Exponential Gain in Quantum Computing of Quantum Chaos and Localization

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We present a quantum algorithm which simulates the quantum kicked rotator model exponentially faster than classical algorithms. This shows that important physical problems of quantum chaos, localization, and Anderson transition can be modeled efficiently on a quantum computer. We also show that a similar algorithm simulates efficiently classical chaos in certain area-preserving maps.

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The massive parallelism of quantum evolution allows one to manipulate simultaneously exponentially many states through entanglement (see reviews [1,2]). That opens new horizons for computations based on quantum mechanics, as was stressed by Feynman [3]. Nevertheless, it is not so obvious if this parallelism can be used to speed up exponentially any given computational algorithm. There is certainly no systematic way to do this, and that is why so much interest has been generated by the Shor quantum algorithm [4] which factorizes large numbers exponentially faster than any known classical algorithm. At present very few other quantum algorithms have been found in which substantial computational gain is achieved compared to classical computing. Among them is the Grover algorithm [5] which significantly accelerates the problem of searching an unsorted database, although the gain is not exponential. In addition, quantum computers can be used as analog machines to simulate some many-body quantum systems which are hardly accessible in usual computer simulations [6]. In this way some systems such as spin lattices can be modeled very naturally, for example, by cold atoms in optical lattices [7]. However, this kind of simulation is restricted to systems whose physical elements are related or similar to the qubits (spin halves) of a quantum computer. At present apart from these natural examples there are no developed quantum algorithms which would allow one to reach exponential gain in the computation of the quantum dynamics of physical systems.

It is therefore desirable to find a quantum algorithm corresponding to a physical model with rich and complex quantum dynamics. During the last decades, it has been understood that generally the dynamics of classical nonlinear systems is chaotic [8]. The corresponding quantum dynamics, called quantum chaos, demonstrates a rich and complex behavior even for systems with only a few degrees of freedom and rather simple Hamiltonians [9]. One of the cornerstone models in the study of quantum chaos is the kicked rotator. In the classical limit, this model reduces to an area-preserving map called the Chirikov standard map [10] which has applications in different fields of physics, such as particle confinement in magnetic traps, beam dynamics in accelerators, comet trajectories, and many others [8]. The map depends on only one parameter, and depending on its value the system can be in the near-integrable bounded regime, with Kolmogorov-Arnold-Moser (KAM) curves, or in the fully chaotic regime with diffusive growth of momentum which statistically can be described by the Fokker-Planck equation. In between these two regimes the phase space of the system has a complex hierarchical structure with integrable islands surrounded by a chaotic sea at smaller and smaller scales. The quantum dynamics corresponding to these different regimes have been intensively studied by different groups in the field of quantum chaos [11]. Many phenomena of general importance are present in this model, including quantum ergodicity, spectral statistics as in random matrix theory, quantum KAM regime, and many others. However, the most unexpected quantum effect is the phenomenon of dynamical localization, in which quantum interference suppresses chaotic diffusion in momentum, leading to exponentially localized eigenstates. This effect has close analogy with Anderson localization of electrons in disordered materials [12], and therefore this model enables one to study also the properties of Anderson localization, a solid-state problem still under intense investigation nowadays. The quantum kicked rotator describes also the properties of microwave ionization of Rydberg atoms [13]. It has been realized experimentally with cold atoms, and the effects of dynamical localization, external noise, and decoherence have been studied experimentally [14].

In this paper we present a quantum algorithm which computes the evolution of the quantum kicked rotator exponentially faster than any classical computation. It simulates the kicked rotator with N levels in $O((\log_2 N)^3)$ operations instead of $O(N \log_2 N)$ for the classical algorithm.

The classical dynamics of the system is given by the Chirikov standard map

$$\bar{n} = n + k \sin\theta; \qquad \bar{\theta} = \theta + T\bar{n}, \tag{1}$$

where (n, θ) is the pair of conjugated momentum (action) and angle variables, and the bars denote the resulting variables after one iteration of the map. In this way the dynamics develops on a cylinder (periodicity in θ) which

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can also be closed to form a torus of length $N = 2\pi L/T$ where L is an integer. The classical dynamics depends only on one single chaos parameter $K = kT$, so that the motion is globally chaotic for $K > 0.9716\ldots$. For $K \gg 1$ the orbits spread diffusively in n with diffusion rate $D = n^2/t \approx k^2/2$ where t is measured in number of iterations (kicks) [8,10]. In the chaos regime, the dynamics is characterized by positive Kolmogorov-Sinai entropy $h \approx \ln(K/2) > 0$, due to which trajectories diverge exponentially and round-off errors grow exponentially with t [15].

The quantum evolution during one period is described by a unitary operator acting on the wave function ψ

$$\bar{\psi} = \hat{U}\psi = e^{-ik\cos\hat{\theta}} e^{-iT\hat{n}^2/2}\psi\,, \qquad (2)$$

where $\hat{n} = -i\partial/\partial\theta$, $\hbar = 1$. In this way the classical limit corresponds to $k \to \infty$, $T \to 0$ while keeping $K = kT = \text{const}$ [11]. The quantum interference leads to exponential localization of the eigenstates $\chi_m(n)$ of the operator $\hat{U}$ in the momentum space n with envelope $\chi_m(n) \sim \exp(-|n - m|/l)/\sqrt{l}$ where m marks also the center of the eigenstate and l is the localization length. In the regime of quantum chaos ($k \gg K \gg 1$) this length is determined by the classical diffusion rate $l = D/2 \approx k^2/4$ [11]. The evolution takes place on N levels with periodic boundary conditions. For $l \gg N$ the eigenstates become ergodic and the level spacing statistics is described by random matrix theory [11]. Therefore depending on the parameters various regimes of quantum chaos can be investigated in this single model.

The evolution operator $\hat{U}$ is the product of two unitary operators $\hat{U}_k = \exp(-ik\cos\hat{\theta})$ and $\hat{U}_T = \exp(-iT\hat{n}^2/2)$ which represent, respectively, the effects of a kick and free rotation. These operators are diagonal in the θ and n representations, respectively. Because of that the most efficient way to simulate the quantum dynamics of this system on a classical computer is to perform forward/backward fast Fourier transforms (FFT) to go from one representation to the other [16], doing diagonal multiplications by U_k and U_T between each FFT. In this way, for a system with N levels, the FFT requires $O(N\log_2(N))$ operations and the diagonal multiplications take $O(N)$ operations, so that evolution on one period is performed in $O(N\log_2(N))$ operations [17]. Our construction of the quantum algorithm keeps the global structure of this classical algorithm, and uses quantum parallelism to speed up exponentially each algorithmic step.

Step I: Preparation of the input state.—We consider a system of n_q qubits; the Hilbert space of dimension $N = 2^{n_q}$ is used to describe N momentum states (eigenstates of the operator $\hat{U}_T$ for $0 \le n \le N - 1$ in binary code) on which evolves the kicked rotator. An initial state $\psi(0) = \sum_{n=0}^{N-1} a_n|n\rangle$ at time $t = 0$ is prepared by rotations of individual qubits and two-qubit gates from the ground state $|0,\ldots,0\rangle$. For example, a typical initial state used in the studies of the kicked rotator dynamics [11], such as $\psi(0) = |N/2\rangle$, requires only one individual rotation. We need also auxiliary registers which will be used later; at the moment they are all in the ground state.

Step II: Action of free propagation operator $\hat{U}_T$.—In the n representation $\hat{U}_T$ is diagonal so that $\hat{U}_T|n\rangle = \exp(-iTn^2/2)\,|n\rangle$. The simultaneous multiplication of the N coefficients can be done in n_q^2 gate operations. Indeed, if $n = \sum_{j=0}^{n_q-1} \alpha_j 2^j$, then $n^2 = \sum_{j_1,j_2} \alpha_{j_1}\alpha_{j_2} 2^{j_1+j_2}$. Therefore $\exp(-iTn^2/2) = \Pi_{j_1,j_2} \exp(-iT\alpha_{j_1}\alpha_{j_2}2^{j_1+j_2-1})$ with $\alpha_{j_{1,2}} = 0$ or 1. As a result, this step can be realized with n_q^2 operations of the two-qubit gate applied to each qubit pair (j_1, j_2) which keeps the states $|00\rangle, |01\rangle, |10\rangle$ unchanged while $|11\rangle$ is transformed to $\exp(-iT2^{j_1+j_2-1})\,|11\rangle$ [18].

Step III: Change from n to θ representation.—In analogy with the classical algorithm, we can use the quantum Fourier transform (QFT) (described in detail, for example, in [1]). The QFT requires $O(n_q^2)$ operations with one-qubit rotations and two-qubit gates similar to the ones described above. After the QFT, we obtain the wave function in the θ representation, $\sum_{i=0}^{N-1} b_i|\theta_i\rangle$, where the θ_i are the binary codes of $N = 2^{n_q}$ discretized angles. We note that the QFT was discussed in [19] for simulating a rather specific model, the quantum baker map.

Step IV: Construction of a supplementary register holding the cosines of angles.—This step transforms $\sum_{i=0}^{N-1} b_i|\theta_i\rangle\,|0\rangle$ into $\sum_{i=0}^{N-1} b_i|\theta_i\rangle\,|\cos\theta_i\rangle$. The second register is, of course, present since step I, but is used only at that step. After these operations, it contains the binary codes of the N values of $\cos\theta_i$, correlated with θ_i in the first register. The number of qubits p in this second register sets the precision of the cosines at 2^{-p}, and should be equal to or greater than n_q. This register will be used in the next step to perform the kick operator $\hat{U}_k$. To realize this transformation, we need a few auxiliary registers which can be erased at the end. First we precompute the $2n_q$ values $\cos(2\pi/2^j), \sin(2\pi/2^j)$, for $j = 1,\ldots,n_q$ with precision 2^{-p}. This can be done quantum mechanically or classically in polynomial time by first computing the case of smallest angle and then using recursive relations, doubling the angle each time. Also, other classical methods converging superexponentially (e.g., Newton's) can be used. We decompose θ_i in binary code $\theta_i = \sum_{j=1}^{n_q} \beta_{ij} 2\pi/2^j$ and use the formula $\exp(i\theta_i) = \Pi_{j=1}^{n_q} \exp(i\beta_{ij}2\pi/2^j) = \Pi_{j=1}^{n_q}[\cos(\beta_{ij}2\pi/2^j) + i\sin(\beta_{ij}2\pi/2^j)]$, with $\beta_{ij} = 0$ or 1, to compute $\cos\theta_i$ and $\sin\theta_i$ in $4n_q$ multiplications. This can be done in parallel for all N values of θ_i in $O(n_q p^2)$ gate operations. We need for that an auxiliary register with p qubits on which $\sin\theta_i$ is built. We start therefore with $\sum_{i=0}^{N-1} b_i|\theta_i\rangle\,|1\rangle\,|0\rangle$, then we perform the transformation $\sum_{i=0}^{N-1} b_i|\theta_i\rangle\,|c\rangle\,|d\rangle \to \sum_{i=0}^{N-1} b_i|\theta_i\rangle\,|\cos(\beta_{ij}2\pi/2^j)c - \sin(\beta_{ij}2\pi/2^j)d\rangle\,|\sin(\beta_{ij}2\pi/2^j)c + \cos(\beta_{ij}2\pi/2^j)d\rangle$ for $j = 1,\ldots,n_q$ (initially $|c\rangle = |1\rangle$, $|d\rangle = |0\rangle$). This transformation needs a controlled multiplier with the qubit j as control qubit. The quantum circuits realizing a controlled multiplier are described in [20], and require $O(p^2)$ gate operations for each multiplier. After n_q transformations we obtain $\sum_{i=0}^{N-1} b_i|\theta_i\rangle\,|\cos\theta_i\rangle\,|\sin\theta_i\rangle$.

The total number of gate operations for step IV is therefore $O(n_q p^2)$. We note again that p determines the precision with which the $\cos\theta_i$ are computed. A reasonable regime is $n_q \leq p \leq 2n_q$ which gives a total number of gate operations for this step of $O(n_q^3)$. Besides the three registers already described, some auxiliary registers are necessary to perform these operations. It can be done with five additional registers of size p, but it is probably possible to decrease this number. After that only the registers holding θ_i and $\cos\theta_i$ will be used, and all others can be erased. The auxiliary registers holding intermediate values of cosines and sines can be reused after each multiplication by $\exp(i\beta_{ij}2\pi/2^j)$ is performed, since they can be erased by using multiplication by $\exp(-i\beta_{ij}2\pi/2^j)$ and subtraction.

Step V: Action of kick operator $\hat{U}_k$.—After the previous steps, the state of the system is $\psi = \sum_{i=0}^{N-1} b_i |\theta_i\rangle |\cos\theta_i\rangle$. In the angle representation, the action of $\hat{U}_k$ is diagonal so that $\hat{U}_k|\theta_i\rangle = \exp(-ik\cos\theta_i)|\theta_i\rangle$. Each state $|\theta_i\rangle$ is entangled with $|\cos\theta_i\rangle$ holding the binary code of $\cos\theta_i = \sum_{j=1}^{p} \gamma_{ij} 2^{-j}$, with $\gamma_{ij} = 0$ or 1. Since $\exp(-ik\cos\theta_i) = \Pi_{j=1}^{p} \exp(-ik\gamma_{ij}2^{-j})$, to perform the multiplication, it is therefore enough to apply to each qubit of the second register the one-qubit gate which takes $|0\rangle$ to $|0\rangle$ and $|1\rangle$ to $\exp(-ik2^{-j})|1\rangle$. Only p gate operations (with $n_q \leq p \leq 2n_q$) are used for this transformation. After this $|\cos\theta_i\rangle$ is reversibly erased. As a result of this step, the state of the system is now $\sum_{i=0}^{N-1} b_i \exp(-ik\cos\theta_i)|\theta_i\rangle|0\rangle$.

Step VI: Change from θ to n representation.—This step is similar to step III, it performs backwards the QFT on the first register $|\theta_i\rangle$ and returns the wave function to the momentum basis in $O(n_q^2)$ operations. This gives the wave function of the kicked rotator after one iteration of map (2) (one kick step).

In this way one kick iteration requires $O(n_q^3)$ gate operations. Subsequent kicks are realized using steps II-III-IV-V-VI, since step I is done only once. As a result, a quantum computer can perform the kicked rotator evolution exponentially faster than a classical computer [which needs $O(n_q 2^{n_q})$ operations per kick]. Several successive measurements after t iterations can give the largest probabilities $|a_i|^2$ in the momentum basis from which, for example, the localization length l can be extracted with only a few measurements. Other average characteristics can be obtained efficiently by performing the QFT followed only by a few measurements, giving, for example, the largest harmonics of the probability distribution.

Some modifications in this algorithm are possible. Instead of the additional register $|\cos\theta_i\rangle$ one can use a register holding a uniform polynomial approximation $P(\theta) \approx \cos\theta$. This is actually the technique used in classical computation, where Chebychev polynomials are used. The construction of the polynomial of degree p is done iteratively, starting from the lowest-degree monom and multiplying it by θ_i to obtain the next one. An additional register holds the current power of θ_i between each step. The coefficients of the polynomial should be precomputed in advance. The transition from one degree to another requires $O(p^2)$ gate operations for p qubits, so that the whole process needs $O(p^3)$ operations. For $p \sim n_q$, this is similar to step IV. After computing the register $|P(\theta_i)\rangle$ the next step is unchanged and performs multiplication by $\exp(-ikP(\theta))$ [21].

The generalized models of kicked rotator, where $k\cos\theta$ is replaced by another function $V(\theta)$, are also of interest. In general, it is not obvious if the register $|V(\theta_i)\rangle$ in step IV can be computed in polynomial time, so uniform polynomial approximations can be the only way. A case of particular interest is $V(\theta) = 2\arctan(E - 2k\cos\theta)$, where E and k are parameters. In this case, the kicked rotator can be exactly mapped on a solid-state system on a chain with only nearest-neighbor hopping, as it had been shown in [12]. This computation can be done via uniform polynomial approximation. It may also be possible that this $V(\theta)$ can be computed directly in parallel from registers $|\cos\theta\rangle|\sin\theta\rangle$.

The generalized kicked rotator can also model the localization properties in higher dimensions. For example, if the parameter E varies from kick to kick, for example, $E = -2k\cos(\omega_1 t) - 2k\cos(\omega_2 t)$ where $\omega_1/(2\pi)$ and $\omega_2/(2\pi)$ are two incommensurate frequencies, then the model can be mapped on the three-dimensional Anderson model which displays a metal-insulator transition [22]. For $k < k_c \approx 0.46$ the dynamics is localized in momentum space, while for $k > k_c$ it becomes diffusive and ergodic over all the available space of size N. Similar effects were observed recently in quasiperiodically driven cold atoms [23]. However, this latter model is still operating on a kicked rotator with 1 degree of freedom. One can consider a d-dimensional version of (2) with $\hat{U}_k = \exp(-ik\sum_{r=1}^{d} \times \cos\theta_r)$ and $\hat{U}_T = \exp[-iT\sum_{r=1}^{d} n_r(n_r + \sum_{r<r'}^{d} n_{r'})/2]$, which is directly related to the d-dimensional Anderson localization problem. The simulation of this model on a system of size $N = 2^{n_q}$ for each momentum n_r requires $O(N^d \log_2 N)$ operations on a classical computer since the total basis contains N^d levels. Even for $d = 2$ this model is hardly accessible for today's computers [24]. On the contrary, our quantum algorithm can be directly extended to higher dimensions by increasing the number of registers by a factor d, and the number of operations becomes only $O(dn_q^3)$. For $d = 2$ by changing $\hat{U}_T$ to $\hat{U}_T = \exp[-iT(n_1^2 + n_2^2)/2 - ig\delta_{n_1,n_2}]$ it is possible to simulate the problem of two interacting particles in a localized phase [25]. We note that usually one needs an exponential number of gates to simulate a quantum map operator, and a simulation in polynomial time is not obvious. For example, for the extensively studied kicked top [26] the QFT cannot be used to change representations.

It is interesting to note that on the basis of the algorithm constructed above, one can simulate also the classical map (1). Indeed, the discretization of the map can be done in a symplectic way [27] on a phase space lattice of size $N \times N$:

$$\bar{Y} = Y + S_N(X); \qquad \bar{X} = X + \bar{Y} (\mathrm{mod} N) \qquad (3)$$

with $S_N(X) = [NK\sin(2\pi X/N)/(2\pi)]$, $[\ldots]$ being the

integer part and X, Y integers. This map is area preserving and invertible. An initial classical phase space density can therefore be modeled by a quantum state $\sum_{i_1,i_2} a_{i_1,i_2}|X_{i_1}\rangle|Y_{i_2}\rangle|0\rangle$. Then we use step IV to transform it in $\sum_{i_1,i_2} a_{i_1,i_2}|X_{i_1}\rangle|Y_{i_2}\rangle|S_N(X_{i_1})\rangle$ in $O(\log_2(N)^3)$ operations, performed only once at the beginning. After that the map is reduced to simple additions in the first two registers and require only $O(\log_2(N))$ operations per iteration, simulating exponentially many trajectories in polynomial time. A simulation on a classical computer requires $O(N^2)$ operations per iteration if one simulates a density distributed over $O(N^2)$ lattice cells. After t iterations a_i give the density probability distribution in phase space. QFT can be used to determine the main harmonics of the density, which can be measured by running the algorithm several times.

In conclusion, the algorithm presented here shows that important systems displaying rich and complex properties like classical and quantum chaos, quantum localization, and ergodicity can be simulated exponentially faster on a quantum computer. This allows one to study the time evolution of these systems and the transition between classical and quantum mechanics in the limit of large quantum numbers (semiclassical limit). Using a few tens of qubits can probe this limit far beyond what is possible on today's computers. The problem of the precision of such quantum computation is crucial, and the effects of imperfections should be studied in detail for different physical properties of the simulated system (some of them can be quite sensitive [28]).

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