses.

One of the most striking predictions of the mean field theory of spin glasses is the existence of a line of transitions in the magnetic-field temperature plane first found by de Almeida and Thouless (AT) \cite{11}. The solution of the mean-field, infinite-range, Sherrington-Kirkpatrick (SK) model in the RS phase below the AT line is complicated and was obtained, in a tour-de-force, by Parisi \cite{12, 13}.

The simplest approach to make a classical Ising model quantum is to add a transverse field $hT$. Here we investigate phase transitions in the quantum SK model including both a transverse field and a longitudinal field $h$. The Hamiltonian is

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z - \sum_{i=1}^{N} h_i \sigma_i^z - hT \sum_{i=1}^{N} \sigma_i^z, \quad (1)$$

where the $\{\sigma_i^z, \sigma_i^z\}, (i = 1, \cdots, N)$ are Pauli spin matrices, the interactions $J_{ij}$, which are between all $N(N-1)/2$ pairs of sites, have a Gaussian distribution with mean and variance given by

$$[J_{ij}]_{\text{av}} = 0, \quad [J_{ij}^2]_{\text{av}} = J^2/N, \quad (2)$$

the longitudinal fields $h_i$ have a Gaussian distribution with mean zero and standard deviation $h$, and the transverse field $hT$ is taken, for simplicity, to be the same on each site. Here the notation $[\cdots]_{\text{av}}$ indicates an average over the quenched disorder.

For $hT = 0$, de Almeida and Thouless \cite{11} showed that one must have replica symmetry breaking (RSB) below a line in the $h-T$ plane, see Fig. I. For $h = 0$, the phase boundary in the $h^T-T$ plane has been extensively studied \cite{15–22}. The question of whether RSB occurs in this plane all the way to $T = 0$ has been controversial. For example, Refs. \cite{16} and \cite{21, 22} argue that there is a low-temperature region with replica symmetry, while Ref. \cite{23} claims that there is region near the spin glass phase boundary with replica symmetry. By contrast, Refs. \cite{13, 20} argue that replica symmetry is broken all the way down to $T = 0$.

Here we investigate the stability of the replica symmetric (RS) solution in the $h^T-\beta$ plane finding that it is unstable all the way down to $T = 0$. As a result there must be a quantum AT (QuAT) line in the $h-h^T$ plane at $T = 0$ which we investigate for small longitudinal fields $h$. If it also occurs in those spin glass models which are used in QA studies, it could affect the performance of QA on spin glass problems in a longitudinal field.

The plan of this paper is as follows. In Sec. II we describe the effective one-dimensional model whose solution gives the behavior of the quantum SK model in the thermodynamic limit. The results of our numerical simulations of this model are described in Sec. III while the conclusions are summarized in Sec. IV.

II. REDUCTION TO AN EFFECTIVE ON-DIMENSIONAL MODEL

It is, by now, standard, \cite{19, 20, 24, 26} to reduce the quantum SK model in the replica-symmetric (RS) phase to an effective, non-disordered, long-range, one-dimensional model in which the dimension corresponds to imaginary time $\tau$, running from 0 to $\beta$, the inverse temperature. The interactions in this model have to be determined self-consistently. For our purposes it will be convenient to discretize imaginary time into $M$ time slices, labeled by $\ell$, each of width $\Delta \tau = \beta/M$.

We consider first the case of zero longitudinal field.
The long-range interactions along the $\tau$ direction, $r(\Delta l)$, have to be determined self-consistently from
\[
 r(\Delta l) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dz e^{-z^2/2} \langle S_{l_0} S_{l_0+\Delta l} \rangle_{\mathbf{M}} ,
\]
where we can use any time slice for $l_0$ because of translational invariance, and $\langle \cdots \rangle_{\mathbf{M}}$ indicates an average over the spins with weight $e^{-\mathbf{M}}$. The order parameter $q$ is determined self-consistently from
\[
 q = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dz e^{-z^2/2} \langle S_{l_0} \rangle_{\mathbf{M}}^2 ,
\]
where again we can use any time slice for $l_0$ because of because of translational invariance.

A breakdown of replica symmetry occurs when a divergence occurs in the spin glass susceptibility $\chi_{SG}$, which is defined as follows. If we change the field on site $i$ by a small amount $\delta h_i$ then the expectation value of $\sigma_j^z$ changes by an amount
\[
 \delta \langle \sigma_j^z \rangle = \chi_{ij} \delta h_i ,
\]
where the susceptibility $\chi_{ij}$ is given, according to linear response theory, by
\[
 \chi_{ij} = \int_0^\beta d\tau [ \langle \sigma_j^z(\tau)\sigma_i^z(0) \rangle - \langle \sigma_j^z \rangle \langle \sigma_i^z \rangle ] ,
\]
where we note that single-spin expectation values are independent of $\tau$. The spin glass susceptibility is then given by
\[
 \chi_{SG} = \frac{1}{N} \sum_{i,j=1}^N [\chi_{ij}]_{av} .
\]
Equivalently, $\chi_{SG}$ gives the change in the spin glass order parameter $q$ when the variance of the random longitudinal field is change by an amount $\Delta$ according to
\[
 \delta q = \chi_{SG} \Delta ,
\]
which demonstrates that $\chi_{SG}$ is the order parameter susceptibility for spin glasses and the symmetry breaking field is the variance of the local longitudinal fields.

The expression for $\chi_{SG}$ in terms of the parameters in the effective one-dimensional model is given in Ref. [28]. One finds
\[
 \chi_{SG} = \frac{\chi_{SG}^0}{1 - J^2 \chi_{SG}^0} ,
\]
where
\[
 \chi_{SG}^0 = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dz e^{-z^2/2} \left[ \sum_{l} \Delta \tau \left( \langle S_{l_0} S_{l_0+l} \rangle_{\mathbf{M}} - \langle S_{l_0} \rangle_{\mathbf{M}}^2 \right) \right] .
\]
The denominator in Eq. (13) is the “replicon” eigenvalue \( \lambda_r \) first calculated by AT [11] for the classical case.

It is straightforward to generalize these results to the case where we include the Gaussian random longitudinal field of standard deviation \( h \) in Eq. (1). From Eq. (4) we see that \( \mathcal{H} \) already has a term with a Gaussian random field of standard deviation \( (\Delta J)^2 / 2 \), so it is sufficient to add another random field of standard deviation \( \Delta \tau h \). These two random fields can be combined into a single random field of standard deviation \( \Delta \tau (J^2 q + h^2)^{1/2} \) and so \( \mathcal{H}(z) \) in Eq. (1) becomes

\[
\mathcal{H}(z) = - (\Delta \tau J)^2 \sum_{\langle l_1, l_2 \rangle} \{ r(|l_1 - l_2|) - q \} S_{l_1} S_{l_2} - K^\tau \sum_l S_l S_{l+1} - \Delta \tau [J^2 q + h^2]^{1/2} z \sum_l S_l. \tag{15}
\]

III. NUMERICAL RESULTS

FIG. 2: The phase diagram in the \( h^T - T \) plane, determined from the vanishing of the denominator of Eq. (13) where \( \chi^0_{SG} \) is given by Eq. (17). The phases are spin glass (SG) and paramagnet (P).

In this section we shall mainly set \( J = 1 \).

First we shall consider the case of no longitudinal field and zero spin glass order parameter \( q \) so we set \( q = 0 \) in Eq. (11). In addition, the expectation value in Eq. (11) does not depend on \( z \), so the \( z \) integral trivially decouples and gives one, and hence

\[
r(\Delta l) = \langle S_{l_0} S_{l_0+\Delta l} \rangle. \tag{16}
\]

Furthermore \( \langle S(0) \rangle \) in Eq. (14) vanishes so

\[
\chi^0_{SG} = \left[ \Delta \tau \sum_l \langle S_{l_0} S_{l_0+l} \rangle \mathcal{H} \right]^2, \tag{17}
\]

and we recall from Eq. (13) that the critical point is when \( J^2 \chi^0_{SG} = 1 \).

We perform standard Metropolis, single spin-flip Monte Carlo on a one-dimensional chain of \( M \) sites with periodic boundary conditions with long-range interactions as specified in Eq. (4) (with \( q = 0 \) for now). In addition to the value of \( M \) we also need to specify the time-slice width \( \Delta \tau \). We have to determine self-consistently the \( M/2 \) parameters \( r(\Delta l) \) where \( \Delta l = 1, 2, \ldots, M/2 \). We start by making a guess for the \( r(\Delta l) \) and then run a high-precision Monte Carlo simulation for these parameters to get the expectation values \( \langle S_l S_{l+\Delta l} \rangle \). Following Eq. (16) these values are used for the next estimate of \( r(\Delta l) \) and we iterate until convergence. We did two hundred iterations, except for the small values of \( M \) where one hundred iterations were performed, and verified that estimates of \( \chi_{SG} \) had converged at a much smaller number of iterations. We averaged over the last quarter of the iterations and performed eight runs to estimate error bars and improve statistics. For \( M \leq 24 \) we were able to use exact enumeration as well as Monte Carlo, which has

FIG. 3: The triangles show results for \( \chi_{SG} \) from our calculations extrapolated to \( \Delta \tau = 0 \) at very low temperature \((T/J = 0.1)\) in the paramagnetic phase. The horizontal axis is \((J/h^T)^2\). On the vertical axis we multiply \( \chi_{SG} \) by \((h^T)^2\) because, for \( h^T \to \infty \), perturbation theory gives \( \chi_{SG} = 1/(h^T)^2 \). The spin glass susceptibility diverges at \( h^T_c/J \simeq 1.51 \) as we shall see later, and this is indicated by the dashed vertical line. For the range of data shown there is a gap in the spectrum so our results converge rapidly as \( T \to 0 \) and we find that \( T/J \simeq 0.1 \) is low enough that the results are almost indistinguishable from those at \( T = 0 \). The line is the result of a 14-term series expansion in powers of \((J/h^T)^2\), evaluated for \( T \) strictly equal to 0. The agreement is excellent until the critical point is approached where (a) we need to be more careful in extrapolating our results to \( T = 0 \) as we shall see later, and (b) the solid line is the “raw” series from Ref. 29 so it does not show a divergence at \( h^T_c \).
the advantage of there being no statistical errors. The exact enumeration results served as a useful check on the Monte Carlo code.

The phase boundary in the $h^T-T$ plane is where the denominator in Eq. (14) vanishes and our results for this are shown in Fig. 2. In the limit of $T \to 0$ we find the critical value of $h^T$ to be

$$h_c^T = 1.51 \pm 0.01 \tag{18}$$

in agreement with earlier work of Yamamoto and Ishii 15 who obtained $h_c^T = 1.506$ from a perturbation expansion. We will discuss the error bar quoted in Eq. (18) in the context of Fig. 4 below.

As a check on our calculations we compare our results in the low temperature limit in the paramagnetic phase with a recent series expansion 20. The leading correction due to a finite value of $\Delta \tau$ in Quantum Monte Carlo simulations varies as $10^{-\Delta \tau}$ (19) (\Delta \tau)^2$, so we extrapolated our results for several values of $\Delta \tau$, to $\Delta \tau = 0$ by doing a linear fit in $(\Delta \tau)^2$. Our results at $T = 0.1$ extrapolated to $\Delta \tau = 0$, are in excellent agreement with the series results as shown in Fig. 3.

To investigate the stability of the RS solution we have to work out this solution in the spin glass phase shown in Fig. 2. Even with no external longitudinal field, the presence of a non-zero spin glass order parameter $q$ requires us to do the $z$ integral in Eqs. (7), (8) and (13), as well as determine $q$ self-consistently. This is in addition to the self-consistent determination of $r(\Delta l)$ which we had before in the paramagnetic phase. Doing the $z$ integral is, in general, quite challenging so we will only get results for small $q$ which means we stay close to the phase boundary in Fig. 2 (and eventually apply only a small longitudinal field).

We perform the $z$-integrals by Gauss-Hermite integration 31 according to the following formula

$$\int_{-\infty}^{\infty} e^{-x^2} f(x) dx = \sum_{j=1}^{L} w_j f(x_j) \tag{19}$$

where the weights $w_j$ and abscissas $x_j$ are tabulated and can also be evaluated from scratch 31. (We used tables available on the internet.) Since the integrands are even functions of $z$ we only need to take positive values of $x_j$. To check for convergence we did calculations with 3, 6, 12 and 24 positive values.

In all cases we found that $\chi_{SG}$ went negative on crossing the phase boundary, indicating that RSB occurs everywhere in the spin glass phase in Fig. 2. We present here only our results at low $T$, where there has been the greatest controversy 16, 18–22, as mentioned above.

FIG. 4: The spin glass order parameter $q$ near the quantum critical point at $T = 0, h^T = h_c^T$. The linear behavior shows that the order parameter exponent $\beta$ has the value $\beta = 1$ in agreement with analytic work 20.

FIG. 5: A plot of $1/\chi_{SG}$, the inverse of the spin glass susceptibility, near the quantum critical point (QCP) at $T = 0, h_c^T \approx 1.51$. One sees that $1/\chi_{SG}$ tends to zero as the QCP is approached from above. Below the QCP the spin glass order parameter becomes non-zero as shown in Fig. 4. Nonetheless, $\chi_{SG}$ is negative for $h^T < h_c^T$. However this is impossible since $\chi_{SG}$ is a positive quantity, and hence the assumption of replica symmetry, made in the calculation, must be wrong.

Firstly we show our results for the spin glass order parameter $q$ near the quantum critical point at $T = 0, h^T = h_c^T$. It clearly vanishes linearly showing that the order parameter exponent $\beta$, defined by $q \propto (h^T - h_c^T)^{\beta}$, has the value

$$\beta = 1 \tag{20}$$

in agreement with analytic work 20. Note that there is no finite-size rounding in this approach since the ef-
effective one-dimensional model we simulate is a representation of the original SK model in the thermodynamic limit. There are clearly small corrections coming from the temperature $T$ and the time slice width $\Delta \tau$ being not precisely zero. Based on the scatter of the data in Fig. 6 we estimate the value of $h^*_T$ to be $1.51 \pm 0.01$, as indicated in Eq. (18).

To investigate the stability of the RS solution (which has been assumed in our calculations) we compute $\chi_{SG}$ in the quantum spin glass phase and show results for this quantity near the quantum critical point (QCP) in Fig. 7. One sees that the computed $\chi_{SG}$ is negative for $h^T < h^*_T$ with very little dependence in this region on the precise values of $\Delta \tau$ and $T$. However $\chi_{SG}$ cannot really be negative so the assumption of replica symmetry, made in deriving the expression for $\chi_{SG}$, must be false. We conclude that replica symmetry must be broken in the quantum spin glass phase even down to $T = 0$.

In the original calculation of AT [11] for the classical spin glass, the negative eigenvalue (the denominator in Eq. (13) which is essentially $1/\chi_{SG}$ near the instability) varies quadratically in the unstable region near the classical critical point. From the data in Fig. 7 it is plausible that the same quadratic variation occurs near the QCP for $h^T < h^*_T$, though we cannot determine the power with much accuracy, mainly because of the uncertainty in the precise value of $h^*_T$.

According to analytical work [25, 26] the spin glass susceptibility should vary as

$$\chi_{SG} \propto \left( \frac{\ln |\delta h^T|}{\delta h^T} \right)^{1/2}, \quad (21)$$

approaching the quantum critical point from the paramagnetic phase, where $\delta h^T = h^T - h^*_T$. Our numerical data fits this very well as shown in Fig. 8.
FIG. 9: A speculative phase diagram for two dimensions. There is no spin glass phase at finite-T but there is quantum spin glass phase at T = 0 up to $h_c^T$, the critical value of $h^T$, so there might possibly be a QuAT line in the $h$-$h^T$ plane at $T = 0$. While perhaps unlikely, one can not rule out this scenario at present.

Including a longitudinal field $h$ we mapped out $1/\chi_{SG}$ against $h$ for different values of $h^T$ at low $T$, see Fig. 8 for an example. We then determined where $1/\chi_{SG} = 0$ for different values of $h_T$ near $h_c^T$ and so were able map out the $T = 0$ QuAT line near the vicinity of the QCP. The results, which are shown in Fig. 8, are largely independent of the values of $T$ and $\Delta T$ shown. The AT line for the classical spin glass has the form $\delta T \propto h^{2/\phi}$ with $\phi = 3$. In the quantum case, writing $\delta h^T \propto h^{2/\phi}$, the data in Fig. 8 indicates that $\phi > 2$ but the precision of the numerics does not allow us to determine the exponent precisely. We note that Ref. [20] finds analytically that same exponent $\phi = 3$ occurs everywhere including $T = 0$.

Finally we note the possibility of a QuAT line even in two dimensions where there is no spin glass phase at finite temperature, see Fig. 9.

IV. CONCLUSIONS

We have shown that the replica symmetric solution of the quantum Sherrington-Kirkpatrick model is unstable everywhere below a surface in the $h$-$h^T$-$T$ parameter space sketched in Fig. 4 in agreement with Refs. [18–20]. We suspect that the contrary results obtained numerically in Refs. [16, 21, 22] is due to inadequate treatment of finite-size effects. In particular, their claim that there is a finite-temperature multi-critical point is probably a mis-interpretation of crossover effects from the zero-temperature quantum critical point. The replica symmetric region found in Ref. [23] is presumably due to the inadequacies of the static approximation used in that paper. We also note that Yao et al. [32], who have performed experiments on a realization of the quantum SK model with sizes $N \leq 16$, find a fast “scrambling” once the spins freeze, which seems to contradict our claim that replica symmetry is broken everywhere in the spin glass phase. However, the sizes in the experiments are very small and may not reflect the behavior in the thermodynamic limit.

In the method adopted here, the thermodynamic limit is taken from the start. In each of the three axis planes there is a line of transitions where replica symmetry is broken. In the $h$-$T$ plane this is the familiar de Almeida-Thouless (AT) line. The phase boundary in the $h^T$-$T$ plane is plotted accurately in Fig. 3. We call the line of transitions in the $h$-$h^T$ plane the quantum de Almeida-Thouless (QuAT) line. If the QuAT line also occurs in systems with short range interactions it may affect the performance of quantum annealers [3] when solving spin glass problems in the presence of a bias (i.e. magnetic field).

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One could also add disorder to the transverse field. We are not aware that this has been studied in detail, but expect that adding some additional disorder to an already strongly disordered Hamiltonian would not change the physics.

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In the classical limit, Eq. (11) gives

\[ \chi_{SG} = \frac{1}{T^2} \frac{1}{N} \sum_{i,j=1}^{N} \left[ \langle \sigma_i^z \sigma_j^z \rangle - \langle \sigma_i^z \rangle \langle \sigma_j^z \rangle \right]^2 \]

It is usual, in classical spin glasses, to omit the factor of $1/T^2$ since it varies smoothly in the vicinity of the finite-$T$ transition, but here we are interested in the behavior of transitions as $T \to 0$, so it is essential to include it.

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