

Concentration Bounds for Quantum States and Limitations on the QAOA from Polynomial Approximations

Anurag Anshu ✉

School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA

Tony Metger ✉

Institute for Theoretical Studies, ETH Zürich, Switzerland

Abstract

We prove concentration bounds for the following classes of quantum states: (i) output states of shallow quantum circuits, answering an open question from [15]; (ii) injective matrix product states; (iii) output states of dense Hamiltonian evolution, i.e. states of the form $e^{iH^{(p)}} \dots e^{iH^{(1)}} |\psi_0\rangle$ for any n -qubit product state $|\psi_0\rangle$, where each $H^{(i)}$ can be any local commuting Hamiltonian satisfying a norm constraint, including dense Hamiltonians with interactions between any qubits. Our proofs use polynomial approximations to show that these states are close to local operators. This implies that the distribution of the Hamming weight of a computational basis measurement (and of other related observables) concentrates. An example of (iii) are the states produced by the quantum approximate optimisation algorithm (QAOA). Using our concentration results for these states, we show that for a random spin model, the QAOA can only succeed with negligible probability even at super-constant level $p = o(\log \log n)$, assuming a strengthened version of the so-called overlap gap property. This gives the first limitations on the QAOA on dense instances at super-constant level, improving upon the recent result [8].

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1 Introduction

Concentration bounds deal with the deviation of random variables from their expectation. Such bounds describe important structural properties of probability distributions that carry low correlation, and as a result have become ubiquitous tools in mathematics, computer science, and physics. A series of recent works has extended concentration bounds to the quantum many-body setting, where weakly correlated quantum states hold physical and



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computational relevance and their concentration properties explain important physical effects. For example, the concentration of expectation values in various quantum states such as product states [23, 24, 1], Gibbs quantum states [16, 30], and finitely correlated states [3] explains the equivalence of ensembles [9, 10, 32, 2] and eigenstate thermalisation [29] in quantum statistical mechanics. Concentration bounds are also an important proof technique in quantum complexity theory: for example, concentration properties of quantum states generated by low-depth quantum circuits have been used to prove circuit lower bounds on low-energy states of quantum Hamiltonians [17], leading to the recent proof of the NLTS conjecture [7, 6, 5]. Furthermore, concentration results play an important role in analysing and bounding the performance of variational quantum algorithms for classical constraint optimisation problems, e.g. the quantum approximate optimisation algorithm (QAOA) [19, 18, 14, 8].

The standard method to prove concentration inequalities is the moment method. The slow growth of the moments of weakly correlated probability distributions or quantum states serves as a signature of concentration. Arguably the simplest example is the classical Chernoff-Hoeffding bound, which shows that the probability that the sum of n independent random variables deviates from its expectation value by more than k is at most $e^{-\Omega(k^2/n)}$. We call this *Gaussian concentration*. The moment method also extends to non-commuting observables with product quantum states [27] or quantum states with exponential decay of correlation [3], albeit sometimes with weaker bounds of the form $e^{-\Omega(k^\alpha/n^\beta)}$ for some $\alpha, \beta > 0$. We call these weaker bounds *exponential concentration*.¹

An alternative to the moment method was introduced in [28]. The idea of this approach is to approximate the quantum state of interest by a local operator and use this approximation to prove concentration bounds. Because the local approximation is usually constructed from low-degree polynomials, we call this the *polynomial-based method*. The strength of the resulting concentration bounds depends on the locality of the approximation. [28] used this method to show exponential concentration of the form $e^{-\Omega(k/\sqrt{n})}$ for local classical observables on the ground states of gapped local Hamiltonians. However, their method was not able to produce Gaussian concentration even for the simplest case of local observables on an i.i.d. distribution (e.g. the sum of i.i.d. random variables), a case in which the Chernoff-Hoeffding bound does give Gaussian concentration results.

1.1 Main results

We extend the polynomial-based method in two ways: we show that in cases where the moment method produces Gaussian concentration, the polynomial-based method can do so, too; and we show that the polynomial-based method can be applied to a much wider class of states, including the output states of shallow quantum circuits, injective matrix product states, and the output states of dense Hamiltonian evolutions (explained below). An example of a dense Hamiltonian evolution is the QAOA for solving classical constraint optimisation problems (COPs). We therefore obtain concentration bounds for the QAOA, and combining this with the so-called *overlap gap property* first introduced in the classical literature [22, 21], we prove strong limitations on the performance of the QAOA even at (admittedly only slightly) super-constant level $p = o(\log \log n)$. Crucially, our method works

¹ Note that with this definition, technically Gaussian concentration is a special case of exponential concentration for $\alpha = 2$ and $\beta = 1$. However, when we say “exponential concentration” it is usually implicit that α and β are such that the bounds are generally weaker than for Gaussian concentration. A typical case is $\alpha = 1$ and $\beta = 1/2$.

for *dense* COPs, which may have constraints between any variables, and our proofs are fairly straightforward. This improves upon the recent work [8], which proved similar results for constant-level QAOA on dense instances using a highly technical proof.

We now describe our main results in more detail. In all cases, concentration bounds are obtained by approximating the quantum state of interest by a local operator, so in sketching the proof ideas, we only focus on the construction of such a local approximation. Below, we only give concentration bounds for the Hamming weight distribution W_ρ of an n -qubit quantum state ρ , i.e. the probability distribution over $\{1, \dots, n\}$ describing the Hamming weight of a computational basis measurement of ρ . More formally, $\Pr[W_\rho = i] = \sum_{x \in \{0,1\}^n: |x|=i} \langle x | \rho | x \rangle$. However, it is straightforward to extend these bounds to other observables that only change slowly as the Hamming weight changes.

■ **Table 1** Main results and comparison with prior work. For each case, we consider a state on n qubits and bound the probability that the Hamming weight of a computational basis measurements deviates by more than $k \in [0, n]$ from its median (or mean). Note that [8] were able to show concentration over both the choice of instance and the randomness of the QAOA output, whereas our bounds, while stronger, only deal with concentration over the latter.

	Prior work	This work
Depth t quantum states	$e^{-\Omega(k/\sqrt{2^{2t}n})}$ (implicit in [28])	$e^{-\Omega(k^2/2^{2t}n)}$
Injective matrix product states	$e^{-\Omega(k/\sqrt{n})}$ ([28, 3])	$e^{-\Omega(k^2/n)}$
Dense Hamiltonian evolution	$o_n(1)$ for the special case of QAOA with level $p = O(1)$ [8]	$e^{-\Omega(n^{1/8})}$ for $k = o(n)$ and level $p = o(\log \log n)$

Shallow quantum circuits

Consider a depth- t quantum circuit, i.e. a circuit comprised of t layers of arbitrary 2-qubit gates applied to the initial state $|0\rangle^{\otimes n}$. We denote the unitary implemented by this circuit by U . The output state of this circuit is the unique maximum-energy eigenstate of a 2^t -local Hamiltonian that is a sum of commuting projectors. To see this, observe that $U|0\rangle^{\otimes n}$ is the unique joint $(+1)$ -eigenstate of the operators $H_i = U|0\rangle\langle 0|_i U^\dagger$, where $|0\rangle\langle 0|_i$ acts as identity on all qubits except i . By a standard lightcone argument, H_i only acts non-trivially on 2^t qubits, so $H = \frac{1}{n} \sum H_i$ is a 2^t -local Hamiltonian with $U|0\rangle^{\otimes n}$ as its unique $(+1)$ -eigenstate. Therefore, the output of the circuit can be written as $U|0\rangle\langle 0|^{\otimes n} U^\dagger = \delta_1(H)$, where $\delta_1(1) = 1$ and $\delta_1(x) = 0$ for $x \neq 1$. We can now approximate $\delta_1(x)$ using a degree- d polynomial P_d constructed in [26, 12, 4]. Polynomials spread the locality of operators in a controllable way. We can therefore show that $P_d(H)$ is a $(d \cdot 2^t)$ -local operator that approximates $U|0\rangle\langle 0|^{\otimes n} U^\dagger$. Hence, we have constructed a local operator approximation to $U|0\rangle\langle 0|^{\otimes n} U^\dagger$ and can use this approximation to show that for any depth- t circuit, the output state $|\psi\rangle\langle\psi| = U|0\rangle\langle 0|^{\otimes n} U^\dagger$ has the following concentration property for $k \in (2^t \sqrt{n}, 2^t n)$:

$$\Pr[|W_\psi - \text{median}(W_\psi)| \geq k] \leq e^{-\Omega\left(\frac{k^2}{2^{2t}n}\right)}.$$

This generalises the Chernoff-Hoeffding bound for product distributions (which correspond to the case $t = 1$) and shows Gaussian concentration for any constant-depth quantum circuit, answering an open question from [15]. Similar statements have also appeared in [7, 6, 5]. Note that the same argument applies to any ground state of a Hamiltonian that is a sum of commuting projectors, not just output states of shallow circuits.

Injective matrix product states

Matrix product states (MPSs) are a widely used tensor network representation of quantum states. Injective MPSs have an additional property that ensures that they are the unique ground state of a local “parent Hamiltonian” with a constant spectral gap. We can therefore approximate an injective MPS as a polynomial of its parent Hamiltonian. Using near-optimal polynomial approximations constructed in [4], we obtain Gaussian concentration bounds for injective MPSs. Our bounds are stronger than previous ones [3, 28], which only showed exponential concentration. We also note that conditionally independent probability distributions can be encoded into injective MPSs, and that in that case our concentration bounds reproduce a (version of) Azuma’s inequality.

Dense Hamiltonian evolution

Concentration bounds are natural for quantum states that have weak long-range correlations such as the output states of shallow quantum circuits. A priori, one would not expect similar bounds to hold for quantum states with long-range correlations. Recently, [8] considered the output distribution of the QAOA (explained below) on random dense COPs, i.e. local COPs that can have constraints between any variables. For dense COPs, the operations implemented by the QAOA can include interactions between any qubits, and as a result the output distribution can have long-range correlations. Remarkably, [8] showed that the variance of the average energy density (averaged over the randomness of the QAOA as well as the choice of random instance) vanishes asymptotically. This means that the energy density of the output, which corresponds to the quality of the COP solution produced by the QAOA, concentrates about the average. However, [8] were only able to prove an asymptotic statement without explicit tail bounds and the proof was highly non-trivial.

We consider a more general class of states that includes the output states of the QAOA as a special case. Specifically, we define the output of a *dense Hamiltonian evolution* as a state of the form $e^{tH^{(p)}} \dots e^{tH^{(1)}} |\psi_0\rangle$ for any n -qubit product state $|\psi_0\rangle$. Here, each $H^{(i)}$ can be any commuting local Hamiltonian (though the different $H^{(i)}$ themselves are of course not required to commute). Importantly, $H^{(i)}$ are allowed to be *dense* Hamiltonians, i.e. Hamiltonians with interactions between any qubits. As explained below, the QAOA applied to a dense COP is a special case of dense Hamiltonian evolution.

For our concentration bounds, we further require each $H^{(i)}$ to satisfy a norm constraint, which limits the norm of the Hamiltonian restricted to a subset of the qubits. In particular, this condition is satisfied with overwhelming probability for the random dense model from [8]. Under this condition, we can prove that the output state of a dense Hamiltonian evolution is ϵ -close in operator norm to a k_p -local operator for

$$k_p \leq c_1^p n^{1-(1-\alpha)^{p/4}}, \quad \epsilon \leq e^{-\Omega(n^{1/8})}.$$

Here, c_1 and $0 \leq \alpha < 1$ are constants and p is *level* of the dense evolution, i.e. the number of unitaries $e^{tH^{(i)}}$ that have been applied. In particular, if we choose $p = o(\log \log n)$, then $k = o(n)$. This implies the following exponential concentration result: for ρ_p the output of a dense Hamiltonian evolution with level $p = o(\log \log n)$ satisfying the above conditions,

$$\Pr[|W_{\rho_p} - \text{median}(W_{\rho_p})| > o(n)] \leq e^{-\Omega(n^{1/8})}.$$

Here, we have only stated the asymptotic result, but we can also derive explicit bounds for any choice of p . This concentration result can also be extended beyond just the Hamming weight of a computational basis measurement: for example, it also holds for the energy density of ρ_p with respect to any classical Hamiltonian satisfying a similar norm constraint to the one mentioned above.

To prove that the output of a dense Hamiltonian evolution can be approximated by a local operator, we again make use of polynomial approximations. Recall that we are interested in states of the form $\rho_p = e^{\iota H^{(p)}} \cdots e^{\iota H^{(1)}} |\psi_0\rangle\langle\psi_0| e^{-\iota H^{(1)}} \cdots e^{-\iota H^{(p)}}$ for a pure product state $|\psi_0\rangle$. As a first step, we approximate $|\psi_0\rangle\langle\psi_0|$ by a local operator. For this, we observe that since $|\psi_0\rangle = \otimes_i |\psi_0\rangle_i$ is a product state, it is the unique ground state of the 1-local Hamiltonian $H = \frac{1}{n} \sum |\psi_0\rangle\langle\psi_0|_i$. If we apply a linear combination of Chebychev polynomials to this Hamiltonian, we obtain a good local approximation to $|\psi_0\rangle\langle\psi_0|$. Then, for each unitary $e^{\iota H^{(i)}}$ in the dense Hamiltonian evolution, we approximate the exponential function by its truncated Taylor series. The fact that the Hamiltonian evolution is applied to an approximately local operator allows us to use the norm constraint mentioned above to obtain an improved error bound for the truncated Taylor series. Therefore, the truncated Taylor series spreads the locality of the state in a controllable way without degrading the quality of the approximation too much. Applying this argument recursively for each layer of the dense Hamiltonian evolution, we obtain a local approximation to the output state ρ_p .

Limitations on the QAOA from concentration bounds

The QAOA [19] is an algorithm for solving local COPs (i.e. COPs consisting of any number of clauses, each with at most $q = O(1)$ variables) on a quantum computer. We can associate a q -local Hamiltonian H with every q -local COP C by replacing the variables in C with Pauli-Z matrices acting on different qubits. The resulting Hamiltonian is diagonal in the computational basis and has the property that for any string $x \in \{0, 1\}^n$, $C(x) = \langle x | H | x \rangle$. The QAOA attempts to find a “good” solution x (i.e. one for which $C(x)$ is as large as possible) by starting from the state $|+\rangle^{\otimes n}$ and then applying p layers of unitaries of the form $e^{\iota\beta_i \sigma_x^{\otimes n}} e^{\iota\gamma_i H}$. Here, β_i and γ_i are real parameters that can be tuned to the problem instance. It is clear that this is a special case of the dense Hamiltonian evolution we have described earlier. Our results will apply for any choice of β_i and γ_i and we will always implicitly consider a family of COPs, one for each number n of input bits, in order to make asymptotic statements.

[8] considered the performance of the QAOA on a random spin model on n qubits, described by the q -local Hamiltonian

$$H_n^q(J) = \frac{1}{n^{(q-1)/2}} \sum_{i_1, \dots, i_q=1}^n J_{i_1, \dots, i_q} \sigma_{i_1}^Z \cdots \sigma_{i_q}^Z, \quad (1)$$

where $J_{i_1, \dots, i_q} \sim \mathcal{N}(0, 1)$ are sampled from i.i.d. standard Gaussians. For this model, [8] were able to show that for constant even $q \geq 4$ and level $p = O(1)$, the value achieved by the QAOA (for fixed β_i, γ_i) in expectation over J and the internal randomness of the QAOA is bounded away from the optimal value by a constant as $n \rightarrow \infty$. They were also able to show the asymptotic concentration property described above.

Here, we use our concentration results to show limitations on the QAOA for a class of COPs that includes the random spin model above. For this, we consider local COPs that have the so-called overlap gap property (OGP) [20], which roughly says that “good” solutions to the COP are clustered in the sense that two good solutions are either close or far in Hamming distance. Combining this with our concentration results for dense Hamiltonian evolution, we can show that for any COP with a sufficiently strong OGP whose associated Hamiltonian satisfies a certain norm condition, if the QAOA produced a good solution with noticeable probability, then the probability distribution over good solutions produced by the QAOA would have to be concentrated on one such cluster. This allows us to show that

the QAOA cannot succeed with noticeable probability on *symmetric* COPs (i.e. COPs that are invariant under flipping all the input bits) that have a strong OGP. This is because the symmetry of the COP is in contradiction with the existence of a single cluster on which most of the probability distribution is concentrated: if such a cluster existed, we could take the strings in that cluster and flip all their bits to produce another cluster which, by symmetry, must have the same probability weight, a contradiction. This argument is similar to [11]. As a result, we obtain the following limitation on the QAOA.

► **Theorem (informal).** *Consider a local symmetric COP $C(x)$ with a sufficiently strong OGP and suppose that the associated Hamiltonian H satisfies a certain norm constraint. Then, the value of the solution to $C(x)$ produced by the QAOA with level $p = o(\log \log n)$ is bounded away from the optimal value by at least a constant except with probability $e^{-\Omega(n^{1/8})}$.*

For even q , the random spin model from Equation (1) is symmetric and satisfies the aforementioned norm constraint with overwhelming probability. Furthermore, it was shown in [13] that it satisfies the OGP with overwhelming probability. However, we note that here we need a stronger version of the OGP than was shown in [13]. This stronger version appears to be implicit in their proof, too, although we leave its formal proof for future work and assume it here as a conjecture. Assuming this stronger OGP, we can show the following.

► **Theorem (informal).** *With probability $1 - O(e^{-n})$ over the choice of J (with i.i.d. Gaussian entries), the value of the solution to the random spin model (Equation (1)) produced by the QAOA with level $p = o(\log \log n)$ is bounded away from the optimal value by at least a constant except with probability $e^{-\Omega(n^{1/8})}$.*

This places strong limitations on the performance of the QAOA because it does not just bound the *expectation* value away from the optimal value as in [8], but instead asserts that the QAOA output is bounded away from the optimal value with overwhelming probability, even at super-constant level $p = o(\log \log n)$.

1.2 Discussion and open questions

We have shown that polynomial approximations can be used to derive Gaussian concentration bounds for the output states of constant-depth quantum circuits and injective matrix product states, and exponential concentration bounds for the output states of dense Hamiltonian evolution. The latter can be used to derive strong limitations on the performance of the QAOA at super-constant level $p = o(\log \log n)$ even on dense instances such as random spin models.

At first sight, it is surprising that the (provably optimal) polynomial approximations [26, 12] we use for shallow quantum circuits are able to reproduce the (likewise provably optimal) Chernoff-Hoeffding bound in the classical case. It would be interesting to explore whether there is a deeper conceptual connection between optimal polynomial approximations and optimal concentration bounds.

On a more technical level, there are a number of interesting improvements one could hope to make to our bounds. Firstly, our bounds for MPSs can only deal with sub-linear deviations $k = O(n^{1-\delta})$ for any $\delta > 0$. It would be desirable to extend this result to arbitrary values of k . Additionally, one could hope to prove similar concentration bounds for PEPSs, the two-dimensional analogue of MPSs.

Secondly, we only achieve exponential, not Gaussian, concentration bounds for dense Hamiltonian evolutions with level $p = o(\log \log n)$. Can one improve these results to Gaussian concentration and also extend them to higher levels, e.g. $p = O(\log n)$ or even $p = O(n^\delta)$ for a

small $\delta > 0$? Furthermore, we show concentration for the output states of dense Hamiltonian evolution for a fixed instance, but we cannot show that for random COPs, the output states also have concentration properties over the choice of random instance, e.g. over the choice of $J_{i_1 \dots i_q} \sim \mathcal{N}(0, 1)$ in the case of the random spin model introduced earlier. [8] do show such a concentration property, albeit only in the asymptotic regime without explicit bounds. Can our polynomial approximation techniques also be used to prove explicit concentration bounds over the choice of random instance? If so, it might be possible to extend the limitations on the performance of dense evolutions for COPs proven in this work beyond symmetric COPs and optimisers.

Finally, our techniques may also be useful for problems in condensed matter physics. As an example, consider the Lieb-Schultz-Mattis theorem [31] and its higher-dimensional generalisation [25], seminal results in condensed matter physics. Their main idea is that sufficient symmetry and non-degeneracy of the ground space prevents a Hamiltonian from being gapped. Inspired by our application to symmetric QAOA, we can ask whether an alternative proof of this result can be obtained using concentration bounds and polynomial approximations, e.g. by showing that the concentration properties of unique gapped ground states are in conflict with the symmetry requirements.

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