Simulation of quantum systems on a realistic quantum computer

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Why Quantum computation ?

- According to Moore's law, chips will scale down to atomic size around 2020. It is thus likely that quantum effects will become important by then.
- Unitary evolution in quantum mechanics is reversible: no energy dissipation on small scale, so no limitation a priori upon computation size caused by power requirements.
- Simulation of physical quantum systems with an exponentially large Hilbert space.
- Some computational problems could be solved by a quantum computer more efficiently than by any classical computer.

Qubit

- *qubit:* elementary unit of quantum information recorded in a two-state quantum system (spin $1/2$, two-level atom, ...)
  these states are labeled $|0\rangle$ and $|1\rangle$
  General state of a qubit: $\alpha|0\rangle + \beta|1\rangle$ with $\alpha^2 + \beta^2 = 1$

- *quantum computer:* ensemble of n coupled qubits $=$ Hilbert space with 2^n orthogonal quantum states
  each basis state is labeled $|i\rangle$ with i n-bit binary number

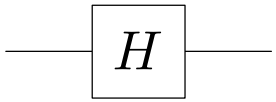
  example for 3 qubits:

$\|000\rangle$	$\|100\rangle$
$\|001\rangle$	$\|101\rangle$
$\|010\rangle$	$\|110\rangle$
$\|011\rangle$	$\|111\rangle$

Quantum gates

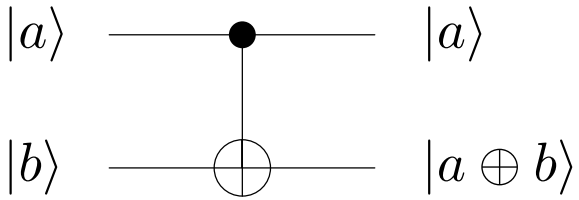
Quantum gate: unitary operation on several qubits

Hadamard



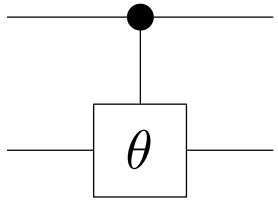
$$\begin{cases} |0\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ |1\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \end{cases}$$

Controlled-NOT



$$\begin{cases} |00\rangle \rightarrow |00\rangle \\ |01\rangle \rightarrow |01\rangle \\ |10\rangle \rightarrow |11\rangle \\ |11\rangle \rightarrow |10\rangle \end{cases}$$

Controlled-Phase



$$\begin{cases} |00\rangle \rightarrow |00\rangle \\ |01\rangle \rightarrow |01\rangle \\ |10\rangle \rightarrow |10\rangle \\ |11\rangle \rightarrow e^{i\theta}\,|11\rangle \end{cases}$$

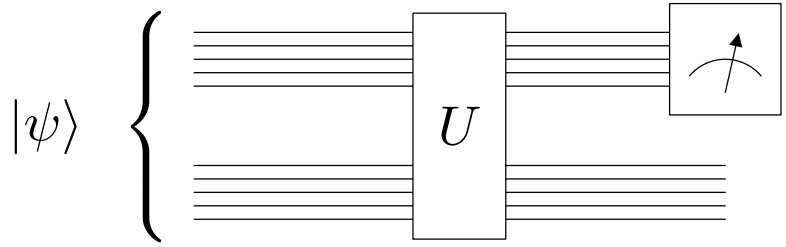
Universal set of gates

Each unitary transformation in the Hilbert space can be decomposed into (for example):

1. Single qubit rotations
2. Two-qubit gate (Controlled-NOT)

Quantum algorithm

A quantum algorithm consists of 3 steps



preparation unitary evolution measure

Quantum Fourier Transform

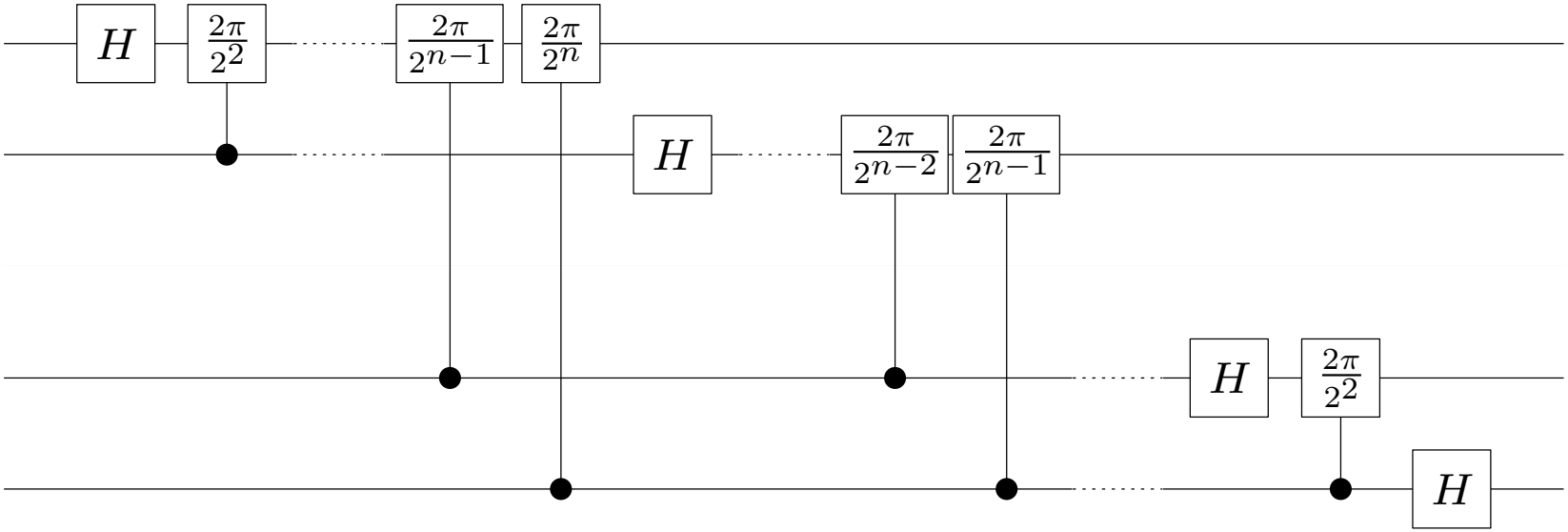
Given a register of n qubits, the QFT operation is defined on each of the $N = 2^n$ states of the Hilbert space by

$$QFT : |a\rangle \mapsto \frac{1}{\sqrt{N}} \sum_{c=0}^{N-1} \exp(2\pi i a c/N) \, |c\rangle$$

With $\tilde{f}$ discrete Fourier transform of f,

$$QFT : \sum_a f(a) \, |a\rangle \mapsto \sum_c \tilde{f}(c) \, |c\rangle$$

QFT can be perfomed with only 2 types of gate: Hadamard and controlled-phase



Thus with n qubits, the number of steps required is: $\frac{n(n+1)}{2} \sim O\left(n^2\right)$

To compare, the classical Fast Fourier Transform requires $\sim O(n2^n)$ operations.

However, even if it does compute the FFT of a complex vector, the result can't be exctracted efficiently. The QFT is not an algorithm by itself, it must be embedded in a larger procedure, like the Shor algorithm.

Quantum algorithms

Factorisation algorithm (Shor, 1994)

Problem: given an integer N, find its prime factors (useful for RSA scheme).

With the best known classical algorithm, the number of computational steps is (with $n = \log_2 N$):

$$O\left(\exp\left(n^{\frac{1}{3}}(\log n)^{\frac{2}{3}}\right)\right)$$

$N \sim 10^{130}$: $t_c \approx 30$ days on a nowadays computer

$N \sim 10^{260}$: $t_c \approx 10^6$ years

Quantum factoring:

$$O\left(n^2 \log n \log(\log n)\right)$$

$t_q \approx 7$ hours (for 2.10^{10} gates on 10^3 qubits, switching rate 1MHz)

$t_q \approx 50$ hours

Quantum algorithms

Search algorithm (Grover, 1996)

Problem: Find a particular item in an unstructered list of N items.

Classical: $O(N)$ Quantum: $O\left(\sqrt{N}\right)$

Simulation of quantum systems

Quantum computers can simulate physical quantum systems without an exponential growth of the needed resources. Algorithms have been proposed to simulate many-body quantum systems, spin systems and quantum maps.

• Experimental NMR implementation of the quantum baker's map by Y. S. Weinstein, S. Lloyd, J. Emerson and D. G. Cory, Phys. Rev. Lett. **89**, 157902 (2002).

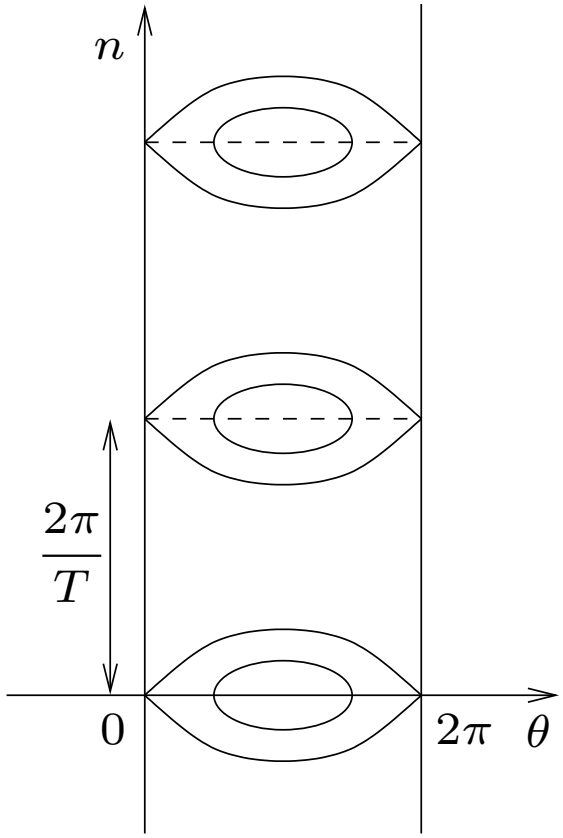
Classical kicked rotator

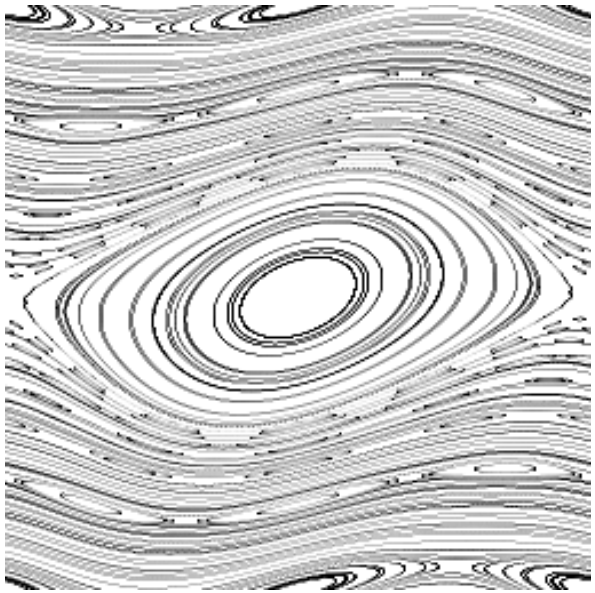
Classical kicked rotator (Chirikov standard map)

$$\begin{cases} \bar{n} &= n + k\sin\theta \\ \bar{\theta} &= \theta + T\bar{n} \end{cases}$$

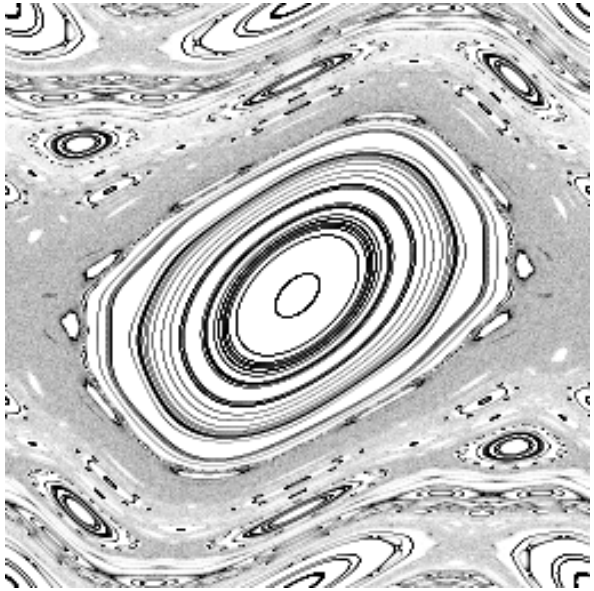
The behaviour of this system depends on $K = kT$

- $K = 0 \Rightarrow$ integrability
- $0 < K < K_g \approx 0.97 \Rightarrow$ mixed phase space, no diffusion in momentum
- $K \gg K_g \Rightarrow$ chaos, classical diffusion of n

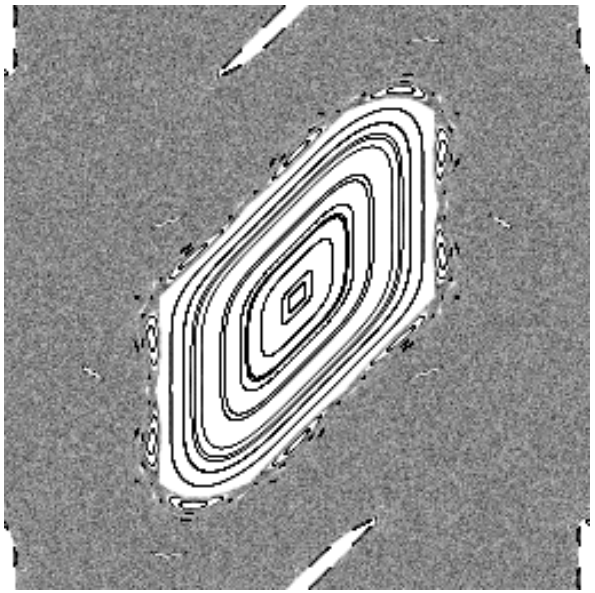




$K = 0.5$



$K = K_g$



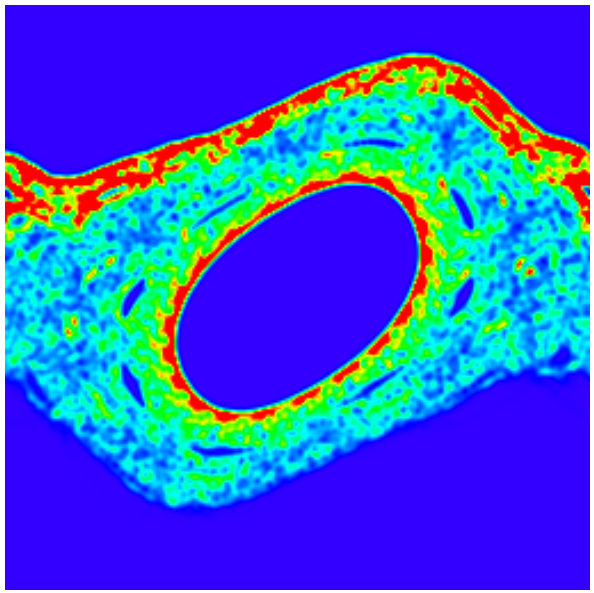
$K = 2$

Quantum kicked rotator

This system displays quantum chaos, and modelizes Rydberg atoms and Anderson localization of electrons in solids. The evolution operator is

$$\hat{U} = e^{-ik\cos\hat{\theta}}\, e^{-iT\frac{\hat{n}^2}{2}}$$

The system's behaviour now depends on 2 parameters: K and T (here $\hbar = 1$).

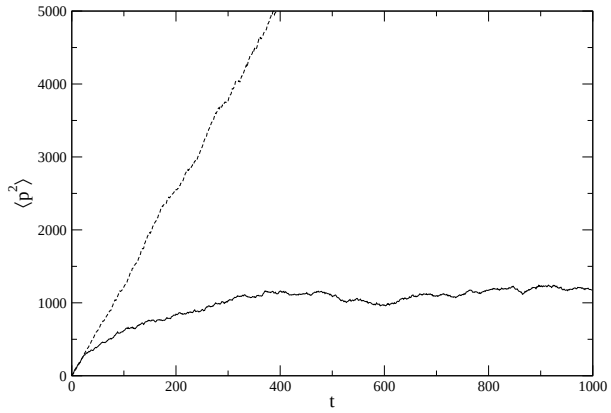


Husimi distribution for $K = K_g$

Dynamical localization

Classical case

Diffusion of momentum p in phase space, for $K > K_g$. The diffusion rate D can be approximated by $D \approx \frac{k^2}{2}$ for $K \gg 1$.



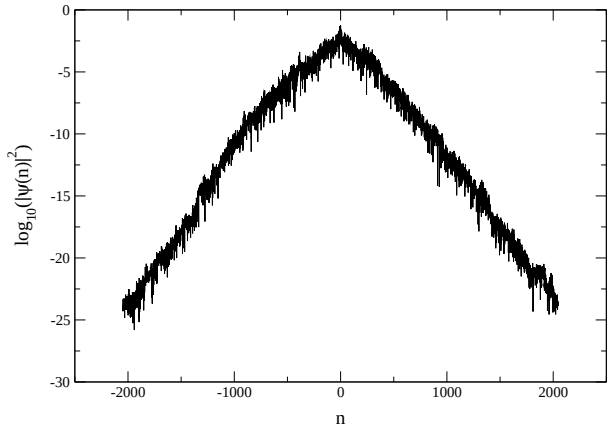
Quantum case

The eigenstates of $\hat{U}$ are exponentially localized

$$\psi(n) \approx \frac{1}{4l} e^{-\frac{|n-n_0|}{l}}$$

with the localization length

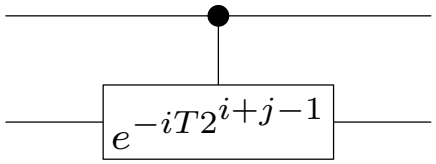
$$l \approx \frac{D}{2}$$



Quantum algorithm

Developped by B. Georgeot and D. L. Shepelyansky, Phys. Rev. Lett. **86**, 2890-2893 (2001).

1. application on every pair of qubits (i, j) of the gate



2. QFT to express ψ in θ representation
3. construction of a supplementary register holding the cosines of angles

$$\sum_{i=0}^{N-1} b_i|\theta_i\rangle|0\rangle \rightarrow \sum_{i=0}^{N-1} b_i|\theta_i\rangle|\cos\theta_i\rangle$$

4. application on each qubit j of the second register of the transformation

$$\begin{pmatrix} 1 & 0 \\ 0 & e^{-ik2^{-j}} \end{pmatrix}$$

5. inverse QFT to switch back to n representation

$O\left(n_q^3\right)$ steps

Classically

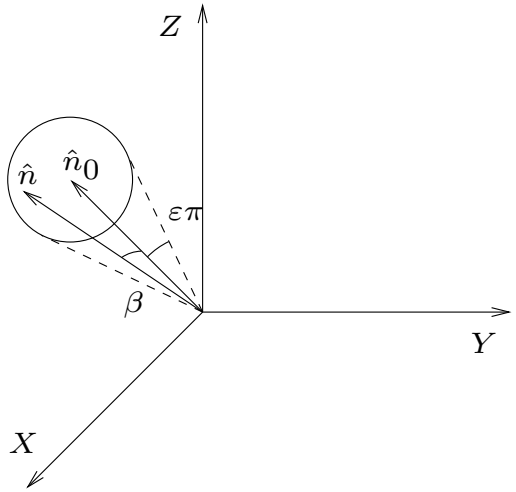
$O(n_q 2^{n_q})$ steps

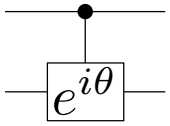
Noisy quantum gates

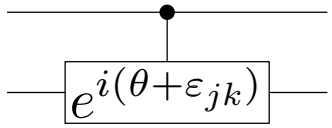
Each basic unitary operation is rotated by a small random angle of amplitude $\varepsilon \ll 1$ (however the kick operator is performed exactly).

Without noise, operation H is written as $\hat{n}_0 \cdot \vec{\sigma}$.

With imperfection $H = \hat{n}_j \cdot \vec{\sigma}$ is achieved by choosing a unit vector $\hat{n}_j$ tilted by an angle ε_j ($\leq \varepsilon$) from $\hat{n}_0$.



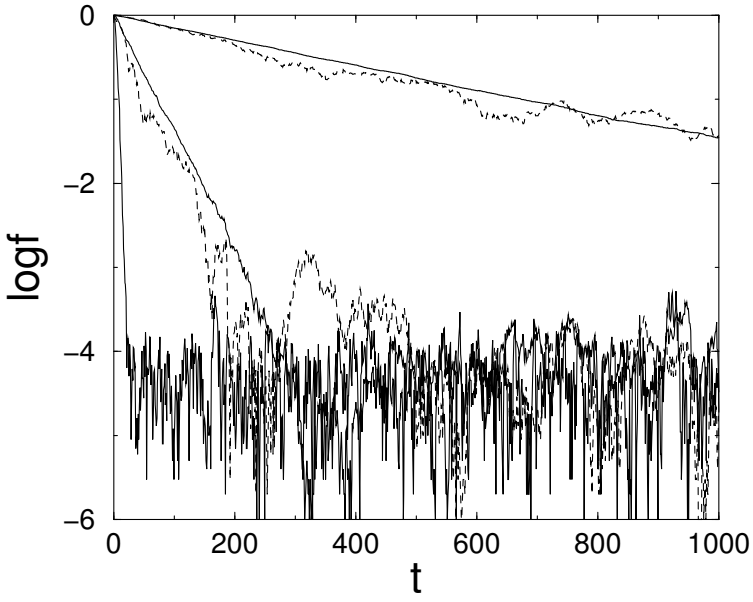
The two-qubit gate 

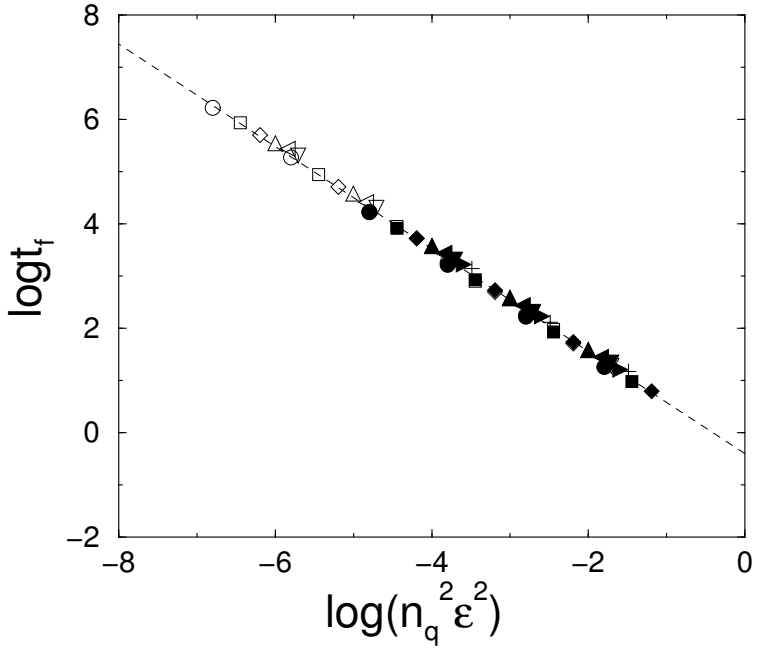
is simply replaced by 

with a random $|\varepsilon_{jk}| \leq \varepsilon$.

Fidelity in presence of errors

The fidelity of the quantum state is defined by $f(t) = \left|\langle\psi_\varepsilon(t)|\psi_0(t)\rangle\right|^2$





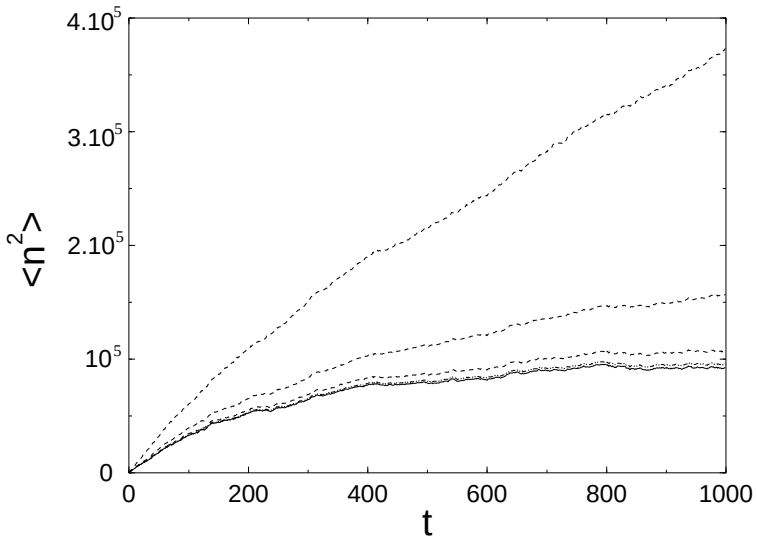
t_f : time for which fidelity drops under 0.5

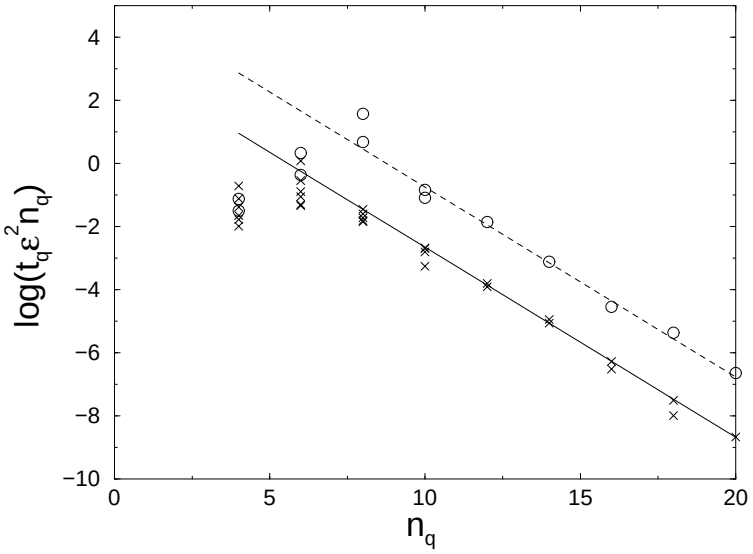
$$t_f \sim \frac{1}{n_q^2 \varepsilon^2}$$ Polynomial in n_q

Second moment in presence of errors

See also P. H. Song and D. L. Shepelyansky, Phys. Rev. Lett. **86**, 2162 (2001)

t_q : time for which $\langle n^2 \rangle$ reaches twice the value without noise





$$t_q \sim \frac{1}{\varepsilon^2 n_q 2^{2n_q}}$$

Exponential in n_q

Effects of noisy gates on Wigner and Husimi functions

The wave function can be represented using Wigner function to allow comparison between classical and quantum cases. The Wigner function is calculated from the wave function represented in θ space (with $\Theta = N\frac{\theta}{2\pi}$)

$$W(\theta, n) = \sum_{m=0}^{N-1} \frac{e^{-\frac{2i\pi}{N}n(m-\Theta/2)}}{2N} \psi(\Theta - m)^* \psi(m)$$

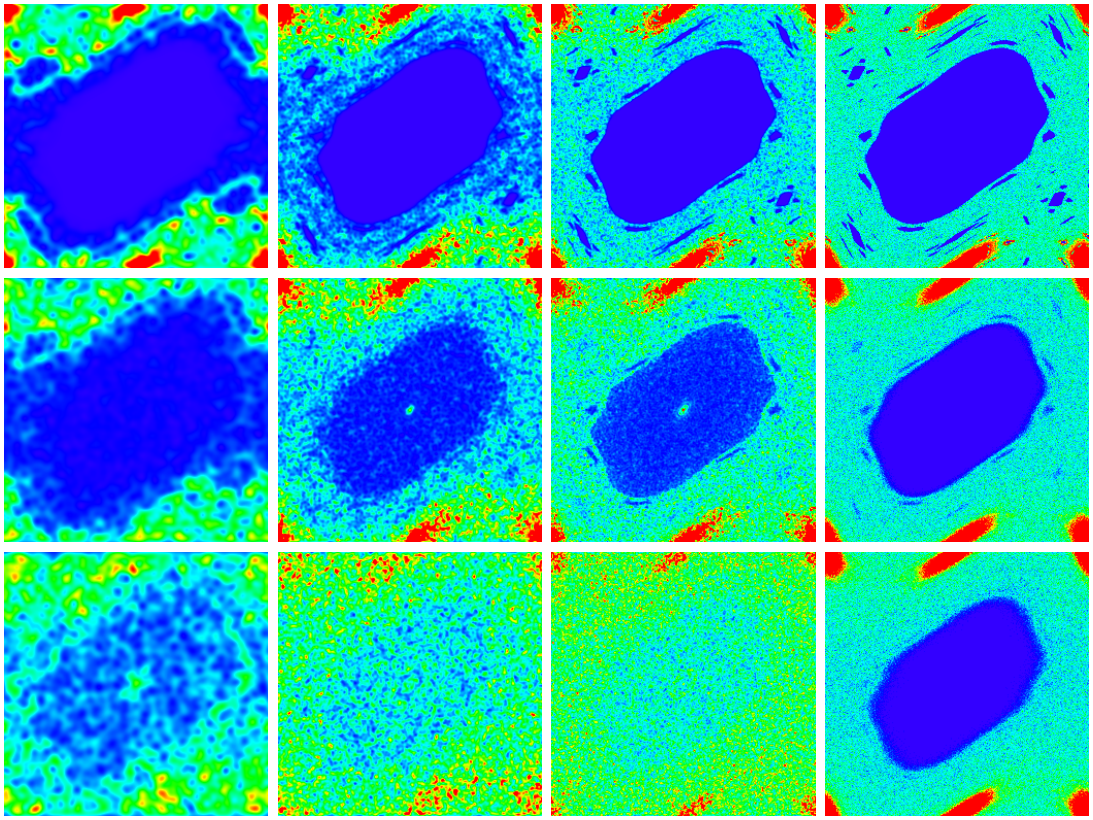
An arbitrary point of the Wigner function can be computed with a quantum algorithm which was proposed in C. Miquel, J. P. Paz, M. Saraceno, E. Knill, R. Laflamme and C. Negrevergne Nature **418**, 59-62 (2002).

$K = 1.3$ $n_q = 9$ $n_q = 12$ $n_q = 14$ Classical

$\varepsilon = 0$

$\varepsilon = 2.10^{-3}$

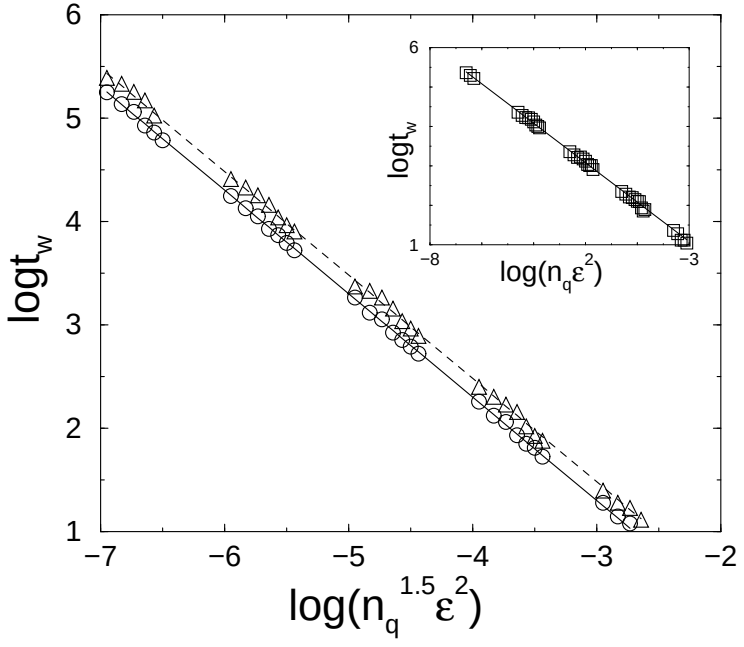
$\varepsilon = 4.10^{-3}$



Husimi distribution (gaussian smoothing of Wigner function)

To evaluate the effects of noise on individual values of the Wigner function, we define the relative error by $\delta W_\varepsilon = \langle |W - W_\varepsilon| \rangle / \langle |W| \rangle$

t_W: time for which δW_ε reaches $1/2$.



$K = K_g$, $T = 2\pi/N$ (one cell), chaotic zone ($\bigcirc$) and integrable zone ($\triangle$).

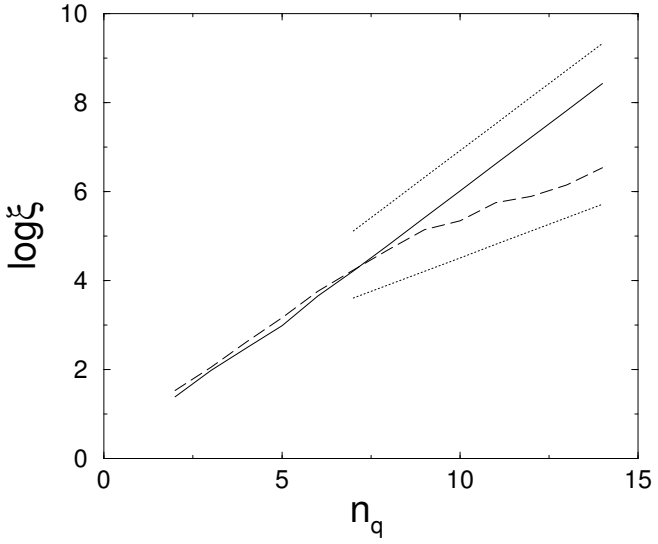
Inset: $T = 0.5$ and $K = 5$, localized zone

$$\boxed{t_W \sim \frac{1}{n_q^\alpha \varepsilon^2}}$$ polynomial in n_q

Efficiency of quantum computation of Wigner function

The value of the Wigner function for a specific point can be measured as the expectation value of the Z observable for an ancilla qubit: $W(q,p) = \frac{1}{2N}\langle Z \rangle$

The inverse participation ratio is defined by $\xi = (\sum W_i^2)^2 / (\sum W_i^4)$. It represents roughly the number of peaks in the Wigner function.

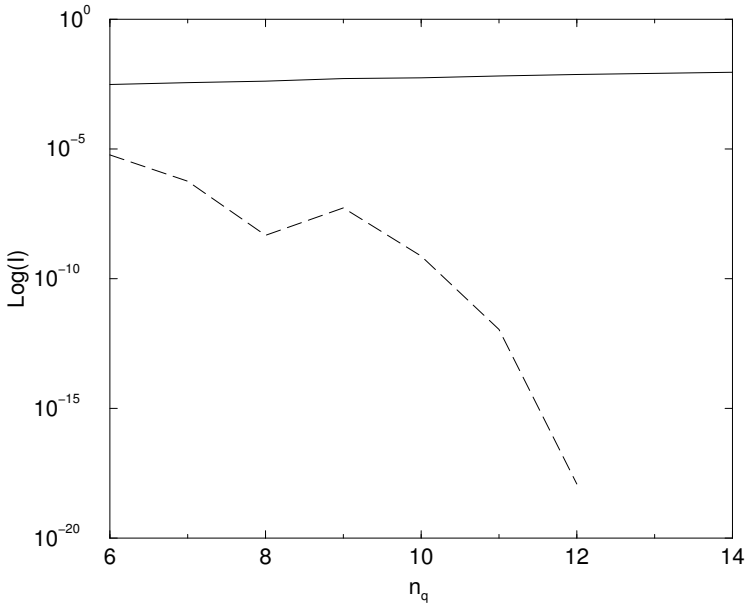


$T = 2\pi/N$ (full line):
$\xi \sim N^2 \Rightarrow \langle Z \rangle \sim \frac{1}{\sqrt{N}}$ Non efficient

T constant ($T = 0.5$, dashed line):
$\xi \sim N \Rightarrow \langle Z \rangle \sim 1$ Efficient

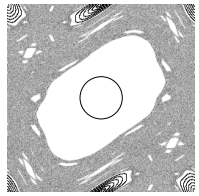
Tunneling into an island of integrability

Invariant curves cannot be crossed classically, and only quantum tunneling can transfer probability inside integrable islands. However, errors in quantum gates can turn the exponential decrease of exact tunneling into a polynomial growth (with respect to n_q).



Scaling of I with n_q (solid line: $\varepsilon = 3.10^{-3}$, dashed line: $\varepsilon = 0$)

$$I \approx \int_{disc} H(q,p)\, dq\, dp$$



With errors:

$$I(t) \sim n_q^{\alpha} \varepsilon^2 t \quad \text{with } \alpha \approx 1.3$$

Kicked Harper Model

Harper model

The Harper model was introduced in 1955 to describe the motion of electrons in a 2-dimensional lattice with a perpendicular magnetic field.

$$H = L\cos p + K\cos q$$

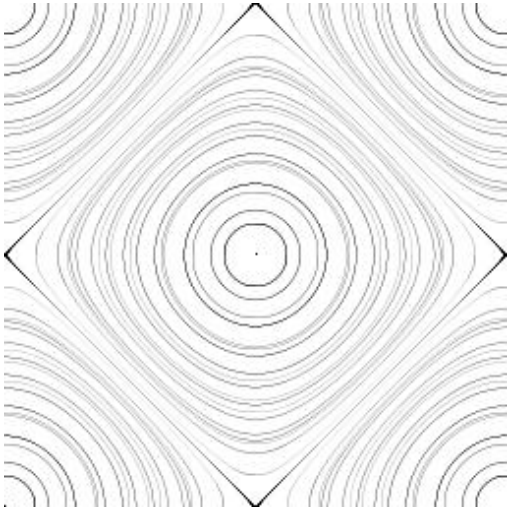
Widely studied, but its dynamics is integrable.

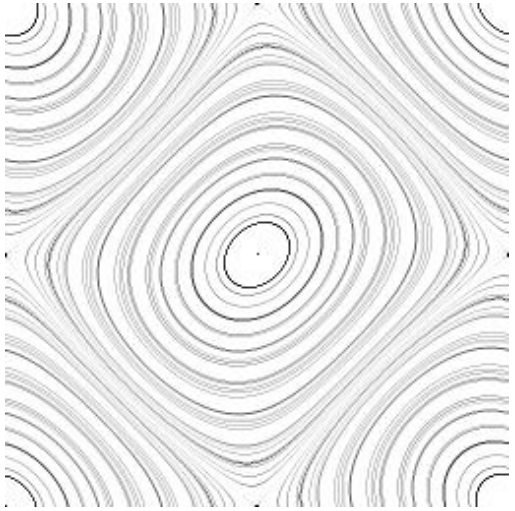
Kicked Harper Model

This model has been related to the motion of electrons in perpendicular magnetic and electric fields, and the stochastic heating of a plasma in a magnetic field.

$$H = L\cos p + K\cos q \sum_{m=-\infty}^{\infty} \delta(t-m)$$

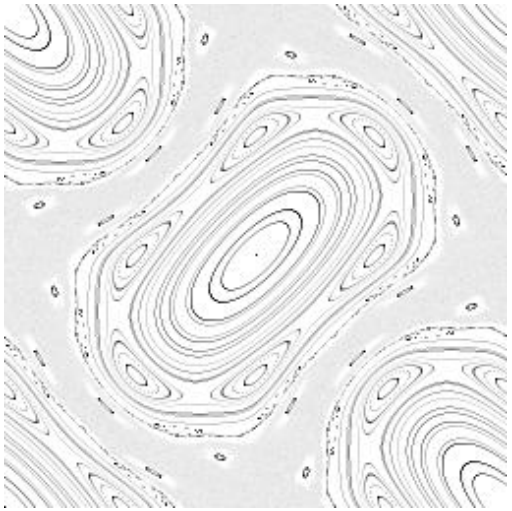
$K = L = 0.001$

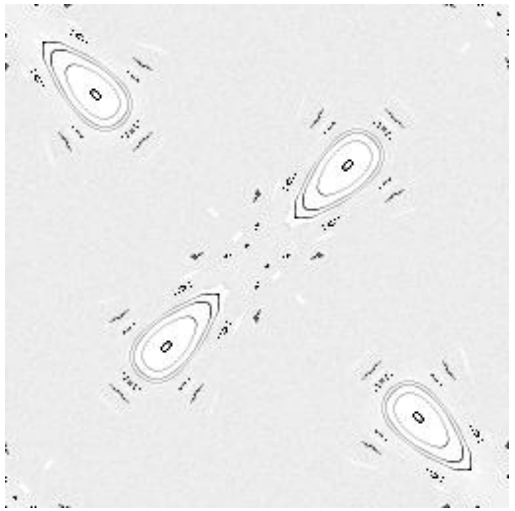




$K = L = 0.5$

$K = L = 1.5$





$K = L = 2.5$

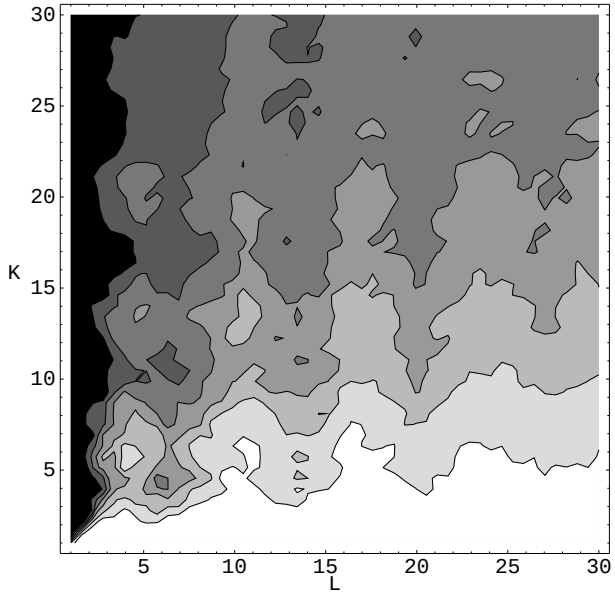
Quantum kicked Harper

The quantized version of the kicked Harper model has the evolution operator

$$\hat{U} = \exp\left(-i\frac{L}{\hbar}\cos\hat{p}\right)\exp\left(-i\frac{K}{\hbar}\cos\hat{q}\right)$$

The system's behaviour now depends on 3 parameters: K, L and $\hbar$.

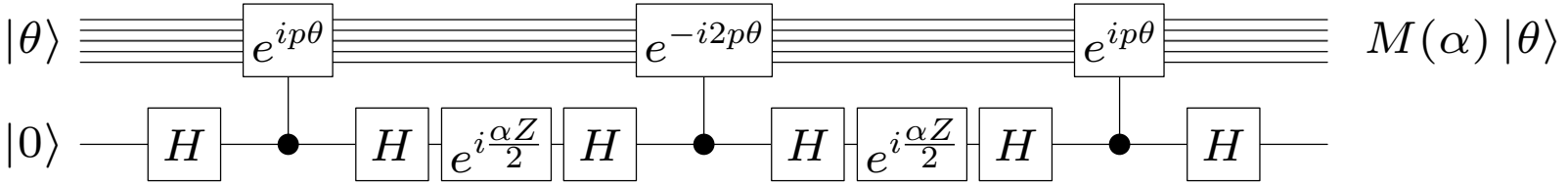
- $K \ll L$ localized momentum eigenstates
- $K < L$ coexistence of localized and delocalized states, ballistic diffusion
- $K \approx L$ anomalous diffusion



Map of inverse participation ratio (white being the lowest value)

Slices

Similar to A. A. Pomeransky and D. L. Shepelyansky, Phys. Rev. A **69**, 014302 (2004).

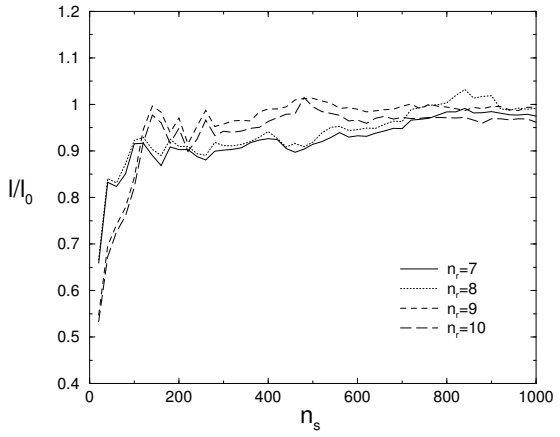


$$M(\alpha) = 1 + i\alpha\cos(p\hat{\theta}) + O(\alpha^2) \approx e^{i\alpha\cos(p\hat{\theta})}$$

We can thus perform the kick operator by repeated application of $M(\alpha)$

$$e^{-ik\cos(p\hat{\theta})} \approx M(\alpha)^{n_s} \text{ with } \alpha = -\frac{k}{n_s}$$

resources needed: $n_q + 1$ qubits and $O(n_s n_q)$ operations



Chebyshev polynomials

Any function can be approximated on $[-1,1]$ by: $\sum_{j=0}^{m} c_j\, T_j(x) - \frac{1}{2}c_0$

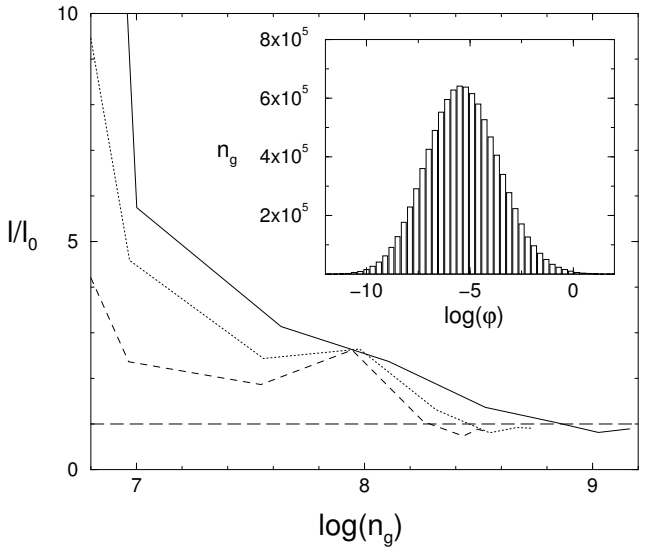
where $T_j(x)$ is the jth Chebyshev polynomial (of degree j), the c_j's suitable coefficients and m the chosen order of the approximation.

If $P(x)$ is a Chebyshev polynomial approximation of $\cos[\pi(x+1)]$, we can approximate the kick operator by $e^{-ik\cos(p\hat{\theta})} \approx e^{-ikP(\hat{\theta}/\pi-1)}$

Each term of the polynomial can be realized with multiply-controlled phase gates

$$e^{i\beta\hat{\theta}^r} = \prod_{j_1\cdots jr} C_{j_1\cdots jr}\left[\beta\left(\frac{2\pi}{N_H}\right)^r 2^{j_1+\ldots+jr}\right]$$

resources needed: n_q qubits and $\boxed{O(n_q^{m+1}) \text{ operations}}$



Static errors

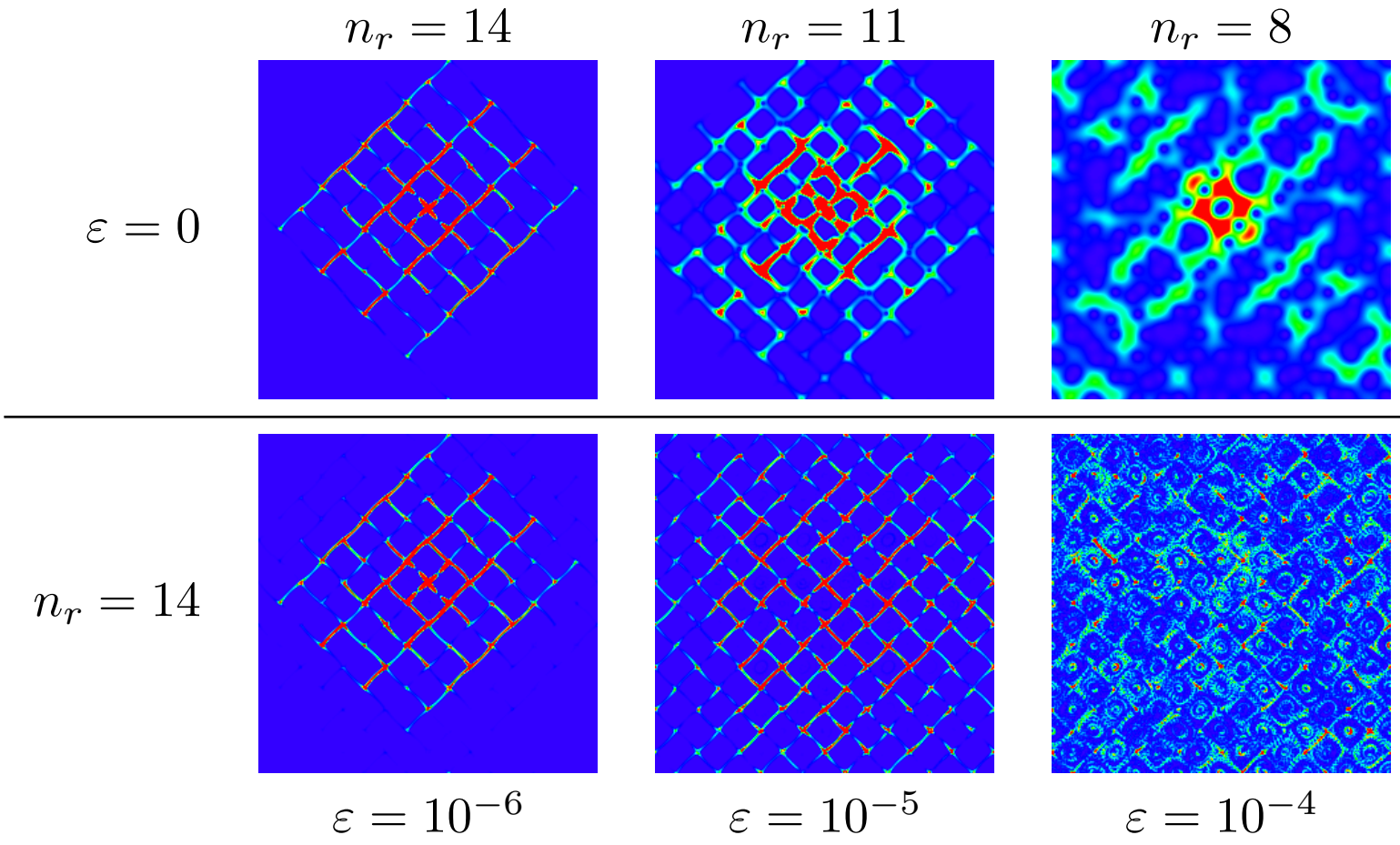
This error model was introduced in *Quantum chaos border for quantum computing*, B. Georgeot and D. L. Shepelyansky Phys. Rev. E **62**, 3504-3507 (2000)

Static errors stem from residual interactions between qubits. Gates are considered as instantaneous, but between the gates the quantum register evolves during the time τ_g according to the hamiltonian

$$H_1 = \sum_i \delta_i Z_i + \sum_i J_i X_i X_{i+1}$$

where δ_i and J_i are randomly and uniformly distributed over the intervals $[-\frac{\delta}{2}, \frac{\delta}{2}]$ and $[-\frac{J}{2}, \frac{J}{2}]$, and we assume periodic boundary conditions. The amplitude of the errors will be described by the rescaled parameter $\varepsilon = \delta\tau_g = J\tau_g$.

$K = L$ small: Stochastic web



Stochastic web

A wave packet will diffuse at a distance s along the stochastic web according to the law

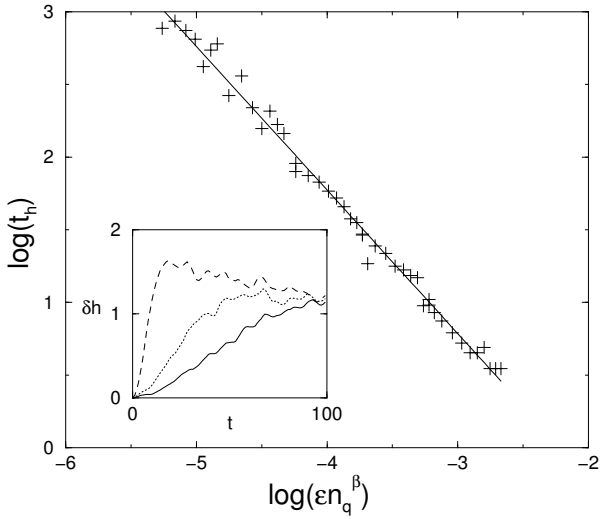
$$\langle s(t)^2 \rangle \approx D_s t$$

For a simulation up to a time t^*, one can get an estimation of D_s with

$$\left.\begin{array}{l} t^*\sqrt{t^*} \text{ classical operations} \\ t^* \text{ quantum operations} \end{array}\right\} \Longrightarrow \text{Polynomial gain}$$

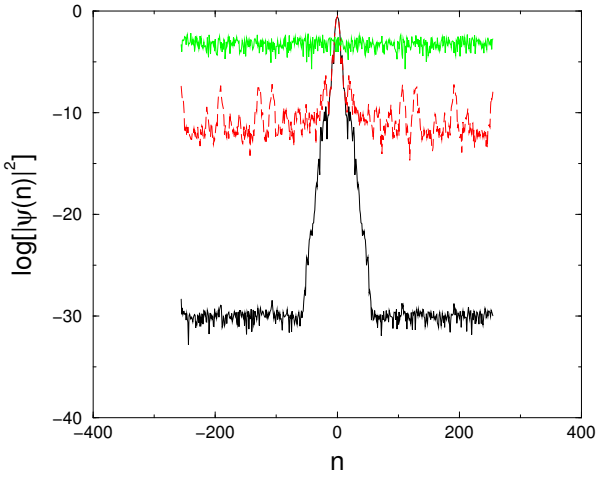
If t_h is the time for which the error on the Husimi function is half its mean value on the stochastic web

$$\boxed{t_h \sim \frac{1}{\varepsilon n_q^\beta}} \quad \text{with } \beta \approx 1.23$$



t_h for $K = L = 0.5$ ($10^{-6} \leq \varepsilon \leq 10^{-4}$ and $5 \leq n_r \leq 14$)

$K \ll L$: Localized regime

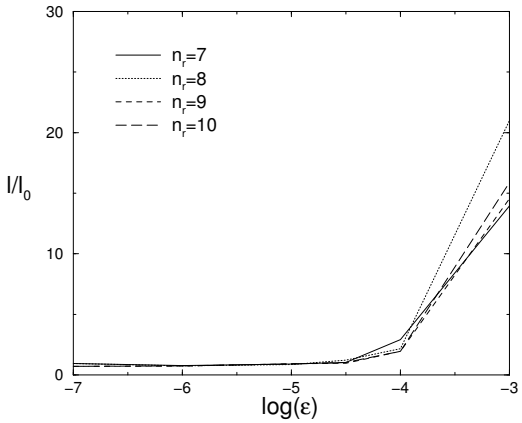


$K = 1$, $L = 5$
$\varepsilon = 0$, 10^{-7}, 10^{-3} from bottom to top

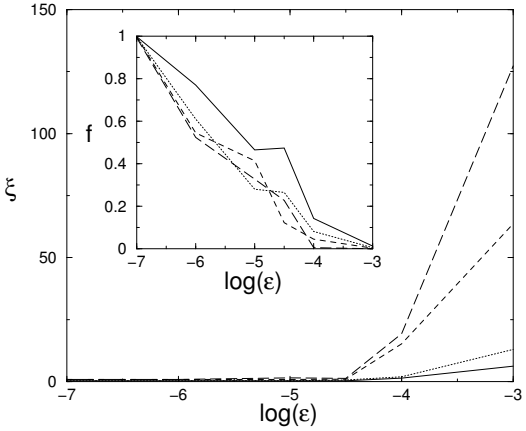
The wave function is spread upon a domain of size $\approx l$.
Classically, the momentum diffuses as $\langle n(t)^2 \rangle \approx Dt$.
To determine l we need

$t^* \sim l$ quantum operations
$l \times t^* \sim l^2$ classical operations
$\Big\}$ $\Longrightarrow$ Polynomial gain

localization length



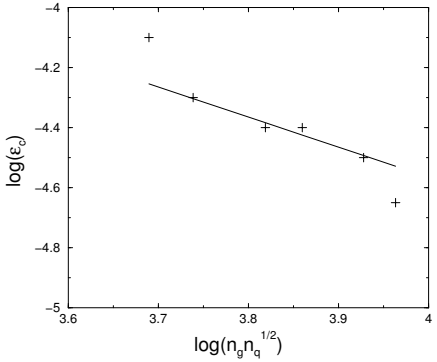
IPR

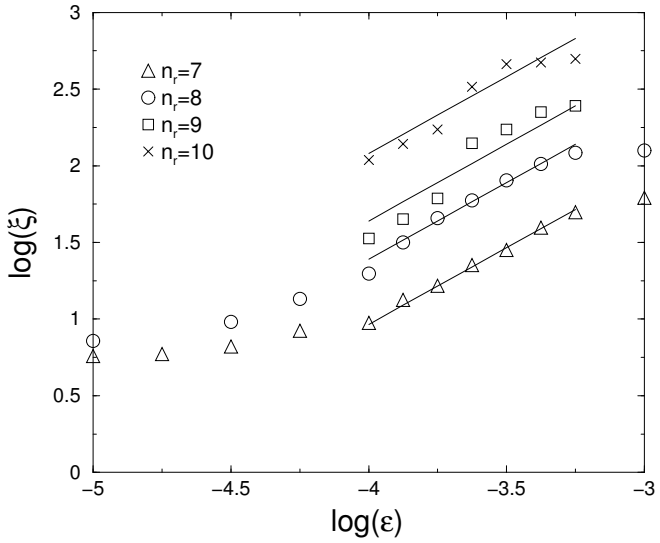


Localized regime

Using perturbation theory, we can estimate the critical error for which the IPR is twice the unperturbed value

$$\varepsilon_c \sim \frac{1}{n_g \sqrt{n_q l}}$$





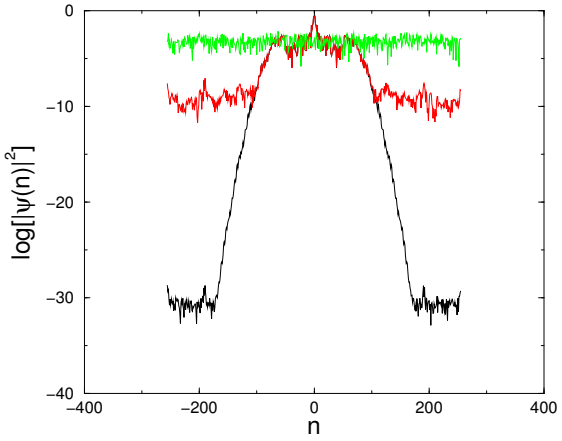
Breit-Wigner regime (Lorentzian LDOS)

$$\xi \sim \varepsilon^2 n_g^2 n_q N$$

Gaussian local density of states – consistent with data

$$\xi \sim \varepsilon n_g \sqrt{n_q} N$$

$K \lesssim L$: Partially delocalized regime



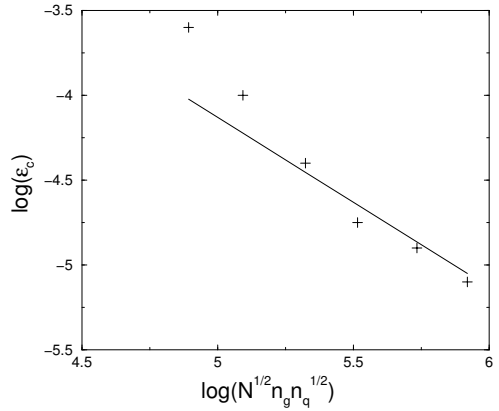
A wave packet initially localized in momentum spreads ballistically. Thus to simulate the system up to a time t^*, one need

$$\left.\begin{array}{l} t^* \text{ quantum operations} \\ t^{*2} \text{ classical operations} \end{array}\right\} \Longrightarrow \text{Polynomial gain}$$

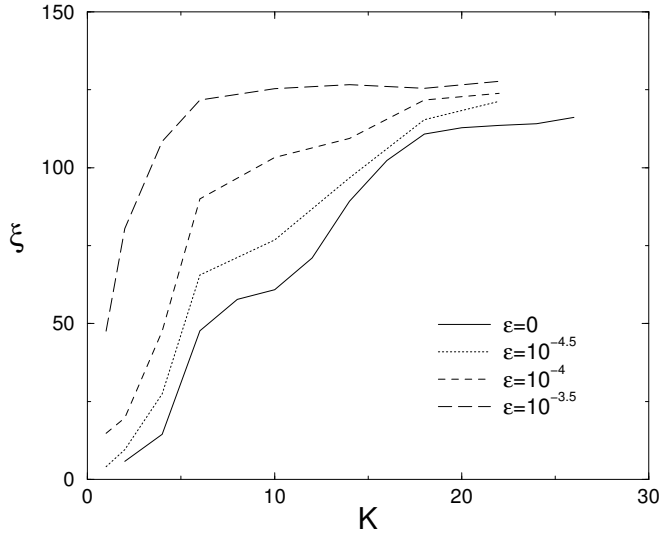
The integrated probability in the delocalized plateau can be obtained after a time $\sim l$

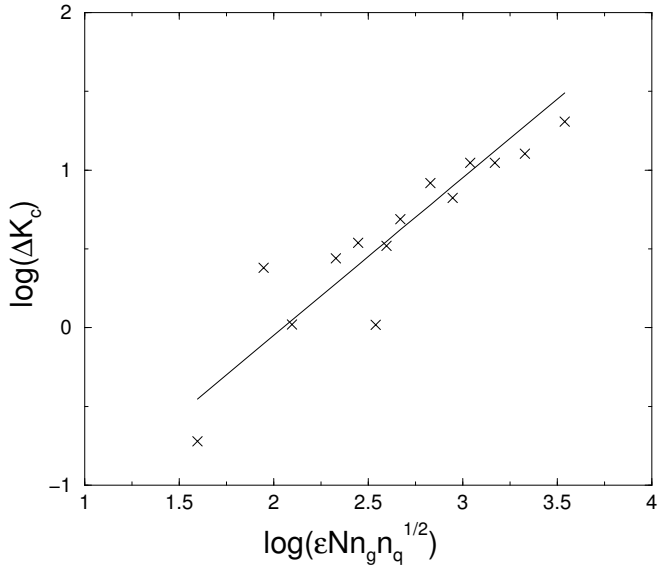
With perturbation theory and numerical simulations, ε_c can be shown to depend exponentially on the number of qubits

$$\boxed{\varepsilon_c \sim \frac{1}{n_g \sqrt{n_q N}}} \qquad \text{with } N = 2_q^n$$



Partially delocalized regime





K_c corresponds to the limit between localized and delocalized states

$$\Delta K_c \sim \varepsilon n_g \sqrt{n_q} N$$

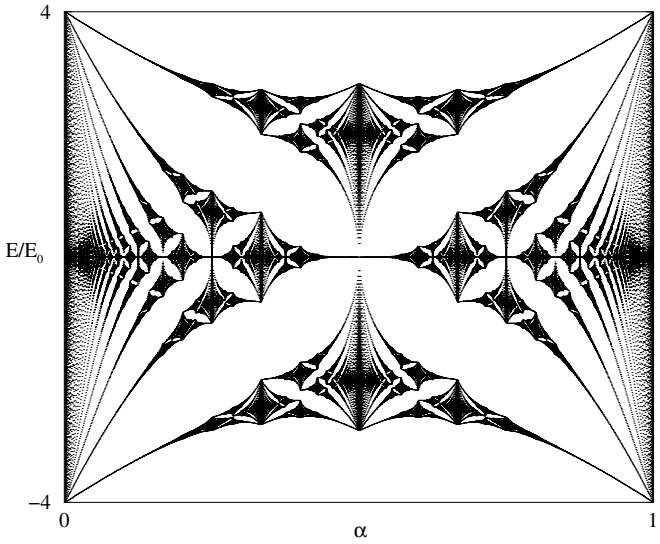
Unlike the Anderson transition, the shift scales exponentially with the number of qubits.

Harper model spectrum

The Harper model has a fractal spectrum known as the Hofstadter butterfly.

$$H = 2E_0 \left(\cos\hat{q} + \cos\hat{p}\right) \text{ with } [\hat{q}, \hat{p}] = i2\pi\alpha$$

Classically, if N is the size of the Hilbert space the spectrum can be computed in $O(N^2 \log N)$ operations.

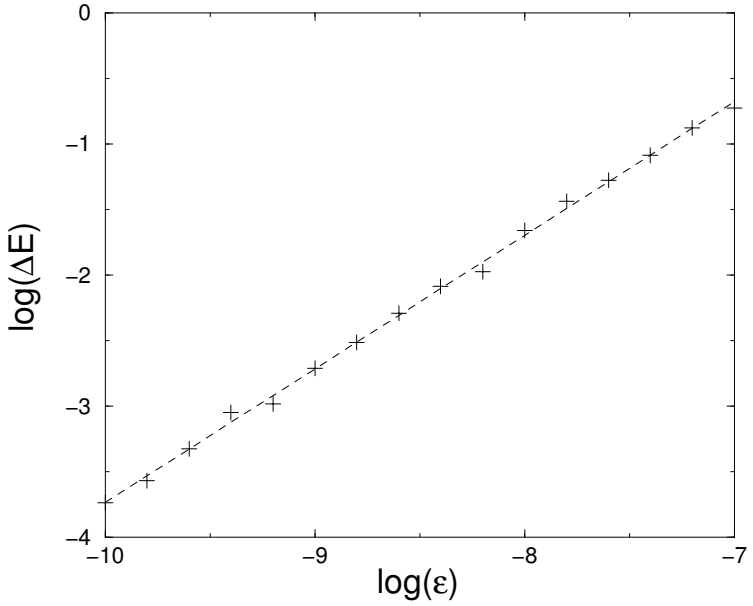


With a quantum algorithm, one needs $O(N)$ operations for the determination of one eigenvalue with unknown precision.

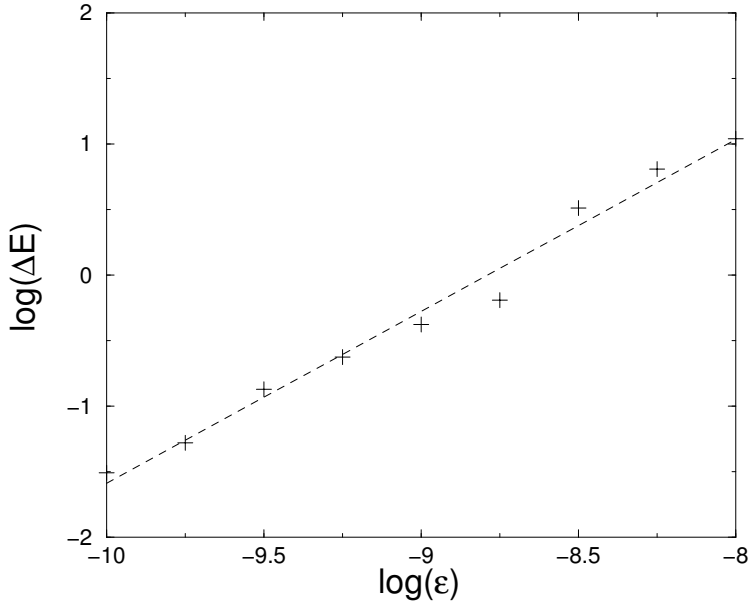
Amplitude amplification (derived from Grover's algorithm)
$\Rightarrow O(N\sqrt{N})$ operations for one part of the spectrum.

Effects of imperfections upon spectrum

We call ΔE the average error on eigenphases due to static errors.



Slices: $\Delta E \sim \varepsilon$



Chebyshev: $\Delta E \sim \varepsilon^{\alpha}$ with $\alpha \approx 1.3$

Conclusion

- Simulation of quantum maps on quantum computers allows to compute interesting quantities with only a few qubits, and with a polynomial gain upon classical computation.
- The scaling of errors with the size of the simulated system depends on the considered quantity.
- The wave function could be protected by using quantum error correcting codes.
- Analytical expressions for the decay laws of some quantities in chaotic régime can be derived using random matrix theory.