A solvable model of quantum random optimization problems

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We study the quantum version of a simplified model of optimization problems, where quantum fluctuations are introduced by a transverse field acting on the qubits. We find a complex low-energy spectrum of the quantum Hamiltonian, characterized by an abrupt condensation transition and a continuum of level crossings as a function of the transverse field. We expect this complex structure to have deep consequences on the behavior of quantum algorithms attempting to find solutions to these problems.

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A large part of theoretical research in quantum computing has been devoted to the development of algorithms that could use quantum properties to perform computational tasks faster than classical devices. A typical problem that is encountered in almost all branches of science is that of optimizing irregularly shaped cost functions $H_P$: two standard examples are $k$-SAT, $H_P$ counting the number of unsatisfied constraints on $k$ boolean variables, and the coloring of a graph with $q$ colors ($q$-COL), $H_P$ then being the number of monochromatic edges. The decision version (whether a solution, i.e. a configuration with $H_P = 0$, exists) of both problems belongs to the class of NP-complete problems. One is mostly interested in the scaling of the difficulty of these problems when the number $N$ of variables involved becomes large. Besides the formal computational complexity theory which classifies the difficulty of problems according to a worst-case criterion, their typical case complexity is often studied through random ensemble of instances, for instance assuming a flat distribution over the choice of $M = \alpha N$ constraints on $N$ variables.

Statistical mechanics tools have provided a very detailed and intricate picture of the configuration space of such typical problem Hamiltonians $H_P$ [1]. A key concept that emerged in this context is that of clustering of solutions. The topology of the space of solutions changes abruptly upon increasing the density of constraints $\alpha$ in the following way: i) at a first threshold $\alpha_q$ it goes from a single connected cluster to a set of essentially disjoint clusters; ii) the number of clusters itself undergoes a transition at $\alpha_c > \alpha_q$ from a phase where it is exponential in $N$, thus defining an entropy of clusters (the complexity), to a phase where the vast majority of solutions are contained in a finite number of clusters; iii) finally, the total entropy of solutions vanishes at $\alpha_c > \alpha_q$, where the problem does not admit a solution anymore (the ground state energy becomes positive). This sequence of transitions (sketched in Fig. 1) has a deep impact on the performances of most classical optimization algorithms, that slow down dramatically deep in the clustered phase.

To solve the optimization problem $H_P$ with a quantum computer, one can choose its Hamiltonian to be

$$H = H_P + \Gamma H_Q,$$

where $H_Q$ does not commute with $H_P$ and induces quantum fluctuations. One can switch off $H_Q$ adiabatically in order to find the ground state of $H_P$ [2]. The question that arises naturally is: what are the consequences of the complicated structure of $H_P$ for the spectrum of $H$? Indeed, we expect the spectrum to be strongly influenced by the clustering phenomenon, and that this should have consequences on the performances of quantum algorithms as it does in the classical case. The influence of $H_P$ should be the strongest, and the easiest to analyze, for small $\Gamma$.

Some initial steps in this analysis have been recently performed in [3]. It was shown that increasing $\Gamma$ can induce level crossings between classical ground states and classical low-energy excited states: in the thermodynamic limit these level crossings can be accompanied by exponentially small (in system size) gaps in the spectrum of $H$ that might be particularly dangerous for a class of quantum algorithms such as the Quantum Adiabatic Algorithm (QAA) [2]. However, the $H_P$ studied in [3] admit a single ground state (see [4] for a recent discussion of this point), and therefore they do not show the complex clustering phenomenon explained above, whose influence on the spectrum of the quantum problems remains unclear.

In this paper, we address this issue by studying the quantum version of a simplified model of random optimization problems introduced in [5], that shares part of the structure with more complex problems, at the same time being fully solvable in the thermodynamic limit.

We find, for this model, that quantum fluctuations have a strong influence on the cluster structure: they lift the degeneracy inside each cluster and the ground state energy is lowered proportionally to the entropy of the cluster. This mechanism is somehow similar to the order-by-disorder phenomenon that is found in some frustrated magnets [6]. Therefore, if the classical energy changes from cluster to cluster, then level crossings are induced between clusters by varying $\Gamma$. These crossings happen over a continuous range of $\Gamma$, giving rise to a complex spin glass phase characterized by a continuously changing ground state (as in classical spin glasses upon chang-
ing the temperature or the coupling constants [7]) and an exponentially small gap. Finally, at large $\Gamma$ the spin glass phase undergoes a first order “delocalization” transition towards a simple quantum paramagnetic phase, of the type discussed in [8–10]. This set of results gives us a consistent picture of the effect of adding quantum fluctuations on top of the complex classical phase space sketched in Fig. 1, and allows to study in the same toy model the interplay between the different phenomena discussed in [3] and [8–10].

Model.— The quantum version of the Random Subcubes model [5] is defined as follows. We take the Hilbert space $\mathcal{H}$ of $N$ spins $1/2$ (qubits), in the basis of the Pauli matrices $\sigma_i^z$, where $\mathcal{A}$ is a subset (subcube) of the Hilbert space $A = \{|\sigma\rangle \mid \forall i, \sigma_i \in \pi \}$, where $\pi$ are independent (set-valued) random variables which encode the authorized values of $\sigma_i$: $\pi_i = \{-1\}$ or $\{1\}$ with probability $p$/2, and $\{-1, 1\}$ with probability $1-p$. The variable $i$ is “frozen” in $A$ in the former case and “free” in the latter. Note that the number of states in a cluster $A$ is equal to $2^{N s(A)}$, where $N s$ is the number of free variables; we call $s(A)$ the internal entropy of a cluster. We next define a set $S$ as the union of $2^{N(1-\alpha)}$ random clusters. We define a Hamiltonian $H_A = N c_0(A) \Sigma_{\mathcal{A}} \langle \sigma | \mathcal{A} \rangle$, for each cluster, and a “penalty” Hamiltonian $H_V = NV \Sigma_{\mathcal{Z} \in S} | \sigma \rangle \langle \sigma |$. The problem Hamiltonian $H = H_V + \Sigma_A H_A$ is then diagonal in the basis $| \sigma \rangle$.

We wish to interpret the states in $S$ as “local minima” of $H_V$ and the others as “excited states”. A sharp distinction between them can be obtained by sending the positive constant $V$ to infinity; for finite $V$, we will always assume that $V \gg \max_A c_0(A)$. As a quantum term we choose here $\Gamma H_Q = -\Gamma \Sigma_{i=1}^N \sigma_i^z$, i.e. a transverse field acting on the spins. Note that taking instead an $H_Q$ proportional to $\Sigma_{i \neq j} \langle \sigma_i | \sigma_j \rangle$ would lead to the simpler multi-solution Grover problem investigated in [11].

Analysis of the classical Hamiltonian.— In [5] it is shown that the set $S$ has the following structure. i) For $\alpha \leq \alpha_d = \log_2(2-p)$, each state $| \sigma \rangle$ belongs to an exponential number of clusters and the space $S$ coincides with $\mathcal{H}$. ii) For $\alpha > \alpha_d$, one has $S \neq \mathcal{H}$. The number of clusters $N \num(s)$ of entropy $s$ is given by

$$\num(s) = N^{-1} \log_2 (N \num(s)) = 1 - \alpha - D(s)|1-p|,$$

where $D(s) = x \log_2(x/y) + (1-x) \log_2(1-x)/(1-y)$.

This expression is restricted to the interval $s \in [s_{\min}, s_{\max}]$ for which $\num(s) \geq 0$. Note that this dependency of the complexity $\num(s)$ on the internal entropy is present in $k$-SAT and $q$-COL but not in XORSAT whose quantum version was studied in [10]. Above $\alpha_d$ there is “ergodicity breaking” in the sense that a local random walk over solutions starting in one cluster takes an exponentially long (in $N$) time to reach another cluster [5].

iii) For $\alpha > \alpha_{\text{sep}} = 1 + \log_2(1-p^2)/2$, the clusters are well separated, in the sense that with probability 1 for $N \to \infty$ the Hamming distance (number of opposed spins) between any two clusters is of order $N$. From now on we focus on the region $\alpha > \alpha_{\text{sep}}$, which is of principal interest for our purposes. Most results are expected to hold more generically for $\alpha > \alpha_d$ (because the effect of overlapping clusters is negligible [5]), yet the arguments used below should be refined in this regime.

One can compute the total number of states in $S$ by observing that

$$|S| = 2^{N s_{\text{tot}}} = \sum_{A} 2^{N s(A)} \sim \int_{s_{\min}}^{s_{\max}} ds 2^{N |\num(s)+s|},$$

therefore $s_{\text{tot}} = \max_{s \in [s_{\min}, s_{\max}]} (\num(s) + s)$. It turns out that for $\alpha_d < \alpha < \alpha_c = p/(2-p) + \log_2(2-p)$, the maximum is at $s^*(\alpha) \in [s_{\min}, s_{\max}]$. Therefore most of the configurations of $S$ belong to one of the exponentially many (in $N$) clusters of size $s^*$. For $\alpha > \alpha_c$, the maximum is in $s^* = s_{\max}$, therefore most of $S$ is supported by the largest clusters whose number is sub-exponential in $N$ since $\num(s_{\max}) = 0$. The order parameter for this condensation transition is the average Hamming distance between two random configurations in $S$, close to $N/2$ for $\alpha < \alpha_c$ and strictly smaller otherwise. Finally, for $\alpha > 1$ there are no more clusters and the set $S$ is empty.

Spectrum of the cluster Hamiltonian.— We will now study the spectrum of the quantum Hamiltonian $H = H_V + \Gamma H_Q$ as a function of $\Gamma$, and we consider first the (“hard”) $V \to \infty$ limit where $H_V$ is infinite for the states that do not belong to $S$: then we can project out these states from the Hilbert space and look to the restriction of $H = \sum_A H_A + \Gamma H_Q$ on $S$, which contains $2^{N s_{\text{tot}}}$ states. Since the matrix $H_Q$ only connects configurations at unit Hamming distance, and different clusters have distance of order $N$, the Hamiltonian $H$ has no matrix elements connecting different clusters. Therefore we can diagonalize $H$ separately in each cluster. The restriction of $H$ to a given cluster $A$ with $Ns(A)$ free spins is equal to $H_A$ plus the Hamiltonian of $Ns(A)$ uncoupled spins in a transverse field, its spectrum is hence made of levels

$$E_k(A) = N c_0(A) + (2k - N s(A)) \Gamma,$$

with $k = 0, \cdots, N s(A)$, each $N s(A)$ times degenerate. In particular the lowest level has energy per spin $c_{\num}(A) = c_0(A) - \Gamma s(A)$, therefore the energy of clusters with larger entropy decreases faster with $\Gamma$.
Quantum paramagnetic state.— Next, we consider a “soft” version of the model in which $V$ is finite (still with $V \gg \max_A e_0(A)$). Therefore now $H$ is defined on the full Hilbert space $\mathcal{H}$. In this case, in addition to the $2^{N s_m}$ energy levels discussed above (that we shall refer to as the S-band), there exists another set of $2^N - 2^{N s_m} \sim 2^N$ levels (the V-band), whose energy is expected to be of order $V$ at small $\Gamma$. For the states in the S-band we use perturbation theory in $\Gamma$; the leading order is of the energy levels discussed above (that we shall refer to as the O-band), and the perturbation analysis [12] shows that the spectrum of the limit. Moreover, an argument based on small rank perturbation analysis [12] shows that the spectrum of the V-band states is close to the one of $N$ free spins in transverse field with classical energy $NV$:

$$E_k^V = NV + (2k - N)\Gamma, \quad k = 0, \ldots, N, \quad (4)$$

with degeneracy close but not equal to $\binom{N}{k}$. In particular the lowest of such levels is the Quantum Paramagnetic (QP) state $|Q\rangle \sim 2^{-N/2} \sum_\mathcal{Q} |\mathcal{Q}\rangle$, which is uniformly extended in the basis $|\mathcal{Q}\rangle$ and has energy per spin $e_\text{QP} = V - \Gamma$.

Level crossings.— We discuss now the zero temperature phase diagram of the model for $\alpha > \alpha_{\text{sep}}$ and $N \to \infty$. To get a meaningful thermodynamic limit, the number of clusters of energy $e_0$ is set to $2^{N \Sigma(e_0)}$, where $\Sigma(e_0)$ is some increasing function of $e_0 \in [0, \epsilon_m]$ (as in most random optimization problems). We assume that $\Sigma(e_m) = 1 - \alpha$ so the total number of clusters in $\mathcal{S}$ is still $2^{N(1-\alpha)}$. Since the frozen variables are chosen independently for each cluster, the complexity of clusters of energy $e_0$ and entropy $s$ is $\Sigma(e_0, s) = \Sigma(e_0) - D(s||1-p)$. It vanishes for a given value $s_{\text{max}}(e_0)$ which is also an increasing function of $e_0$. The S-band, or Spin Glass (SG), ground state energy is

$$e_\text{SG} = \min_{e_0 \in [0, \epsilon_m]} \min_{s \in [s_{\text{max}}(e_0), s_{\text{max}}(e_0) - (e_0 - \Gamma s)]} (e_0 - \Gamma s) \quad (5)$$

The minimum is in $e_0 = 0$ as long as $\Gamma < \Gamma_c = 1/(s_{\text{max}}^{\text{max}}(0))$. Above this value, the minimum is in a different $e_0$ for each value of $\Gamma$: in this region the ground state changes abruptly from one cluster to another upon changing $\Gamma$ by an infinitesimal amount [7], see the inset of Fig. 2. Since the clusters have Hamming distance proportional to $N$, we expect these crossings to be avoided at finite $N$ producing exponentially (in $N$) small gaps [3, 9]. Note that in some relevant cases the slope of $\Sigma(e_0)$ in $e_0 = 0$ is infinite, therefore $\Gamma_c = 0$ and level crossings happen at all $\Gamma$.

The energy $e_{\text{QP}}$ crosses $e_{\text{SG}}$ given by Eq. (5), giving rise to a first order phase transition between the spin glass and the quantum paramagnet [8–10] at a critical $\Gamma \propto V$, see Fig. 2. As a consequence, the transverse magnetization $m_x = de/d\Gamma$ has a jump at the transition [10].

![Figure 2: Low energy spectrum of the model for $\alpha_{\text{sep}} < \alpha < \alpha_c$. As an example we choose (following [5]) $p = 0.7, \alpha = 0.85$, and $\Sigma(e_0) = (1 - \alpha)[2 + e_0/\epsilon_m - (e_0/\epsilon_m) \ln(e_0/\epsilon_m)]/3$ for $e_0 \in [0, \epsilon_m]$ with $\epsilon_m = 0.1$. Main panel: Energy of the SG (cluster) ground state [Eq. (5), full line] and of the QP state $e_{\text{QP}} = V - \Gamma$ for $V = 1$ (dashed line). A first order transition between the two states happens at $\Gamma \sim 2$. Inset: Level crossings in the SG state. For better readability we plot $e_{\text{SG}} + \Gamma s_{\text{max}}(0)$ [Eq. (5), full line] and show the energy $e_0 - \Gamma s_{\text{max}}(0)$ of two different clusters with $e_0 = 0.05, 0.2$ (dot-dashed lines).](image)
the zero-energy clusters is \( \Sigma(e_0) \) as in Fig. 2, and \( \beta = 1 \) (full lines). The vertical line corresponds to \( \alpha_{ep} = 0.797 \) for this value of \( p \). The higher \( \Gamma \) line is the first order transition between SG and QP. Above the lower \( \Gamma \) line \( \alpha_c(\Gamma, \beta = 1) \) the system is in the condensed phase. The condensation transition lines \( \alpha_c(\Gamma, \beta) \) are also reported (dashed lines) for different values of \( \beta \), showing that the non-condensed phase disappears for \( \beta \to \infty \). The complexity of the zero-energy clusters is \( \Sigma(e_0 = 0) = 2(1 - \alpha)/3 \), hence one has \( \alpha_c(\Gamma = 0, \beta = \infty) = \frac{2}{3} p + \frac{1}{2} \log_2(2 - p) = 0.875 \).

**Conclusions.**— In this paper we introduced the quantum version of a simple toy model of optimization problems [5]. In the classical case \( \Gamma = 0 \), the model captures the essential structure of the space of solution of random optimization problems, and displays several phase transitions that are present also in more realistic problems such as \( k \)-SAT and \( q \)-COL, at least at large \( q, k \). We explored the consequences of this complex structure on the spectrum of the quantum Hamiltonian at \( \Gamma > 0 \), and we showed that: 

- i) Quantum fluctuations lower the energy of a cluster proportionally to its size.
- ii) As clusters have an energy distribution, level crossing between different clusters are induced as a function of \( \Gamma \) in the spin glass phase, due to a competition between energetic and entropic effects. These crossings happen in a continuous range of \( \Gamma \), giving rise to a complex spin glass phase characterized by a continuously changing ground state. Since the clusters are separated by an extensive Hamming distance, as were individual solutions considered in [3], we expect an exponentially (in system size) small gap everywhere in this phase. 
- iii) At large \( \Gamma \sim V \) the spin glass phase undergoes a first order transition towards a quantum paramagnetic phase [8–10], corresponding to the complete delocalization of the ground state in the computational basis \(|\sigma\rangle\).
- iv) At finite temperature, there is a line of condensation transitions \( \alpha_c(\Gamma, \beta) \) that shrinks to \( \Gamma = 0 \) at low temperatures: indeed, at zero temperature the condensation transition becomes abrupt. While at \( \Gamma = 0 \) the space of solutions is dominated by an exponential number of clusters of intermediate size, for any \( \Gamma > 0 \) the biggest clusters contain the ground states.

Overall, this toy model shows that the low energy spectrum of quantum optimization problems can be very complex, and characterized by different level crossings: internal level crossings in the spin glass phase, or the crossing between the spin glass and the quantum paramagnet giving rise to a first order phase transition. Moreover, both entropic and energetic effects are important. We expect that this complex structure of the low-energy spectrum of the quantum Hamiltonian will have deep consequences on the behavior of quantum algorithms: for instance, the Quantum Adiabatic Algorithm proposed in [2] should run into difficulties because of the exponentially small gaps that are expected at the crossings.

We expect these results to be also relevant for the physics of quantum glasses: indeed, mean-field lattice glass models fall in the same class of random optimization problems. In this context the glass transition corresponds to the condensation transition discussed above. The phase diagram we reported in Fig. 3, characterized by a re-entrance of the glass transition line, has been found using different approaches [13]. Extending these results to more realistic optimization problems, and further investigating the connection between the spectrum and the performances of quantum algorithms, are two lines of research that should be developed in the future.

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