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Avoiding quantum chaos in quantum computation

G. P. Berman,[1] F. Borgonovi,[2] F. M. Izrailev,[3] and V. I. Tsifrinovich[4]
[1]*Theoretical Division and CNLS, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*
[2]*Dipartimento di Matematica e Fisica, Universitá Cattolica, via Musei 41, 2512 Brescia, Italy and INFM, Unitá di Brescia and INFN, Sezione di Pavia*
[3]*Instituto de Fisica, Universidad Autonoma de Puebla, Apartado Postal J-48, Puebla 72570, Mexico*
[4]*IDS Department, Polytechnic University, Six Metrotech Center, Brooklyn, New York 11201*
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We study a one-dimensional chain of nuclear 1/2 spins in an external time-dependent magnetic field, considered as a possible candidate for experimental realization of quantum computation. According to the general theory of interacting particles, one of the most dangerous effects is quantum chaos that can destroy the stability of quantum operations. The standard viewpoint is that the threshold for the onset of quantum chaos due to an interaction between spins (qubits) strongly decreases with an increase of the number of qubits. Contrary to this opinion, we show that the presence of a nonhomogeneous magnetic field can strongly reduce quantum chaos effects. We give analytical estimates that explain this effect, together with numerical data supporting our analysis.

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Much attention has been paid in recent years to the idea of quantum computation (see, for example, [1–3] and references therein). The burst of interest in this subject is caused by the discovery of a fast quantum algorithm for the factorization of integers [4] demonstrating the effectiveness of quantum computers in comparison to the classical ones. Nowadays, there are different projects for the experimental realization of quantum computers, based on interacting two-level systems (qubits). One of the most important problems widely discussed in the literature, is the problem of decoherence that arises in many-qubit systems due to the influence of an environment [5]. However, even in the absence of the environment, the interaction between qubits may lead to the onset of quantum chaos [6].

The latter subject of quantum chaos in closed systems of interacting particles has been developed recently in application to nuclear, atomic, and solid state physics (see, e.g., [7] and references therein). When the (two-body) interaction between particles exceeds a critical value, fast transition to chaos occurs in the Hilbert space of many-particle states [8]. Different aspects of this transition are now well understood, such as a statistical description of eigenstates and the onset of thermalization in finite systems (see, e.g., [9] and references therein).

Direct application of quantum chaos theory to a simple model of quantum computer [6] has shown that for a strong enough interaction between qubits, the onset of quantum chaos is unavoidable. Although for $L=14-16$ qubits the critical value J_{cr} for quantum chaos threshold is quite large, with an increase of L it decreases as $J_{cr}\sim 1/L$. From the viewpoint of the standard approach to closed systems of interacting particles, the decrease of chaos threshold with an increase of qubits looks generic. However, in this paper we demonstrate that this conclusion is not universal and the quantum chaos can be avoided, for example, with a proper choice of the external magnetic field.

Our consideration is based on the model of one-dimensional chain of L identical nuclear 1/2 spins, for example, proton spins in a high magnetic field [10]. The constant magnetic field, which points in the positive z direction is slightly nonuniform: $B^z=B^z(z)$. The angle θ between the direction of the chain and z axis satisfies to the condition: $\cos\theta=1/\sqrt{3}$. In this case the dipole-dipole interaction is suppressed, and the main interaction between nuclear spins is the Ising interaction mediated by chemical bonds. The gyromagnetic ratio for a proton $\gamma/2\pi$ is approximately 43 MHz/T. If the distance between neighboring spins is 0.2 nm and the frequency difference between them is 1 kHz, then the corresponding gradient of the constant magnetic field dB^z/dz is approximately 2×10^5 T/m. Such a gradient is experimentally achievable; see, e.g., [11]. In our model the spin chain is also subjected to the transversal circular polarized magnetic field. The expression for the total magnetic field has the following form [12]:

$$\vec{B}(t)=[b_\perp^p\cos(\nu_p t+\varphi_p),-b_\perp^p\sin(\nu_p t+\varphi_p),B^z].$$

Here B^z is a constant magnetic field oriented in the positive z direction, $b_\perp^p$, ν_p, and φ_p are the amplitudes, frequencies, and phases of a circular polarized magnetic field. The latter is given by the sum of $p=1_i\ldots,P$ rectangular pulses of the length $t_{p+1}-t_p$, rotating in the (x,y) plane and providing a quantum computer protocol. The quantum Hamiltonian of this system has the form

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

where the "pulse function" $\Theta_p(t)$ equals 1 only during the pth pulse, for $t_p<t\leqslant t_{p+1}$. The quantities $J_{k,n}$ stand for the Ising interaction between two qubits, ω_k are the frequencies of spin precession in the B^z magnetic field, Ω_p is the Rabi

frequency of the pth pulse, $I_k^{x,y,z}=(\frac{1}{2})\sigma_k^{x,y,z}$, the latter being the Pauli matrices, and $I_k^{\pm}=I_k^x \pm iI_k^y$.

For the pth pulse, the Hamiltonian (1) can be represented in the coordinate system that rotates with the frequency ν_p. Thus, for the pth pulse, and $t_p<t\leqslant t_{p+1}$ our model can be reduced to the *stationary* Hamiltonian,

$$\mathcal{H}^{(p)}=-\sum_{k=0}^{L-1}\left[\xi_k I_k^z+(\alpha I_k^x-\beta I_k^y)+2\sum_{n>k}J_{k,n}I_k^z I_n^z\right], \quad (2)$$

where $\xi_k=(\omega_k-\nu_p)$, $\alpha=\Omega_p\cos\varphi_p$, and $\beta=\Omega_p\sin\varphi_p$.

A typical quantum protocol can require a regime of both *selective*, $\Omega_p\ll J_{k,n}\ll\delta\omega_k\ll\omega_k$, and *nonselective*, $\Omega_p\gg\delta\omega_k\gg J$, excitations, where $\delta\omega_k=|\omega_{k+1}-\omega_k|$ [10]. In this paper we mainly concentrate on the latter, however, the theory developed here can be extended to the former one. Nonselective excitation provides the simplest way to prepare a homogeneous superposition of 2^L states needed for implementation of both Shor and Grover algorithms. In what follows, for simplicity, we consider the case when $\varphi_p=\pi/2$ and $\Omega_p=\Omega$, $\nu_p=\nu$. Our main interest is in the nearest neighbor interaction (*N interaction*) between qubits for two different cases, the *dynamical* one when all coupling elements are the same, $J_{k,n}=J\delta_{n,k+1}$, and the case when all values $J_{k,k+1}$ are random (*random model*). We also briefly discuss another case when all qubits interact to each other (*A interaction*) with random $J_{k,n}$.

For the dynamical N interaction and $\nu=\omega_0$, $\omega_k=\omega_0+ak$ $(a>0)$, the Hamiltonian takes the form

$$H=\sum_{k=0}^{L-1}[-\delta_k I_k^z+\Omega I_k^y]-2I\sum_{k=0}^{L-2}I_k^z I_{k+1}^z. \quad (3)$$

where $\delta_k=ak$. In the z representation the Hamiltonian matrix of size $N=2^L$ is diagonal for $\Omega=0$. For $\Omega\neq 0$, we have, $H_{kn}=H_{nk}^*=i\Omega/2$ with $n>k$. The matrix is very sparse, and it has specific structure in the basis, reordered according to an increase of the number s, written in the binary representation, $s=i_{L-1},i_{L-2},\ldots,i_0$ (with $i_s=0$ or 1, depending on whether a single-particle state of ith qubits is the ground state or the excited one).

For $\Omega\gg J$ the spectrum consists of $L+1$ narrow bands with large gaps of size approximately Ω between the bands. Since the most interesting energy region for the preparation of the homogeneous wave function is in the middle of the energy spectrum, we consider below only the central band and the corresponding eigenstates for L even.

In the absence of interaction, $J=0$, all eigenstates in the z representation are fully extended with the value of components $|\psi_n|$ close to $1/\sqrt{N}$. Typical structure of eigenstates in the central band is shown in Fig. 1 for different values of J. One can see that with an increase of J interaction, the probabilities $w_n=|\psi_n|^2$ deviate from the unperturbed value $w_n=1/N$, thus resulting in quantum computation errors. The data demonstrate the transition from *regular* states for a weak interaction, $J\leqslant 0.1$, to *strongly chaotic* ones for $J\approx 100$.

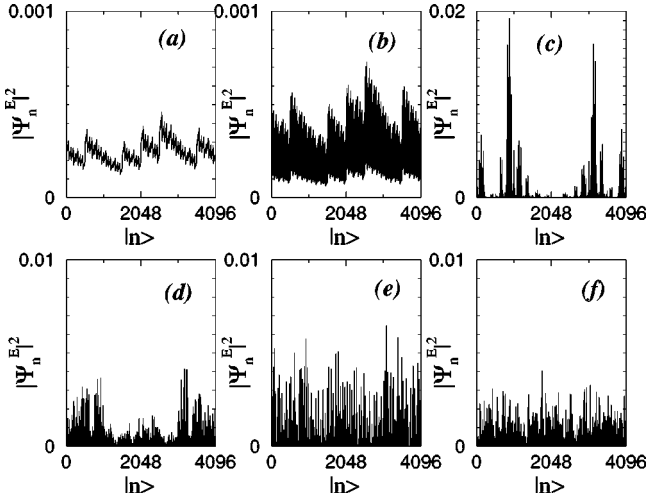

FIG. 1. Typical structure of eigenfunctions for $J=0$, 2×10^{-4}, 0.1, 1, 10, and 100 denoted by (a, b, c, d, e, f) respectively. Eigenstates are taken from the central energy band for $L=12$, $\Omega=100$, and $a=1$.

Global properties of eigenstates can be characterized by the number $N_{\rm pc}$ of principal components, determined through the *inverse participation ratio*, $N_{\rm pc}(E)=[\Sigma_n|\psi_n(E)|^4]^{-1}$, where $\psi_n(E)$ is the nth component of a specific eigenfunction. For zero interaction $N_{\rm pc}$ is equal to N, and it decreases with an increase of interaction, thus giving the measure of the destruction of unperturbed $(J=0)$ eigenstates. Note that for completely chaotic eigenstates with Gaussian fluctuations for ψ_n, one has $N_{\rm pc}=N/3$ [7].

Numerical data for the dependence of $N_{\rm pc}$ on the interaction J reveal different regions, see Fig. 2. The first region (very weak interaction) corresponds to completely extended eigenstates with $|\psi_n|\approx 1/\sqrt{N}$. Here the energy spectrum is characterized by many close quasidegenerate levels. In the

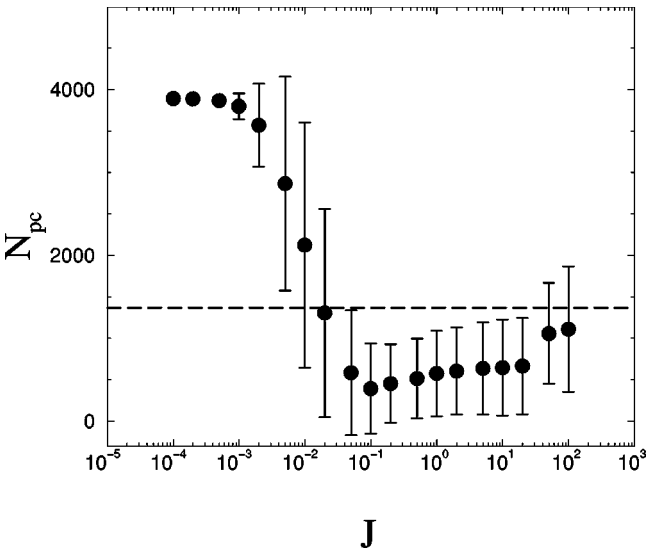

FIG. 2. The average number of principal components $N_{\rm pc}$ as a function of J for the parameters of Fig. 1; the horizontal line corresponds to $N/3$. The average is taken over the eigenfunctions from the central band only.

second region with $N_{pc} \ll N$ all eigenstates are strongly influenced by the interqubit interaction. We call it the region of *weak chaos* since a kind of irregularity emerges in the structure of eigenstates. However, this region has nothing to do with *quantum chaos*. Indeed, here the level spacing distribution $P(s)$ is quite close to the Poisson, known to be a fingerprint of the integrability of a system. From the practical point of view the *weak chaos* that occurs for $J \geqslant J_{cr} \approx 0.05$, should be avoided in quantum computation because of large deviations of eigenstates from the unperturbed ones, see Figs. 1(c) and 1(d).

A second transition to *strong quantum chaos* occurs for $J \geqslant J_{band} \gg J_{cr}$ with $J_{band} \approx 20$. By this term we denote the situation when the level spacing distribution has the Wigner-Dyson form and fluctuations of components ψ_n are close to the Gaussian ones with $N_{pc} \approx N/3$. Analysis shows that this transition corresponds to the overlapping of the central energy band with the nearest ones. Quite unexpectedly, the randomization of the interaction strength in the interval $[-J,J]$ does not change the results: the transition to strong quantum chaos occurs only due to the overlapping of the energy bands for a very large interaction. This means that for both the dynamical and random N interaction, our system is close to an integrable one for $J \leqslant J_{band}$.

The above *numerical* analysis for $L=12$ shows that the *weak chaos* can significantly influence the structure of eigenstates, but the regime of *strong chaos* is not achievable in quantum computation. However, according to a common belief, the thresholds for *both* weak and strong chaos are expected to decrease with an increase of L, thus, leading to a destruction of unperturbed states even in the presence of a relatively weak interaction J [13].

We show now *analytically*, that contrary to the standard viewpoint, in this model the weak chaos border. I_{cr} *is independent* of the number of qubits. In order to explain this unexpected phenomena, it is convenient to represent the Hamiltonian (3) in the basis in which it is diagonal for noninteracting $(J=0)$ qubits,

$$H = H_0 + JV_0. \tag{4}$$

Here the ''effective field'' Hamiltonian H_0 is determined by the sum of L individual Hamiltonians H_k,

$$H_0 = \sum_{k=0}^{L-1} H_k = \sum_{k=0}^{L-1} \sqrt{\delta_k^2 + \Omega^2} I_k^z, \tag{5}$$

and the interaction between new ''quasiparticles'' is given by $V_0 = V_{drag} + V_{band} + V_{off}$. Here $V_{drag} = -2\Sigma_k b_k b_{k+1} I_k^z I_{k+1}^z$ stands for the diagonal interaction, $V_{band} = -2\Sigma_k a_k a_{k+1} I_k^y I_{k+1}^y$ describes the coupling within the band and with its neighbor bands, and $V_{off} = 2\Sigma_k (a_k b_{k+1} I_k^y I_{k+1}^z + a_{k+1} b_k I_k^z I_{k+1}^y)$ refers to the coupling between next-to-neighbor different bands. The amplitudes a_k and b_k are given by the relations, $a_k = \Omega/A$, $b_k = (\nu - \omega_k)/A$, and $A = \sqrt{\delta_k^2 + \Omega^2}$.

Under the condition $\delta_k = ak \ll \Omega$ we have the following expression for single-particle ''quasienergies'' ϵ_k corresponding to the Hamiltonian H_0,

$$\epsilon_k = \pm \frac{1}{2} \sqrt{\delta_k^2 + \Omega^2} \simeq \pm \frac{1}{2} \left(\Omega + \frac{a^2 k^2}{2\Omega} \right). \tag{6}$$

Note, that each ''quasiparticle'' can have $2L$ different ''quasienergies'' ϵ_k while qubits have two. The above expression allows us to construct many-particle unperturbed quasienergies, $E_c = \Sigma_{k=0}^{L-1} \epsilon_k$, inside the central band. Indeed, for $ak \ll \Omega$ all many-particle levels have (for L even) $L/2$ positive and $L/2$ negative values of ϵ_k. As a result, the total number N_{cb} of many-body states in the central band is given by $N_{cb} = L![(L/2)!(L/2)!]^{-1}$, and the size can be estimate as twice the maximum energy, $(\Delta E)_{cb} = 2E_c^{max} = a^2 L^2 (L-1)/8\Omega$.

Now, we can estimate the mean level spacing δE between those many-body states that are directly coupled by V_{band}. The value δE can be estimated as the ratio $\delta E = (\Delta E)_f / M_f$ where $M_f \approx L/2$ is the number of many-body states coupled by V_{band}. One should stress that the energy range $(\Delta E)_f$ within which these states are coupled, is much less than the total energy width $(\Delta E)_{cb}$ of the central band, due to the two-body nature of interaction. This value $(\Delta E)_f$ can be estimated as the maximal difference between the energies $E_c^{(2)} = \Sigma_k^{(2)} \epsilon_k$ and $E_c^{(1)} = \Sigma_k^{(1)} \epsilon_k$ of two many-body states $|1\rangle$ and $|2\rangle$ of H_0, that have the coupling $\langle 1|V_{band}|2\rangle$ different from zero. From the expression (6) one finds, $(\Delta E)_f = a^2 L/\Omega$. As a result, for $L \gg 1$ we have $\delta E = \Delta E_f / M_f \approx 2a^2/\Omega$.

Now, δE should be compared with the typical perturbation strength $V = JV_0$ [9]. The latter can be found from V_{band} as $V \approx J/2$. Therefore, we finally obtain

$$J_{cr} \approx \frac{4a^2}{\Omega}. \tag{7}$$

Note that in the ''effective field'' representation J_{cr} determines the *delocalization border*. Namely, for $J \leqslant J_{cr}$ the eigenstates are δ-like functions with $N_{pc} \approx 1$, and above this border, for $J \geqslant J_{cr}$, the value of N_{pc} increases fast with an increase of the interaction.

Remarkably, the threshold J_{cr} to *weak chaos* contrary to [6], does not depend on the number L of qubits. The origin of this phenomenon is that the width $(\Delta E)_f$ and M_f both increase linearly in L. This effect is entirely related to the constant gradient of the magnetic field in the original Hamiltonian thus leading to a quadratic growth of the energy in Eq. (6) in dependence on k. One can show that for a homogeneous magnetic field we get the same L dependence as in [6].

Numerical data for the number N_{pc} of principal components of eigenstates in the new basis [where H_0 is diagonal for $J=0$, see Eq. (4)] are given in Fig. 3 as a function of J/J_{cr}. One can see that below the border, $J < J_{cr}$, there is a scaling dependence of N_{pc} on L and Ω that confirms our estimate (7). On the other side, for $J > J_{cr}$, the value of N_{pc} saturates to its maximal value $N_{cb}/3$ in correspondence with

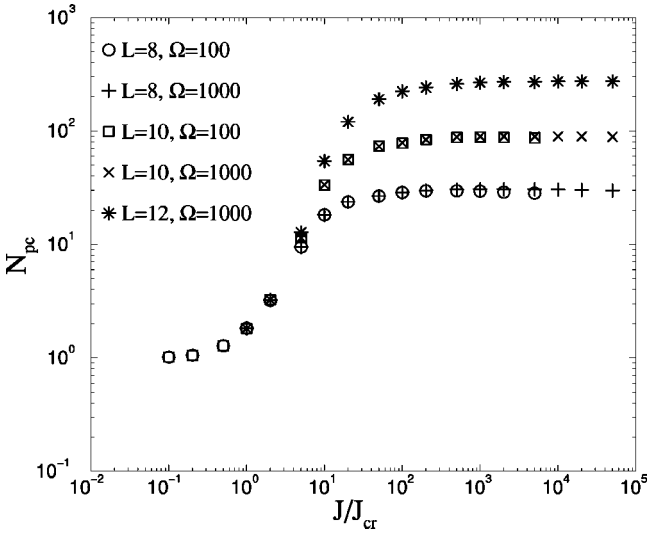

FIG. 3. The average number of principal components for the dynamical N interaction as a function of J/J_{cr}, in the central band in the H_0 basis, for different Ω and L.

random matrix predictions [7]. We have to stress that the transition to extended states in the ''effective field'' representation, which occurs for $J>J_{cr}$, corresponds to the transition to *weak chaos* for the eigenstates in the z representation, see Fig. 2.

Data for random N interaction turn out to be similar to that shown in Fig. 3. This indicates that the model is, indeed, close to the integrable one, independent of whether the interaction is dynamical or random. This phenomenon can be explained analytically. Indeed, on neglecting the interband interaction V_{off}, the Hamiltonian (4) is *rigorously* integrable, see [14] and references therein. Therefore, the onset of quantum chaos for N interaction is only possible when energy bands are overlapped.

Now we have to take into account that with an increase of L, the width $(\Delta E)_{cb}$ of the central band can exceed the distance Ω between the nearest ones, which leads to strong quantum chaos. The estimate for the critical value, L_{cr}, which corresponds to the band overlapping in absence of the J interaction reads as $L_{max}\sim(\Omega/a)^{2/3}\gg 1$.

It can be shown that for the interaction between *all qubits* (A interaction) there is no relevance to the integrability, and the *delocalization border* (7) corresponds to the onset of *strong quantum chaos* manifested by the Wigner-Dyson distribution for $P(s)$. In this case the estimate for the energy width $(\Delta E)_f$ is $(\Delta E)_f=L^2a^2/2\Omega$, and $M_f=L^2/4$. Therefore, we get $\delta E=(\Delta E)_f/M_f\approx 2a^2/\Omega$ which is the same as for the N interaction. This is an unexpected result since generically, the chaos border for A interaction is much lower than for N interaction ($J_{cr}\propto 1/L^2$, see, e.g., [13]). Our numerical data for the A interaction in Eq. (3) confirm the above prediction.

In conclusion, we have shown that, in contrast to general belief, the chaos border in the model of L interacting qubits does not decrease with an increase of L, in the presence of a magnetic field with constant gradient in the x direction. The quantum chaos that emerges for a very strong interaction between qubits is irrelevant to quantum computation as far as a short range interqubits coupling is concerned. The mechanism of strong chaos for the N interaction is due to band overlap only, and can be avoided even for a very large number of qubits. It is interesting to note that a similar analysis for an inhomogeneous gradient of magnetic field ($\omega_k\propto k^4$), give rise to a chaos border proportional to L. The region of parameters for quantum computation with *selective excitation* requires additional analysis.

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