Title: Onset of Chaos in a Model of Quantum Computation

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Recently, the question of a relevance of the so-called quantum chaos has been raised in applications to quantum computation \cite{2,3}. Indeed, according to the general approach to closed systems of finite number of interacting Fermi-particles (see, e.g. \cite{4,5}), with an increase of an interaction between qubits a kind of chaos is expected to emerge in the energy spectra and structure of many-body states. Specifically, the fluctuations of energy levels and components of the eigenstates turn out to be very strong and described by the Random Matrix Theory. Clearly, if this happens in a quantum computer, it may lead to a destruction of the coherence of quantum computations due to internal decoherence inside many-body states. It is important to stress that quantum chaos occurs not only in the systems with random interaction, but also for purely dynamical interaction. In the latter case, the mechanism of chaos is due to a complex (non-linear) form of a two-body interaction represented in the basis of non-interacting particles.

Numerical analysis \cite{2} of a simplest model of quantum computer (2D model of 1/2-spins with a random interqubit interaction $J$) shows that with an increase of the number $L$ of qubits, the chaos threshold $J_{\text{cr}}$ decreases as $J_{\text{cr}} \propto 1/L$. On this ground, it was claimed that the onset of quantum chaos could be dangerous for quantum computers, since their effectiveness requires $L \gg 1$. On the other hand, in \cite{3} it was argued that in order to treat this problem properly, one needs to distinguish between chaotic properties of stationary states, and the dynamical process of quantum computation.
Below, we report our main theoretical and numerical results for the realistic model of quantum computer, suggested in [1]. We consider both stationary and dynamical approaches to the model in the region of a non-selective excitation which prepares a homogeneous superposition of \( N = 2^L \) states needed for the implementation of both Shor and Grover algorithms.

The model describes a 1-dimensional chain of \( L \) interacting 1/2-spins in the constant magnetic field \( B^z \), subjected to a sum of \( p = 1, \ldots, P \) time-dependent rectangular pulses of a circular polarized magnetic field rotating in the \( x,y \)-plane. Each of the pulses has the amplitude \( b_p \), frequency \( \nu_p \), phase \( \varphi_p \) and lasts during the period \( T_p = t_{p+1} - t_p \). Therefore, the Hamiltonian has the form,

\[
H = -\sum_{k=0}^{L-1} (\omega_k I_k^z + 2 \sum_{n>k} J_{k,n} I_k^z I_n^z) - \frac{1}{2} \sum_{p=1}^{P} \Theta_p(t) \Omega_p \sum_{k=0}^{L-1} \left( e^{-i\nu_p t - i\varphi_p} I_k^- + e^{i\nu_p t + i\varphi_p} I_k^+ \right),
\]

where the “pulse function” \( \Theta_p(t) \) equals 1 during the \( p \)-th pulse. The quantities \( J_{k,n} \) stand for the Ising interaction between two qubits, \( \omega_k \) are the frequencies of spin’s precession in the \( B^z \)-field, and \( \Omega_p \) is the Rabi frequency corresponding to the \( p \)-th pulse. The operators \( I_k^\pm \) are defined by the relations \( I_k^\pm = I_k^x \pm i I_k^y \), and \( I_k^{x,y,z} = (1/2) \sigma_k^{x,y,z} \), the latter being the Pauli matrices.

The Hamiltonian for a single pulse can be written in the coordinate system, rotating around \( z \)-axes with the frequency \( \nu_p \). Thus, for one pulse the model is described by the stationary Hamiltonian (below, \( \varphi_p = \pi/2, \Omega_p = \Omega, \nu_p = \nu \)). We mainly study the nearest neighbor interaction (\( N \)-interaction) between qubits for the dynamical case, \( J_{k,n} = J \delta_{n,k+1} \), and when all \( J_{k,k+1} \) are random. In contrast to the model [2] with homogeneous magnetic field, we consider the constant gradient magnetic field with a linear dependence on the position of the \( k \)-th qubit, \( \delta_k = |\omega_{k+1} - \omega_k| \ll \omega_k = ak \), with \( \Omega_p, J_{k,n}, \delta \omega_k \ll \omega_k \). Thus, for the dynamical \( N \)-interaction the Hamiltonian reads,

\[
H = \sum_{k=0}^{L-1} \left[ -\delta_k I_k^z + \Omega I_k^y \right] - 2J \sum_{k=0}^{L-2} I_k^x I_{k+1}^x; \quad \delta_k = \omega_k - \nu.
\]

For this Hamiltonian we have developed the theory [6,7] which predicts two transitions
in dependence on the interaction $J$. The first one was termed in [7] the delocalization border which corresponds to the transition to a weak chaos for

$$J > J_{cr} \approx \frac{\alpha^2}{\Omega}$$

(3)

By the weak chaos we mean a kind of randomness in many-body states, together with the absence of the Wigner-Dyson (WD) distribution $P(s)$ for the spacings between energy levels of the Hamiltonian (2). The latter distribution is a strong evidence of the quantum chaos in the energy spectra of chaotic quantum systems, and typically it emerges above the delocalization border [5]. Instead, the form of $P(s)$ in our model is very close to the Poisson which is known to occur in integrable systems. Our analytical approach allows one to explain this unexpected result by showing that, indeed, the model (2) is close to an integrable one, even in the case of completely random $N$-interaction [7].

The estimate (3) turns out to be very different from that obtained in [2] for the homogeneous magnetic field. Indeed, according to (3), the (weak) chaos border is independent of the number of qubits. Therefore, magnetic field with a constant gradient strongly reduces dangerous effects of the quantum chaos. Numerical data show that one needs to have a relatively weak interaction, $J \ll J_{cr}$, in order to avoid big errors in the structure of many-body states, which appear as a result of weak chaos.

Another unexpected analytical prediction which is confirmed by the numerical data, is that the delocalization border (3) remains the same for the case when all qubits interact one to each other. However, in this case, the delocalization border (3) coincides with the onset of strong chaos. The latter is characterized by strong (almost gaussian) fluctuations of the components of eigenstates, and by the WD-distribution for $P(s)$.

A theoretical analysis, supported by numerical computations ([6,7]), predict a transition to strong haos in presence of $N$-interaction too. Nevertheless it should be noticed that in this case strong chaos is due to a strong overlap of energy bands.

We have also studied the errors that arise when preparing the uniform many-body state from the ground one. For this, we computed the evolution of the wave function in the
model (1), during one pulse with $\varphi = \pi/2$. Without the interaction, $J$, at the end of the pulse all components of the wave function are the same $\psi_n^0 = 1/\sqrt{N}$. The interaction results in some errors in amplitude and phase which can be characterized by $\eta = \langle ||\psi_n| - \psi_n^0|| \rangle_n$ and $\phi = \langle \arctan(Im\psi_n/Re\psi_n) \rangle_n$, where $\langle \ldots \rangle_n$ means the average over the different $n$ components.

Numerical data show that the errors decrease with an increase of $\Omega$ respectively as $\eta \propto \Omega^{-2}$, and $\phi \propto \Omega^{-1}$ in agreement with simple analytical estimates. As one can see, the delocalization border does not influence the errors. This means that the weak chaos is not important for this kind of the evolution of our system. Indeed, this evolution lasts quite short time compared with the inverse distance between nearest levels inside the energy band. Therefore, until the bands are non-overlapped, the weak chaos does not influence the dynamics. On the other hand, with the decrease of $\Omega$, the bands start to overlap which could strongly increase errors in the wave function.

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