Quantum algorithms for complex dynamics in presence of imperfections

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Abstract

This poster presents some recent results concerning analytical and numerical studies of the effects of imperfections on a class of quantum algorithms which allow for the polynomial simulation of some aspects of the rich and nontrivial quantum dynamical behaviour of quantum maps. We have studied the decay of entanglement in an operating quantum computer, with numerical experiments for the sawtooth map up to 20 qubits, and we have shown that the residual level of entanglement is exponentially sensitive to imperfections in the chaotic regime. We have also studied the dynamics of a map based on the quantum wavelet transform and its fidelity timescale, evidencing that for self-interaction in the quantum memory the threshold for error correction is significantly decreased with respect to the case of imperfect gates. Our attention was also focussed on the Anderson metal-insulator transition: already 7 qubits are sufficient to study the physics of this transition in disordered solid-state systems; we were able to observe also here the characteristic signature of static errors.

A need for practical algorithms

While there is already a number of results for ideal (noiseless) quantum computers which prove the superiority of this computational model over the classical one, no scalable quantum computer has been built so far, and the technological and (maybe) fundamental problems concerning their design indicate that in the foreseeable future the quantum computer community will not have access to devices with a memory larger than 10-15 qubits. It is therefore interesting, for the time being, to design and study quantum algorithms with very limited memory requirements, which could however be used as a test-ground for error correction strategies. In this context, the quantum algorithms for the simulation of chaotic maps are ideal candidates, because they satisfy the previous requirement and allow for the investigation of non-trivial physical phenomena.

Classical and quantum (chaotic) maps

We study time-dependent Hamiltonian systems with periodic conditions on q and on p, which can show the phenomenon of dynamical chaos. The discretised dynamics, determined by the parameters K and L, can be understood as a "kick" followed by a free evolution:

$$\begin{cases} \bar{q} &= q + \bar{p} \mod 2\pi \\ \bar{p} &= p - K\frac{dV}{dq} \mod 2\pi L \end{cases} \qquad H(t) = \frac{p^2}{2} - KV(q)\sum_n \delta(t-n)$$

In the quantum case one must consider also the number of levels N (with $\hbar = 2\pi L/N$). The Floquet operator (evolution operator corresponding to one iteration of the map) is a product of two terms, which are diagonal respectively in $\hat{p}$ and $\hat{q}$.

$$\boxed{U_F = e^{-i\hat{p}^2/2\hbar} e^{-iK\,V(\hat{q})/\hbar}} = \exp\left[-i\frac{\pi L}{N}\hat{n}_p^2\right] \cdot \exp\left[-i\frac{K}{L}\left(\frac{2\pi}{N}\right)^{\alpha-1}\mathcal{P}_\alpha(\hat{n}_q)\right]$$

Since the Floquet operator is a composition of operators diagonal in the position and momentum space, it is easily implemented using the QFT ($\mathcal{F}$) to move from one representation to the other:

$$U_F = \mathcal{F}^\dagger \circ e^{-i\alpha x^2} \circ \mathcal{F} \circ e^{-i\beta\hat{V}(x)}$$

Unlike the classical case, this allows for an efficient simulation of the evolution of the system for one time step on a quantum computer, for those potentials which are polynomials, by considering $x = \sum_{j=0}^{n-1} a_j 2^j$:

$$e^{-2\pi i\gamma x^\alpha} = \prod_{j_1\cdots j_\alpha} e^{-2\pi i\gamma a_{j_1}\cdots a_{j_\alpha} 2^{j_1+\ldots+j_\alpha}} = \prod_{j_1\cdots j_\alpha} \mathtt{RPC}_{j_1\ldots j_\alpha}\left(\gamma 2^{j_1+\ldots+j_\alpha}\right)$$

where $\mathtt{RPC}_{j_1\ldots j_\alpha}(\beta)$ is a controlled phase shift, which multiplies a basis state times $\exp(-2\pi i\beta)$ if the qubits $j_1\ldots j_\alpha$ are in $|1\rangle$ and acts as the identity otherwise. If $\alpha = 1$ this is a plain phase shift.

Complexity and efficiency of the quantum map algorithms

It is easily seen that, if n_q is the number of qubits the wave function is expanded on, the exponentiation circuit requires n_q^α gates, and that it is the most expensive subroutine of the quantum double-well algorithm. Thus these algorithms can calculate one time step in the quantum map in polynomial time (with respect to n_q), while classical algorithms cannot do better than $n_q 2^{n_q}$ (since they are limited by fast Fourier transforms).

The speed-up in the simulation of one map step is not, of course, the whole story, since measurements in general (but note always → M.Terraneo and D.L.Shepelyansky, *A measurement that preserves quantum localisation*, in preparation) destroy the coherence of the system and the computation must be restarted from scratch, and in order to sample a generic wave function $O(2^{n_q})$ measurements are necessary. Nonetheless, some features can be efficiently extracted.

For instance, the entanglement of a pair of qubits can be determined by a number of measurements which depends only on the required precision. Moreover, quantum maps in the appropriate regime show the phenomenon of dynamical localisation or Anderson localisation, i.e. the wave function is spread over a constant number of basis states, independently of n_q.

Developing with a quantum programming language

The algorithms in this poster were implemented using a quantum language developed by one of the authors [4], and the numerical experiments have been performed up to $n_q \sim 20$ qubits. This quantum language complements a generic general purpose classical language with a set of quantum primitives. The underlying scheme involves a run-time environment which calculates the byte-code for the quantum operations and pipes it to a simulator. This language can compactly express existing quantum algorithms and reduce them to sequences of elementary operations; it also easily lends itself to automatic, hardware independent, circuit simplification. All controlled and multi-controlled high level primitives are automatically broken down into one or two qubit primitives (Hadamard gates, phase shifts and controlled phase shifts) by the language. For further details see [4].

Error models: noisy gates and static errors

For the evolution of a realistic quantum computer we have considered two types of imperfections. **Noisy gates** correspond to an imperfect external control: each elementary (hardware) gate in a quantum circuit is still a unitary operation, but its parameters are slightly modified. This can be achieved in two equivalent ways: either the perfect gate is followed by a one-qubit rotation around a random axis of a small angle $\eta \in [-\epsilon/2, \epsilon/2]$, or the eigenvalues of the gate are perturbed of an amount η in the basis where it is diagonal. **Static errors** correspond to a residual interaction among the qubits of the quantum computer memory. In our simulations, only next-neighbour interactions are considered, so that the overall number of couplings grows like the number of qubits n_q. Static errors are implemented by letting the Hamiltonian $\mathcal{H}\tau/\hbar = \delta^\mu\sigma_z^\mu + J^{\mu\nu}\sigma_x^\mu\sigma_x^\nu$ act after the application of each elementary gate. The coefficients δ^μ and $J^{\mu\nu}$ are chosen in $[-\delta/2, \delta/2]$ and $[-J, J]$ respectively. The **error intensity** ϵ is a parameter which measures the strength of the imperfections; for noisy gates it exactly the upper limit for $|\eta|$, i.e. $\epsilon^2 \sim \sigma^2(\eta)$; for static errors it is a mixture of the coefficients for the Zeeman terms and the coupling terms, i.e. $\epsilon^2 \sim \sigma^2(\delta^\mu) + \sigma^2(J^{\mu\nu})$.

Entanglement and the sawtooth map

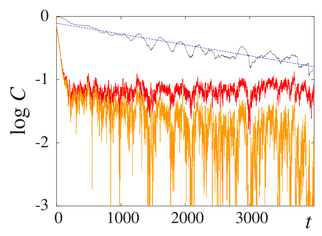
The first study we describe [1] concerns the sawtooth map, characterised by the potential $V(q) = -q^2/2$. It is easy to understand that for positive K the potential behaves repulsively and the classical map become globally chaotic. Due to the discontinuity of $V'(q)$ the KAM theorem does not apply. We have tried to investigate the evolution of "entanglement" in the memory of the quantum computer during the execution of this non-trivial algorithm. A study of the amount of entanglement is important because many researchers think that it must be linked to the power of quantum computation. Without this resource, one should resort to an exponentially large memory, to measurement devices with exponential precision or incur into other exponential costs.

We have chosen to study the evolution of the entanglement of formation of the two most significant qubits, using a functionally dependent quantity (indeed, almost the same quantity), the *concurrence* C, which depends only on the reduced density matrix ρ of the two qubits. If one defines $\tilde{\rho} = (\sigma_y\otimes\sigma_y)\rho^*(\sigma_y\otimes\sigma_y)$, then C is $\max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$ where the λ_i are the square roots of the eigenvalues, in decreasing value order, of $\sqrt{\tilde{\rho}}\rho\sqrt{\tilde{\rho}}$. The initial state we use is $|\psi\rangle = \frac{|00\rangle+|11\rangle}{\sqrt{2}}|\phi\rangle$, for which $C = 1$, and L is always a multiple of 4.

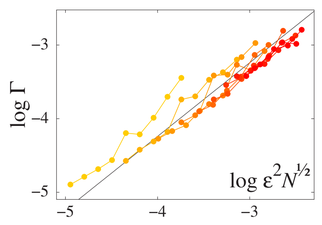
It is clear that this quantity does not account for the overall entanglement of the quantum memory, but it has been proven to be linked to interesting physical properties (like quantum phase transitions), and its degradation due to "errors" in the computation should be correlated to the powerfulness of the computation. In any case, for the more general case of multi-partite systems, no satisfactory definition has been found up to now (the additivity properties are not yet clear too → A.Pomeransky, *Strong superadditivity of the entanglement of formation follows from its additivity*, [5]).

Numerical experiments up to ~ 20 qubits have shown that on a perfect quantum computer the concurrence C decays exponentially (with a decrease rate proportional to the classical diffusion rate) until it reaches a plateau, characterised by large fluctuations. The average residual level for the concurrence is roughly proportional to $1/\sqrt{g}$, where $g = DN/L^2$ is the *Thouless conductance*. We attribute the presence of strong fluctuations to the fact that the value $\bar{C}$ is averaged only over the time but there is no averaging over the parameters. Thus, from the point of view of disordered systems $\bar{C}$ represents only one value for one realisation of disorder.

Noisy gates and entanglement degradation



What is the effect of noisy gates on the residual level of concurrence? This picture illustrates the procedure for extracting numerically the induced decay rate. The two lower curves show the dependence $C(t)$ for the perfect (red) and noisy (yellow) algorithm. In the latter case the average is done over 20 noise realizations. The black curve in the upper part shows the ratio of the two $C(t)$; this ratio is averaged over a 100 kick moving window to reduce fluctuations. The dashed straight line shows a fit of the ratio to an exponential decay $e^{-\Gamma t}$.



This picture illustrates the dependence of the decay rate on the error intensity (ϵ increases from yellow to red) and the number of qubits. The straight line shows the averaged behaviour $\Gamma = 0.58\epsilon^2\sqrt{N}$. Quite naturally we find that $\Gamma \propto \epsilon^2$ (see, for instance, [6]). This scaling becomes better and better for large ϵ values where Γ is larger. However, more surprisingly there is an exponential growth of $\Gamma \propto \sqrt{N}$.

This result is very different from those obtained in other papers (see [6] and [7]), where the time scale for the fidelity and the decoherence rate for tunnelling oscillations varied polynomially with n_q. A possible explanation is that the eigenstates are exponentially sensitive to imperfections due to the chaotic structure of the wave functions (see e.g. [8]), but more investigation is required. Summarising the results of this study:

- **the law $\Gamma \sim \epsilon^2$, which was already known to be valid for the fidelity degradation, is confirmed;**
- **a quantum algorithm can remain efficient even if the bipartite entanglement becomes exponentially small;**
- **entanglement timescales can be exponential in a chaotic regime → the sensitivity to noisy gates depends on the algorithm.**

A wavelet transform based map

The second study we describe [2] concerns the effects of various imperfections in a quantum computation of a simple dynamical model based on the quantum wavelet transform (QWT). The wavelet transform (WT) was chosen because of its similarities with the Fourier transform (FT). Wavelets are obtained by translation and dilation of an original function and they allow high resolutions for microscopic details, both in frequency and space. It is well accepted that the Fourier transform (FT) and WT are the main instruments for data treatment, and it has been shown that in many applications the performance of WT is much higher compared to the Fourier analysis. The discrete WT can be implemented with high computational efficiency and provide a powerful tool for treatment of digital data. In this study we use the 4-coefficient Daubechies WT.

The sensitivity of the quantum Fourier transform (QFT) to imperfections was tested in various numerical simulations and the time-scales for reliable computation of the algorithm were established. In order to estimate the degree of generality for these results, it is important to investigate the stability and the accuracy of QWT in similar conditions. This test is non-trivial since the functions of the wavelet basis have singularities in the derivatives (in contrast to analyticity of Fourier waves) that may enhance the effects of perturbations.

For this investigation we developed an algorithm essentially based on multiple applications of the QWT. The algorithm is almost identical to that for the sawtooth map, but the QFT are replaced by QWT. As for the QFT, polynomial size circuits exist for the implementation of the QWT on quantum computers. The wavelets transforms are the most expensive sections of the algorithm, since their implementation requires $O(n_q^3)$ elementary gates (and one auxiliary qubits), to be compared to $O(n_q^2)$ and no auxiliary qubit for the QFT.

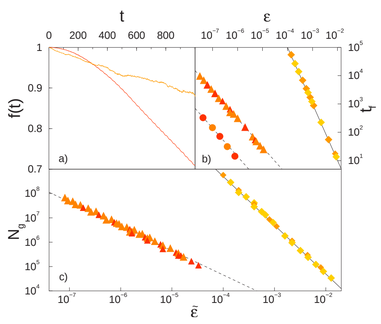
In the studied regime, the numerical simulations of the ideal quantum algorithm for the wavelet map show that the wave function is essentially localised on a few states of the computational basis. This localisation is clearly seen from the Inverse Participation Ratio (IPR) $\xi = 1/\sum_n |\psi_n|^4$ which is a standard quantity to characterise localisation in mesoscopic systems. It directly provides the number of sites on which the probability is concentrated. The phenomenon of localisation would permit to extract the shape of the probability distribution for the wavelet map on a quantum computer with a constant number of measurements.

Effects of imperfections on the fidelity of a wavelet map

Noisy gates and static imperfections act in a radically different way. With noisy gates the localisation is destroyed: the average value of the momentum squared increases with t (diffusion) up to saturation due to the finite size of the system. For static errors instead the IPR shows modified bounded oscillations, but the localisation is not completely destroyed. The qualitative difference between two types of imperfections becomes clear from the analysis of the fidelity, defined as $f(t) = |\langle\psi_\epsilon(t)|\psi(t)\rangle|^2$, the squared modulus of the projection of the perfect evolution onto the noisy one after t map steps. We determine the time scale t_f for accurate computation by fixing a threshold for the fidelity as $f(t_f) = 0.9$.

What we find numerically is that, for **noisy gates**, $\boxed{t_f \propto 1/(\epsilon^2 n_g)}$, where n_g is the number of gates per map iteration. The physical origin for this scaling is related to the fact that after each gate an amount of probability of the order of ϵ^2 is transferred from the ideal state to all other states. This leads to an exponential decay of the fidelity $f(t) \approx \exp(-A\epsilon^2 n_g t)$, where A is a constant.

On the other hand, for **static imperfections** we find $\boxed{t_f = 1/(\epsilon n_g\sqrt{n_q})}$, which is a significantly smaller timescale with respect to noisy gates. Physically, this happens due to the coherent action of static imperfections, which lead to effective Rabi oscillations proportional to $\cos(\epsilon n_g t)$ for each qubit. For n_q qubits this gives $f(t) \propto [\cos(\epsilon n_g t)]^{n_q}$ and for small ϵ we obtain a Gaussian drop of the fidelity $f(t) \sim \exp(-n_q(\epsilon n_g t)^2)$. The effects of static imperfections are dominant for all range of imperfection strengths studied.



Panel a) shows an example of fidelity decay for static errors (orange) and noisy gates (yellow). Panel b) shows the dependence of the time scale t_f on the imperfection strength ϵ for noisy gates (diamonds) and static imperfections (triangles and circles). For clarity data are shifted in ϵ-axis by factor 10 to the left. Panel c) gives the dependence of the total number of gates $N_g = tn_g$ which is possible to simulate reliably versus $\tilde{\epsilon}$. For noisy gates (diamonds) $\tilde{\epsilon} = \epsilon$ and for static imperfections (triangles) $\tilde{\epsilon} = \epsilon\sqrt{n_q}$.

We note that similar scalings were discussed and numerically demonstrated in many other quantum algorithms, thus showing that they are generic and not very sensitive to the singularities in the derivatives of the wavelets. Similar scalings for N_g should also be valid for other quantum algorithms, *e.g.* Grover's and Shor's algorithms. These scalings are important for the quantum error correction threshold; indeed the accuracy border for large scale quantum computation is obtained in the assumptions of random noisy errors and gives a threshold $\epsilon < \epsilon_r \sim 10^{-2}$. This approach intrinsically uses the fact that, for noisy gates, the fidelity remains close to one for a number of gates $N_g = C/\epsilon_r^2$. In the case of static imperfections it is natural to assume that this number should remain approximately the same. Therefore, for static imperfections the accuracy border ϵ_s must be approximately $D\epsilon_r^2/(C\sqrt{n_q})$ This is a significant decrease of the threshold: for the parameters of our numerical studies we obtain that for the noisy error rate $p_r = \epsilon_r^2 \approx 10^{-4}$ the rate induced by static imperfections should be less than $p_s = \epsilon_s^2 \approx 10^{-9}$. The spin echo techniques used in NMR might play here an important role. Summarising the results of this study:

- **for static imperfections the threshold for fault-tolerant quantum computation is decreased by a few orders of magnitude compared to the case of random errors;**
- **static imperfections are dangerous for quantum maps (periodic algorithms) because they can introduce spurious "physical" effects;**
- **new strategies for error correction should be developed to deal with static imperfections.**

A model for the Anderson transition

The third study we describe [3] concerns a quantum algorithm for the simulation of the Anderson metal-insulator (i.e. localised/delocalised) transition in disordered solids, and its sensitivity to static imperfections. In the past, various numerical studies allowed to obtain some values of critical exponents in the vicinity of the transition and to study certain system characteristics at the critical point. These numerical simulations are performed with the help of modern supercomputers and are at the border of their computational capacity.

In [9] it was shown that the evolution propagator in a regime of dynamical or Anderson localisation can be simulated efficiently on a quantum computer. However, this algorithm requires an amount of resources which is not accessible for current experimental implementations of quantum computers. We propose here a cheaper algorithm which can detect the Anderson transition with as little as $7-10$ qubits. The propagation on a unit time step is performed in $O(n_q^2)$ elementary quantum gates while in any known classical algorithm the number of gates scales as $O(2^{n_q})$. Our attention focuses on the vicinity of the critical point (because it is physically interesting), where the algorithm gives a quadratic speedup for the computation of the diffusion rate and the localisation length

The model we chose for this study is the generalised kicked rotator model. With respect to the basic kicked rotator, which is a quantum Hamiltonian map with $V(q) = \cos(q)$, the generalised map introduces a time dependent coefficient, so that $K \to \kappa(t) = [1 + \lambda\cos(\omega_1 t)\cos(\omega_2 t)]$, and replaces the free evolution Hamiltonian $\hat{p}^2/2\hbar$ with a generic function $H_0(\hat{p})$, such that the rotation phases $H_0(n)$ are randomly distributed in the interval $[0, 2\pi)$. For ω_1 irrational with respect to ω_2, this model shows the phenomenon of Anderson transition at some value $K = K_c$.

Implementation of the generalised kicked rotator

The random phase rotations $\exp[-iH_0(n)]$ are performed with the help of a pseudo-random circuit which applies (in temporal order): a) random phase shifts to all the n_q qubits; b) M controlled NOTs + random phase shifts on the target qubit on random locations; c) the sequence of the M controlled NOTs in the reverse order. We use $M \sim n_q$ that according to our tests generates good random phase values (more specifically, we have tested that K_c is the same as for truly random phases), thus this circuit involves $O(n_q)$ gates.

For the construction of the circuit for $V(q,t) = \kappa(t)\cos(q)$, it is convenient to single out the most significant bit of q, i.e. to use the notation $q = \pi a + \bar{q}$, where $a = 0$ or 1. Due to the relation $\cos(q) = (-1)^a\cos(\bar{q}) = \sigma_z\cos(\bar{q})$, with σ_z being the Pauli matrix acting on the first qubit, the kick operator takes the form $U_k = \exp[-i\sigma_z\kappa(t)\cos(\bar{q})]$. Let $S = e^{ia\bar{q}}$; as already shown, this is easily implementable with $n_q - 1$ controlled phase shifts. We want to show that U_k can be approximated to an arbitrary precision by a sequence of one-qubit gates applied to the first qubit and the diagonal operators S. To this aim we introduce the unitary operator

$$R_\gamma(\bar{q}) = HS^1H\, e^{-i\frac{\gamma}{2}\sigma_z}\, HS^{-2}H\, e^{-i\frac{\gamma}{2}\sigma_z}\, HS^1H$$

(H is the Hadamard gate on the first qubit). This operator can be exactly reduced to the form $\cos^2(\frac{\gamma}{2}) - \sin^2(\frac{\gamma}{2})\cos(2\bar{q}) - i\sigma_z\sin(\gamma)\cos(\bar{q}) + i\sigma_x\sin^2(\frac{\gamma}{2})\sin(2\bar{q})$ and hence for small γ we have

$$R_\gamma(\bar{q}) = e^{-i\sigma_z\gamma\cos(\bar{q})} + \frac{i\sigma_x\gamma^2}{4}\sin(2\bar{q}) + O(\gamma^3).$$

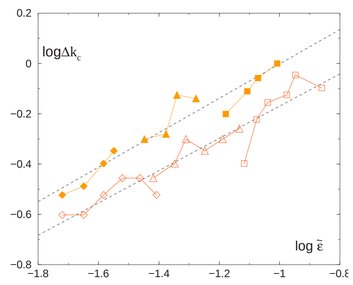
The term with γ^2 can be eliminated using the symmetric representation

$$\mathcal{P} = R_{\frac{\gamma}{2}}(\bar{q})R_{\frac{\gamma}{2}}(-\bar{q}) = e^{-i\sigma_z\gamma\cos(\bar{q})} + O(\gamma^3).$$

Thus the kick operator can be approximated by $U_k = \mathcal{P}^l + O(l\gamma^3)$, with $l = \kappa(t)/\gamma$. In our numerical experiments we used $\gamma \approx 0.2$. Thus, both the kick operator and the random phase evolution are implemented by simple circuits, whose depth is $O(n_q)$. The cost for one step of the generalised kicked rotator map is therefore determined by the Fourier transforms, i.e. it is $O(n_q^2)$. This algorithm does not use auxiliary qubits, and is to be preferred to that described in [9] for moderate values of $\kappa(t)$ (i.e. when l does not grow too much).

Static errors and the shift of the critical point

We focussed our studies on the effects of static errors, due to the fact that this type of imperfection was proven to be the most dangerous. We investigated the properties of the simulated system in the vicinity of the Anderson transition. In particular, we analysed the Inverse Participation Ratio (IPR) ξ, i.e. the number of levels on which the wave function is concentrated. ξ shows a sharp jump from $\xi \sim 1$ to $\xi \sim N = 2^{n_q}$, which takes places in a narrow interval of K values around the "critical point" K_c. This is a manifestation of the Anderson transition from localised to delocalised states. The critical point determined by a simulation on an imperfect quantum computer, $K_c(\epsilon)$, is shifted with respect to the perfect case. A method for detecting the position of the critical point is to measure the two most significant qubits in the momentum representation. This allows for the determination of the probability $W = \sum_{n=N/4}^{3N/4}|\psi_n|^2$ (the initial state is $|0\rangle$), which shows a sharp jump $W = 0 \to 0.5$ around K_c.



This figure shows the dependence of the shift of the critical point $\Delta K_c(\epsilon) = K_c - K_c(\epsilon)$ on the rescaled imperfection strength $\tilde{\epsilon} = \epsilon n_g\sqrt{n_q}$ for various values of ϵ and n_q. Open/full symbols are for $J = 0$ and $J = \delta$ respectively. The dashed lines show the scaling relation

$$\Delta K_c(\epsilon) \propto \tilde{\epsilon}^{\,\alpha} \qquad \text{with} \qquad \alpha \simeq 0.65$$

This result is consistent with our previous studies on static imperfections: all the effects can be understood in terms of the timescale of the fidelity, $t_f \sim 1/\tilde{\epsilon}$.

The coarse-grained characteristics of the probability distribution can be determined from few measurements of the most significant qubits, thus, even if each map step is simulated efficiently, the speedup is only quadratic near the critical point (see the paper for details). Above the critical point the speedup is even stronger. Summarising the results of this study:

- **we have shown an $O(n_q^2)$ algorithm for a non-trivial quantum map with a non-polynomial potential which does not use ancillae;**
- **the analysis of the shift of the critical point K_c under the effects of static errors confirm that the only relevant parameter is the fidelity timescale $t_f \sim 1/(\epsilon n_g\sqrt{n_q})$.**

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