Simple Glass Models and Their Quantum Annealing

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We study first-order quantum phase transitions in mean-field spin glasses. We solve the quantum random energy model using elementary methods and show that at the transition the eigenstate suddenly projects onto the unperturbed ground state and that the gap between the lowest states is exponentially small in the system size. We argue that this is a generic feature of all ''random first-order'' models, which includes benchmarks such as random satisfiability. We introduce a two-time instanton to calculate this gap in general, and discuss the consequences for quantum annealing.

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Solving hard combinatorial problems by temperature annealing is a classic strategy in computer science [1]. A major question is whether annealing a *quantum mechanical* kinetic term [2,3] or a transverse magnetic field Γ can be an efficient strategy. Experimentally this question was studied in an Ising spin glass (SG) [4], an archetype for difficult systems in physics. A quantum first-order transition was observed at very low temperatures, as had been previously found in model systems [5,6]. Here we address several open questions: What is the underlying behavior of the wave functions at the quantum SG transition? Is quantum annealing efficient in solving these difficult optimization problems? We thus first solve a simple quantum version of a SG model, the random energy model (REM) [7]. Despite its simplicity, it reproduces many properties of mean-field glasses [7] and allows one to model the behavior of a wide variety of phenomena such as the ''ideal'' glass transition [8] and random heteropolymer folding [9]. The REM also captures aspects of the phenomenology of random satisfiability [10] and is closely related to the random code ensemble in coding theory [11]. All these problems belong to the so-called ''random first-order'' (RFO), or ''one-step replica symmetry breaking,'' class. To show that in all of these systems the minimal spectral gap Δ between the ground and first excited states is exponentially small in size, we set up an instanton calculation that allows one to compute the gap. The minimal spectral gap in turn yields a lower bound $\tau \propto \Delta^{-2}$ [2] on the time needed to find the ground state.

Quantum SGs have been investigated over the past 30 years [12] using an elaborate mathematical formalism combining the replica [13] and the Suzuki-Trotter methods [5,14] in order to introduce disorder and quantum mechanics. The quantum transition has been found to be first order at low temperature for all RFO models [5,6,14]. We show here first that the quantum version of the random energy model (QREM) can be solved analytically using only basic tools of perturbation theory, a derivation whose simplicity provides a detailed understanding of the quantum glass transition. The minimal gap Δ is found to be exponentially small in N. Next, we show that this result holds for all RFO models, making quantum annealing an exponentially slow algorithm in those cases.

QREM model.—Consider N Pauli spins σ in a transverse field Γ with the Hamiltonian:

$$\mathcal{H}(\{\sigma\}) = E(\{\sigma^z\}) + \Gamma \sum_{i=1}^{N} \sigma_i^x = \mathcal{H}_0 + \Gamma V,$$

where $E(\{\sigma^z\})$ is a function that takes 2^N different values for the 2^N configurations of the N spins. These values are taken randomly from a Gaussian distribution of zero mean and variance $N/2$, as in the REM [7]. A concrete implementation is $E(\{\sigma^z\}) = \lim_{p\to\infty} \sum_{i_1,\ldots,i_p} J_{i_1,\ldots,i_p} \sigma_{i_1}^z \cdots \sigma_{i_p}^z$, where the $J_{i_1,\ldots,i_p}$ are random Gaussian variables. In the σ^z representation $\mathcal{H}$ is a $2^N \times 2^N$ matrix whose diagonal entries are the 2^N classical energies. The matrix elements of $\mathcal{H}_0^{\alpha\alpha} = E_\alpha^{\mathrm{REM}}$ and $\mathcal{H}_0^{\alpha\neq\beta} = 0$, while $V_{\alpha\beta} = 1$ if α and β are two configurations that differ by a single spin flip and zero otherwise. $\mathcal{H}$ is sparse and can be studied numerically rather efficiently even for large matrix sizes using Arnoldi and Ritz methods [15].

Two easy limits.—The model is trivially solved in the limit $\Gamma \to 0$ and $\Gamma \to \infty$. For $\Gamma = 0$, we recover the classical REM with N Ising spins and 2^N configurations, each corresponding to an energy level E_α [7]: Call $n(E)$ the number of energy levels belonging to the interval $(E, E + dE)$; its average over all realizations is easily computed: $\overline{n(E)} = 2^N P(E) \propto e^{N(\ln 2 - E^2/N^2)} = e^{Ns(E/N)}$, where $s(e) = \ln 2 - e^2$ (with $e = E/N$). There is therefore a critical energy density $e_0 = -\sqrt{\ln 2}$ such that, if $e < e_0$, then with high probability there are no configurations, while if $e > e_0$ the entropy density is finite. A transition between these two regimes arises at $\frac{1}{T_c} = \frac{ds(e)}{de}|_{e_0} = 2\sqrt{\ln 2}$ and the thermodynamic behavior follows: (i) For $T < T_c$, $f_{\mathrm{REM}} = -\sqrt{\ln 2}$ and the system is frozen in its lowest energy states. Only a finite number of levels (and only the ground state at $T = 0$) contribute to the partition sum. The energy gap

between them is finite. (ii) For $T > T_c$, $f_{\rm REM} = -\frac{1}{4T} - T\ln 2$; exponentially many configurations contribute to the partition sum.

In the opposite case of very large values of Γ, the REM contribution to the energy can be neglected. In the σ^x basis, we find N independent classical spins in a field Γ; the entropy density is just given by the log of a binomial distribution between $-\Gamma N$ and $+\Gamma N$ and the free-energy density is $f_{\rm para} = -T\ln 2 - T\ln(\cosh\Gamma/T)$.

Perturbation theory.—What happens between these two extreme cases? The perhaps surprising answer for the thermodynamics is *nothing*. At low value of Γ, the free-energy density is that of the classical REM, while for larger values it jumps to the quantum paramagnetic (QP) value $f_{\rm QP}$; a first-order transition separates the two different behaviors at the value Γ such that $f_{\rm REM} = f_{\rm QP}$ (see center panel of Fig. 1). This can be easily understood using Rayleigh-Schrödinger perturbation theory [16,17]. Consider the set of eigenvalues E_k and eigenvectors $|k\rangle$ of the unperturbed REM, when $\Gamma = 0$. The series for a given perturbed eigenvalue $E_i(\Gamma)$ reads

$$E_i(\Gamma) = E_i + \langle i|\sum_{n=0}^{\infty}\Gamma V\left[\frac{Q}{E_i - \mathcal{H}_0}(E_i - E_i(\Gamma) + \Gamma V)\right]^n|i\rangle,$$

where the projector $Q = \sum_{k\neq i}|k\rangle\langle k|$ so that

$$E_i(\Gamma) = E_i + \Gamma V_{ii} + \sum_{k\neq i}\frac{\Gamma^2 V_{ik}V_{ki}}{E_i - E_k} + \cdots. \qquad (1)$$

Since $V_{ij} \neq 0$ if and only if i and j are two configurations that differ by a single spin flip, odd order terms do not contribute in Eq. (1) as one requires an even number of flips to come back to the initial configuration in the sums. Noting that $\sum_{k\neq n}|V_{nk}|^2$ reduces to a sum over the N levels connected to E_i by a single spin flip, one obtains, starting from an *extensive eigenvalue* [$E_i = O(N)$], that

$$\sum_{k\neq i}\frac{V_{ik}^2}{E_i - E_k} = \frac{1}{E_i}\sum_{k=1}^{N}\left(1 + \frac{E_k}{E_i} + \cdots\right) = \frac{N}{E_i} + O\left(\frac{1}{N}\right),$$

where we have used that the E_k are random and typically of order $\sqrt{N}$. Higher nth orders are computed in the same spirit and are found to be $O(N^{n/2-1})$. Therefore, to all (finite) orders, we have

$$E_i(\Gamma) = E_i + \frac{N\Gamma^2}{E_i} + O\left(\frac{1}{N}\right). \qquad (2)$$

This analytic result compares well with a numerical evaluation of the eigenvalues (left panel of Fig. 1). Note that the energy density of all extensive levels is independent of Γ to leading order in N as are hence $s(e)$ and $f(T)$.

The expansion can also be performed using ΓV as a starting point and $\mathcal{H}_0$ as a perturbation. Consider the ground state with eigenvalue $E_0(\Gamma)$ and the unperturbed ground state with $E_0^V(\Gamma) = -\Gamma N$. In the base corresponding to the eigenvalues of ΓV, we find

$$E_0(\Gamma) = E_0^V(\Gamma) + \langle 0|\mathcal{H}_0|0\rangle + \sum_{k\neq 0}\frac{|\langle k|\mathcal{H}_0|0\rangle|^2}{E_0^V(\Gamma) - E_k^V(\Gamma)} + \cdots.$$

The first-order term gives $\sum_{\alpha=1}^{2^N} E_\alpha^{\rm REM}|v_\alpha|^2$. Since the energies of the REM are random and uncorrelated with v_α this sums to $O(\sqrt{N}2^{-N/2})$. For the second-order term, one finds

$$\sum_{k\neq 0}\frac{|\langle k\,|\,\mathcal{H}_0\,|\,0\rangle|^2}{E_0^V(\Gamma) - E_k^V(\Gamma)} = \frac{1}{E_0^V(\Gamma)}\sum_{k\neq 0}\frac{|\langle k\,|\,\mathcal{H}_0\,|\,0\rangle|^2}{1 - E_k^V(\Gamma)/E_0^V(\Gamma)}$$
$$\approx \frac{1}{E_0^V(\Gamma)}\langle 0\,|\,\mathcal{H}_0^2\,|\,0\rangle$$
$$= \frac{N}{2E_0^V(\Gamma)} + o(1). \qquad (3)$$

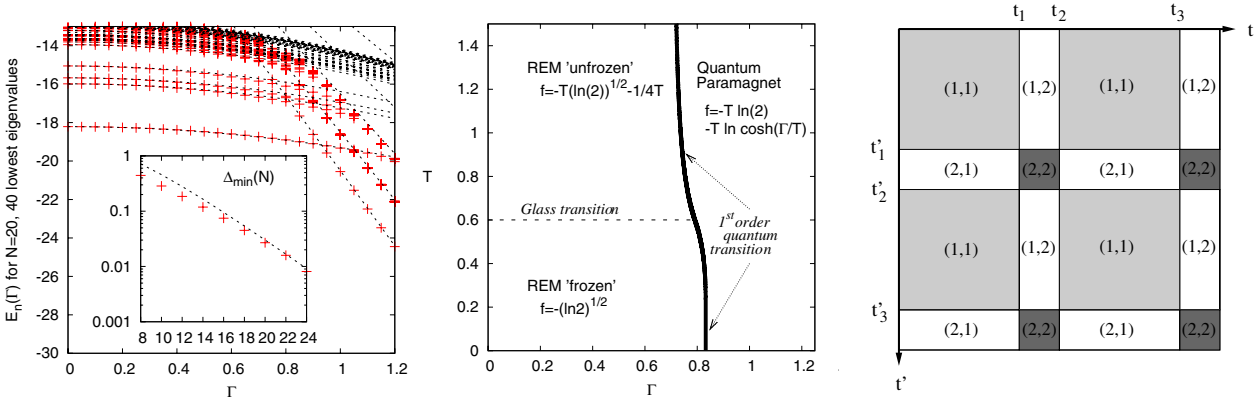

FIG. 1 (color online). Left: Evolution of lowest energy levels for a single realization of the QREM with $N = 20$ spins (dots) compared with analytical predictions (lines). Inset: Evolution of the ensemble averaged minimal gap at the transition. Center: Phase diagram of the QREM in temperature T and transverse field Γ. At $T = 0$ the quantum transition arises at $\Gamma_c = \sqrt{\ln 2}$ while the classical glass transition for $\Gamma = 0$ is at $T_c = \sqrt{\ln 2}/2$. Right: A multi-instanton configuration for the two-times overlap $q_{t,t'}$ and the two-time Lagrange multipliers $\tilde{q}_{t,t'}$. Far from the jump times, the functions $q_{t,t'}$ and $\tilde{q}_{t,t'}$ take the same form as those computed at those times for the glass phase [the regions (1, 1)], for the quantum paramagnet [in the regions (2, 2)], and are zero in the mixed regions (1, 2)-(2, 1). In the large p limit the problem can be solved completely using the so-called "static approximation" [5,14] within the (1, 1) regions, and, in addition, the fact that $\tilde{q}_{t,t'}^d$ and $\tilde{q}_{t,t'}$ become either infinity or zero, with sharp interfaces.

Subsequent terms are treated similarly and give vanishing corrections so that $E_0(\Gamma) = -N\Gamma - \frac{1}{2\Gamma} + o(1)$. Again this derivation holds for other states with extensive energies $E_i^V(\Gamma)$, the only tricky point being the degeneracy of the eigenvalues [18], and for these excited eigenstates, the perturbation starting from the large Γ phase yields $E_i(\Gamma) = E_i^V(\Gamma) - \frac{1}{2\Gamma} + o(1)$. Again, to leading order in N, energy, entropy, and free-energy densities are not modified by the perturbation.

Quantum transition.—This derivation sheds new light on the physics of the transition: The wave function in the QP phase is delocalized over the classical configurations in the σ^z base. The first-order transition amounts to a sudden localization of the wave function into an exponential number of classical states for $T > T_c$ and a finite number of frozen states for $T < T_c$ (and to the ground state at $T = 0$).

Focusing on $T = 0$ and on the avoided level crossing near the transition, we compute the gap $\Delta(N)$ as follows: Consider a value of Γ such that *for that sample* the SG ground state and the quantum paramagnet are degenerate. We lift the degeneracy by diagonalizing $\mathcal{H}$ in the corresponding two-dimensional space

$$\mathcal{H}\,|\phi\rangle = [E_0|\mathrm{SG}\rangle\langle\mathrm{SG}| - \Gamma N|\mathrm{QP}\rangle\langle\mathrm{QP}|]|\phi\rangle = \lambda|\phi\rangle. \quad (4)$$

The gap is given by the difference of the eigenvalues, so that

$$\Delta(N,\Gamma)^2 = (N\Gamma - E_0)^2 - 4[-E_0 N\Gamma + E_0 N\Gamma\langle\mathrm{SG}|\mathrm{QP}\rangle^2]$$

and at the transition when $\Gamma = -\sqrt{\ln 2} = E_0/N$, it yields

$$\Delta_{\min}(N) = 2|E_0|2^{-N/2}, \quad (5)$$

where we have used the fact that $\langle\mathrm{SG}|\mathrm{QP}\rangle = 2^{-N/2}$. This agrees well with numerics, even for small values of N (see left panel of Fig. 1). Similar results are known for number partitioning [19].

Generic case and instanton.—A first-order quantum transition being a generic feature in all RFO models, we expect these arguments to hold *qualitatively* in all such models, so that the gap closes exponentially with N, much in the same way that a *thermal* mean-field first-order transition implies an exponential activation time and metastability. Indeed, quantum annealing works by *tunneling* between quantum states, but in first-order transitions these states are usually "far" from each other. In order to *quantitatively* compute the gap, perturbation theory is of no use in the generic case and one has to resort to instantonic computations [20]. We now discuss how this can be done in disordered systems using the replica method. To introduce the instanton, we use the expansion of the evolution operator and, denoting $\varepsilon = \langle\mathrm{QP}|H|\mathrm{SG}\rangle$, write

$$\mathrm{Tr}\, e^{-\beta H} = \sum_{k\ \mathrm{even}} \frac{1}{k!} \int dt_1 \ldots dt_k e^{-[t_{\mathrm{tot}}^{\mathrm{SG}} H_{\mathrm{SG}} + t_{\mathrm{tot}}^{\mathrm{QP}} H_{\mathrm{QP}}]} \varepsilon^k, \quad (6)$$

where the system jumps at $t_1, \ldots, t_k$ between the states $|\mathrm{SG}\rangle$ and $|\mathrm{QP}\rangle$, $t_{\mathrm{tot}}^{\mathrm{SG}}$ and $t_{\mathrm{tot}}^{\mathrm{QP}}$ is the total time spent in each. Following the standard strategy [5,6,14], the trace is computed via the Suzuki-Trotter and the replica trick. One obtains an effective replicated free energy as a function of the overlaps $q_{t,t'}^{\mu\nu}$ between the replicas at two (imaginary) times and some corresponding Lagrange multipliers $\tilde{q}_{t,t'}^{\mu\nu}$, for which a particular ansatz must be proposed [5,6]. Equation (6) tells us that if we find a solution that interpolates between $|\mathrm{SG}\rangle$ and $|\mathrm{QP}\rangle$ by jumping k times $t_1, \ldots, t_k$ and yields $\ln \mathrm{Tr}[e^{-\beta H}] \sim -t_{\mathrm{tot}}^{\mathrm{SG}} F_{\mathrm{SG}} - t_{\mathrm{tot}}^{\mathrm{QP}} F_{\mathrm{QP}} - kG$, then by simple comparison $\ln\varepsilon \sim G$ leads to $\Delta \sim e^G$: An extensive value of G implies an exponentially small gap and the value of G is thus proportional to the free-energy cost of an interface in a two-time plane. For disordered systems, the computation can be performed by using a special two-time instanton ansatz as shown in the right panel of Fig. 1. We now refer to the presentation and notation of [14]. We calculate the free energy per spin $f = F/N$ of the replicated systems in the $N \to \infty$ limit by the saddle point method. In the one-step replica symmetry ansatz, we divide replicas μ in n/m sets of size m: we denote the parameters $q_{tt'}^{\mu\nu}$ as (i) $q_{tt'}^d$ if $\mu = \nu$ [21], (ii) $q_{tt'}$ if $\mu \neq \nu$ but belong to the same block and zero otherwise. This corresponds to the SG and the QP that have been widely studied [5,6,14]:

$$-\beta f = \int dt dt' \Big\{ -\frac{\beta^2 J^2}{4}(1-m) q_{tt'}^p + \frac{(1-m)}{2} \tilde{q}_{tt'} q_{tt'} + \frac{\beta^2 J^2}{4} [q_{tt'}^d]^p - \tilde{q}_{tt'}^d q_{tt'}^d \Big\} - W_0. \quad (7)$$

An expression for W_0 is given below. We consider a solution corresponding to the low-Γ phase in the interval $(0, t_1)$, (t_2, t_3) that jumps to the high-Γ phase in the intervals (t_1, t_2), (t_4, t_5), and so on.

As a proof of principle, let us rederive the large-p case. The saddle point equations imply that for large p either $(q_{tt'}, q_{tt'}^d, \tilde{q}_{tt'}, \tilde{q}_{tt'}^d) = (1, 1, \infty, \infty)$ or $(q_{tt'}, q_{tt'}^d, \tilde{q}_{tt'}, \tilde{q}_{tt'}^d) = (<1, <1, 0, 0)$. This implies that the form of the instanton configuration of $\tilde{q}_{tt'}^d$ and $\tilde{q}_{tt'}$ is the same as the one of $q_{tt'}$ and $q_{tt'}^d$ but with the values jumping from 0 to ∞. In addition we make the "*static approximation*" that assumes that inside each time interval the parameters q^d and $\tilde{q}^d$ are constant. We conclude that we can write

$$2\tilde{q}_{t't'}^d - \tilde{q}_{t't'} = r_t^d r_{t'}^d, \qquad \tilde{q}_{t't'} = r_t r_{t'}, \quad (8)$$

where r_t and r_t^d are large in the time intervals when the system is in the SG state, and drop to zero when it is not. (The solutions in the literature correspond to a time-independent value of r: large for the glass and small for the QP phase, respectively). Because $q_{t't'}^d$, $q_{t't'}$ are either zero or one, we have

$$\int dt dt' q_{tt'} \tilde{q}_{tt'} \sim \int dt dt' \tilde{q}_{tt'} = I^2$$
$$2\int dt dt' \tilde{q}_{tt'}^d q_{tt'}^d = 2\int dt dt' \tilde{q}_{tt'}^d = I_d^2 + I^2, \quad (9)$$

with the definitions $I \equiv \int dt r(t)$ and $I_d \equiv \int dt r^d(t)$. We further decouple the replicas in the single-spin term in the usual way [5]:

$$W_0 = \ln \mathrm{Tr} \exp(-H_{\mathrm{eff}}) = -\frac{1}{m} \ln \left\{ \int Dz_2 \left[\int Dz_3 \, \mathrm{Tr} \left(\mathcal{T} e^{\int dt' (A(t') \sigma^z + \beta\Gamma \sigma^x)} \right) \right]^m \right\}, \tag{10}$$

where $\mathcal{T}$ denotes time order (a necessity here because of the time dependence in the exponent), and $A(t) \equiv (z_3 r_t^d + z_2 r_t)$. At low temperatures, the "field" in the x direction $\beta\Gamma$ is strong, while the field in the z direction $|A(t)|$ is either zero or $|A(t)| \gg \beta\Gamma$. The single quantum spin then switches from being completely polarized along $|z\rangle$ and along $|x\rangle$, in the periods in which $A \neq 0$ and $A = 0$, respectively. The trace in (10) can then be calculated by switching the single-spin basis from $|x\rangle$ to $|z\rangle$. Denoting $t^{\mathrm{SG}} = \Theta\beta$ the time when $q_t = q_t^d = 1$, and $t^{\mathrm{QP}} = (1 - \Theta)\beta$ the rest, the action becomes

$$-\beta f = \Theta^2 \left\{ -\frac{\beta^2 J^2}{4} (1 - m) + \frac{\beta^2 J^2}{4} \right\} - \frac{1}{2} I_d^2 - \frac{m}{2} I^2 W_z + (1 - \Theta)\beta\Gamma + (\text{number of jumps}) \times \ln |\langle x | z \rangle|, \tag{11}$$

where the terms $|\langle x|z\rangle|$ come from a change of basis, and

$$W_z = -\frac{1}{m} \ln \left\{ \int Dz_2 \left[\int Dz_3 e^{|z_2 I + z_3 I_d|} \right]^m \right\}.$$

This can be evaluated by the saddle point [5,14], a short calculation yields $W_z \sim \frac{1}{2} I_d^2 + \frac{m}{2} I^2 + \ln 2$. Taking a further saddle point with respect to m gives $m = \frac{2\sqrt{2}}{\Theta\beta J}$ and thus

$$-\beta f = \Theta \sqrt{\ln 2} \frac{\beta J}{2} + (1 - \Theta)\beta\Gamma + k \ln |\langle x | z \rangle|. \tag{12}$$

This is exactly the contribution to $\mathrm{Tr}[e^{-\beta H}]$ of the process with k jumps spending a fraction Θ in the glass state and $(1 - \Theta)$ in the paramagnetic state. We finally have $G = N \ln |\langle x|z\rangle| = -N \ln(2)/2$ and we recover Eq. (5).

In a generic problem with a first-order transition, one has to extremize the free energy (7) and from there compute the gap as a free-energy cost of an interface that is generally nonzero.

Conclusion.—Starting from the quantum random energy model, we have discussed the quantum glass transition. The gap is exponentially small at the transition. We introduce a method that allows us to show that this result holds for all models of the random first-order kind; presumably including benchmark problems such as random satisfiability. Our results imply that quantum annealing is exponentially slow at finding the ground state of these random NP-hard (nondeterministic-polynomial-time-hard) problems. Although this seems to contradict recent numerical results [22], the problems considered there were *not* randomly chosen from a flat distribution and are therefore different from what has been considered in the present study and in the computer science literature of random constraint satisfaction problems.

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