Entropy production and fidelity for quantum many-body systems with noise

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We study dynamical properties of systems with many interacting Fermi-particles under the influence of static imperfections. Main attention is paid to the time dependence of the Shannon entropy of wave packets, and to the fidelity of the dynamics. Our question is how the entropy and fidelity are sensitive to the noise. In our study, we use both random matrix models with two-body interaction and dynamical models of a quantum computation. Numerical data are compared with analytical predictions.

I. INTRODUCTION

There are two sources for the appearance of statistical properties in quantum isolated systems. The first one which serves as a base for the traditional statistical mechanics, is the thermodynamic limit in which the number of particles is infinitely large. In this case even integrable systems may be treated statistically. The origin of this effect is an infinite number of independent frequencies in the dynamics of a system. It is clear that in this case any small interaction between particles, or with a heat bath, gives rise to strong statistical properties.

Another situation occurs when the number of particles is finite and not very large. In this case the role of interaction is crucial, and chaos arises under some conditions. For systems with the well defined classical limit, this chaos is known as quantum chaos and can be compared with the classical one. This situation is known in literature as many-body chaos, in contrast to the thoroughly studied case of one-body chaos which refers to a single particle in an external field. The well known example is the hydrogen atom in a strong magnetic field.

In many-body systems the density of many-particle energy levels increases extremely fast (typically, exponentially), both with an increase of the number of particles and excitation energy. For this reason, the interaction between particles can lead to a strong mixing between many-particle basis states, thus resulting in chaotic eigenstates. The latter term refers to the fact that the components of such eigenstates can be practically treated as pseudo-random variables, this leads to strong statistical properties such as the relaxation of the system to a steady-state distribution. Typical examples of such systems are compound nuclei, complex atoms, isolated quantum dots, etc.

Recent calculations for complex atoms [1], multicharged ions [2], nuclei [3], Bose-Einstein condensates [4], and spin systems [5,6] have confirmed the dynamical origin of statistical laws in isolated systems (see details in [7,8] and the review [9]).

The onset of chaos for highly excited states and for many-particle spectra has been thoroughly studied by making use of the Two-Body Random Interaction (TBRI) model which was invented long ago [10]. In this model all two-body matrix elements are assumed to be independent and random variables, however, the model is essentially different from standard random matrix models where the two-body nature of interaction is not taken into account. One of the important results obtained in the frame of this model (see, for example, [11] and references therein), is the Anderson-like transition which occurs in the space determined by many-particle states of the unperturbed part $H_0$. Due to a random character of the perturbation, this delocalization transition can be treated as the transition to a global chaos. Above some critical value of the perturbation, the number $N_{pc}$ of principal components in eigenstates is typically large. For example, $N_{pc} \approx 150$ in the Ce atom [1] and $N_{pc} \approx 10^4 - 10^5$ in heavy nuclei [3].

Recently, the theory of many-body chaos has been extended to quantum computers. One can naturally expect [12,13] that due to a very high density of energy levels, any kind of perturbation may lead to decoherence effects thus destroying the quantum computation. For this reason it is very important to search for the conditions when the role of chaos can be significantly reduced [14,15]. So far, the study of the many-body chaos has been mainly restricted by statistical properties of the energy spectra and eigenstates. On the other hand, in view of experimental applications, one needs to know what are the dynamical properties of quantum systems with strongly interacting particles. Especially, this is very important for quantum computation [16], for which quantum protocols assume a high stability of a long-time dynamics under the influence of an environment or any kind of static imperfections.

Below, we analyze how the static disorder influences the dynamical properties of quantum systems with complex behavior.
II. DYNAMICS OF SYSTEMS WITH TWO-BODY INTERACTION

In what follows we assume that the models under consideration can be represented by the Hamiltonian separated in two parts,

\[ H = H_0 + V \]  \hspace{1cm} (1)

where \( H_0 \) describes the “unperturbed” part and \( V \) stands for the “perturbation”. Then \( V \) can be represented as

\[ V_{lk} = \langle l | V | k \rangle, \]  \hspace{1cm} (2)

where \( |l) \) and \( |k) \) stand for basis states of \( H_0 \) (or, “unperturbed” states). Correspondingly, exact states \( |\alpha) \) of the total Hamiltonian \( H \) are expressed as

\[ |\alpha) = C_\alpha^k |k). \]  \hspace{1cm} (3)

The coefficients \( C_\alpha^k \) give the expansion of an exact state in terms of the basis states (for \( \alpha \) fixed), or the expansion of a basis state in terms of the exact states (for \( k \) fixed).

In the case when the Hamiltonian \( H \) corresponds to a system of interacting Fermi-particles, basis states can be constructed as \( |k) = a_{k_1}^\dagger \ldots a_{k_n}^\dagger |0\rangle \) from the ground state \( |0\rangle \) with \( a_k^\dagger \) as the creation operator. In application to quantum computer models the Hamiltonian \( H_0 \) typically describes a number of non-interacting qubits, and \( V \) stands for the inter-qubit interaction needed for quantum computation (for other variants, see below). In this case the basis state \( |k) \) is a product of single qubit states, with \( a_k^+ \) as the spin-raising operator (if the ground state \( |0\rangle \) corresponds to all spins down).

In principle, the knowledge of the state matrix \( C_n^m \) and of the corresponding energy spectrum \( E_\alpha \) gives a complete information about the system. In particular, if an initial state \( \Psi(0) \) is some basis state \( |k_0) \), the evolution of the \( \Psi \)-function is described by the expression,

\[ \Psi(t) = \sum_{n,m} C_n^m C_m^\alpha |\Psi(0)\rangle \exp(-iE_\alpha t). \]  \hspace{1cm} (4)

Here and below we assume that \( \hbar = 1 \). As one can see, the probability

\[ w_m = |A_m|^2 = |\langle m | \Psi(t) \rangle|^2 \]  \hspace{1cm} (5)

to find the system at time \( t \) in the state \( |m) \) is determined by the amplitude

\[ A_m = \langle m | \exp(-iHt) |m \rangle = \sum_\alpha |C_m^\alpha|^2 \exp(-iE_\alpha t). \]  \hspace{1cm} (6)

When the perturbation is weak, only the component \( A_m \) with \( m = k_0 \) is large, therefore, the evolution of the system is close to the periodic one. However, with an increase of the perturbation strength, the number of components \( A_m \) with relatively large amplitudes increases, and the dynamics of wave packets can be quite complicated. In order to characterize the dynamics of a system in the unperturbed basis \( |k) \), one uses different quantities. The main interest is to known how many unperturbed states are involved in the dynamics depending on time. One of the commonly used quantities is the Shannon entropy of the packet,

\[ S(t) = - \sum_m w_m \ln w_m = -W_0 \ln W_0 - \sum_{m \neq 0} w_m \ln w_m; \]  \hspace{1cm} \[ \sum_m w_m = 1. \]  \hspace{1cm} (7)

Here we introduced the return probability \( W_0(t) = |A_0(t)|^2 \) for the system to be in the initial state \( |k_0) \), due its special role in global properties of the dynamics. One can see that the effective number \( N_p \) of unperturbed states involved in the dynamics can be estimated as \( N_p \approx \ln S(t) \).

Another quantity which nowadays is under the close investigation, is the so-called fidelity,

\[ \mathcal{F}(t) = |\langle \Psi_p(t) | \Psi_u(t) \rangle|^2 \]  \hspace{1cm} (8)

where \( \Psi_u(t) \) stands for the \( \Psi \)-function of the unperturbed system, and \( \Psi_p(t) \) for that of the perturbed one. In the case when perturbation is weak, this quantity serves as a measure of the sensitivity of the system to a given perturbation [17]. There are many results obtained for the fidelity, both analytical and numerical ones, obtained for
different systems (see, for example, [18] and references therein). The main interest is whether the fidelity can serve as a good indicator of the quantum chaos. Note, that the fidelity depends both on the type of the perturbation, and on the form of an initial packet. In what follows, we discuss this quantity in application to systems of interacting Fermi-particles and to a model of quantum computation.

By comparing the definition (8) with Eqs.(5) and (6), one can see that in the case when the initial state is a specific basis state \( |k_0\rangle \), the fidelity is nothing but the return probability [19],

\[
\mathcal{F}(t) = W_0(t) = |A_0(t)|^2; \quad A_0(t) = \sum_\alpha |C^{\alpha}_{k_0}|^2 \exp(-iE^\alpha t) \approx \int P_{k_0}(E) \exp(-iEt)dE.
\]

Here we replaced the summation by the integration that can be done when the number of components \( C^{\alpha}_{k_0} \) is large for a fixed \( k_0 \). Generically, these components fluctuate strongly, therefore, they can be treated as pseudo-random quantities. In fact, this condition of a large number of pseudo-random components in exact eigenstates can be used as the definition of chaos in quantum systems. In this case, the time dependence of \( W_0(t) \) is entirely determined by the Fourier representation of \( P_{k_0}(E) = P(E, E_{k_0}) \) where \( E \) is the energy of exact eigenstates and \( E_{k_0} \) is the energy corresponding to the unperturbed state \( |k_0\rangle \). This quantity is known in the literature as the strength function (SF), or, as the local spectral density of states,

\[
P(E, E_{k_0}) \equiv \frac{|C^{(\alpha)}|^2}{\rho(E)}
\]

where \( \rho(E) \) is the density of states of the total Hamiltonian \( H \), and the average is performed over a number of states with energies close to \( E \). In next Section we discuss main properties of the fidelity (9) in application to close system of interacting Fermi-particles [19].

III. INTERACTING FERMI-PARTICLES

A. Two-body random interaction model

Let us assume that our model consists of finite number \( N_p \) of Fermi-particles that occupy \( M \) single-particle states \( |s\rangle \) characterized by the corresponding energies \( \epsilon_s \). Then the unperturbed Hamiltonian \( H_0 \) describes non-interacting particles, and the interaction between particles is represented by \( V \). In this case the basis many-body states \( |k\rangle \) can be constructed by the Slater determinant, \( |k\rangle = a_{s_1}^\dagger \ldots a_{s_{Np}}^\dagger |0\rangle \), and the Hamiltonian takes the form

\[
H_0 = \sum_{s=1}^M \epsilon_s a_{s}^\dagger a_s.
\]

Correspondingly, the interaction term can be represented in this basis as

\[
V = \frac{1}{2} \sum_{s_1 s_2 s_3 s_4} V_{s_1 s_2 s_3 s_4} a_{s_1}^\dagger a_{s_2}^\dagger a_{s_3} a_{s_4}
\]

where \( a_{s_j}^\dagger \) and \( a_{s_j} \) are the creation-annihilation operators.

The total Hamiltonian \( H = H_0 + V \) with (11) and (12) appears in many physical applications such as complex atoms, nuclei, atomic clusters etc. In fact, the form of \( H \) discussed above is known as the mean field approximation for complex quantum systems of interacting particles. In this description, the unperturbed part \( H_0 \) represents the zero-order mean field for the excited states with the ground state \( E_1 \), and the residual two-body interaction is given by \( V \). Therefore, the single-particle energies \( \epsilon_s \) in such applications are, in fact, renormalized quasi-particle energies (see details, for example, in Ref. [21]). The considered model turns out to be very useful for understanding of the onset of many-body chaos due to a two-body interaction.

For the analytical analysis one assumes that all two-body matrix elements \( V_{s_1 s_2 s_3 s_4} \) are random Gaussian numbers with the zero mean and the variance \( V_0^2 = \langle V_{s_1 s_2 s_3 s_4}^2 \rangle \). Although this assumption of the randomness is quite strong, however, it was found that many of the properties of this TBRI model are quite generic and occur in different dynamical (without any random parameters) systems. The results obtained in the frame of this model can be also extended to interacting Bose-particles, see, for example, Ref. [20]

Without the loss of generality one can assume that the single-particle spectrum is non-degenerate, with the constant mean level spacing \( d_0 = (\epsilon_{s+1} - \epsilon_s) = 1 \). Therefore, the model is defined by four parameters, \( M, N_p, d_0 \) and \( V_0 \).
Note that the number $N$ of many-body states increases very strongly with an increase of number of particles $N_p$ and number $M$ of single-particles states, $N = \frac{M!}{N_p!(M-N_p)!}$. For this reason even for a relatively small number of particles the size of the Hamiltonian matrix is large, and exact eigenstates may consist of many unperturbed basis states, thus providing us with a possibility to describe the system statistically.

Due to a two-body nature of the interaction, the Hamiltonian matrix has features that are different from those of the standard random matrices that are typically used when studying chaos in quantum systems. Specifically, the $H -$matrix is sparse, the off-diagonal matrix elements of $V$ in the representation of many-particle basis states are not completely independent, and the global structure is a band-like (see details in Refs. [22,8]). This makes the analysis more complicated, on the other side, such matrices give a better description of real physical systems, in comparison with standard random matrix ensembles.

One of the important results obtained recently in the frame of this model is the Anderson-like transition which occurs in the Fock space determined by many-particle states of $H_0$ (see, for example, [11] and references therein). The critical value $V_{cr}$ for this transition is determined by the density of states $\rho_f = \frac{1}{g^2}$ of those basis states which are directly coupled by the two-body interaction. When the interaction is very weak, $V_0 \ll d_f$, exact eigenstates are very close to the unperturbed ones, consisting of a small number of basis states. With an increase of the interaction the number $N_{pc}$ of principal basis components in exact eigenstates increases, and for $V_0 \geq d_f$ the eigenstates may be treated as pseudo-random ones. In this case the number $N_{pc}$ can be estimated as $N_{pc} \sim \Gamma / D$ where $\Gamma$ is the spreading width of the strength function (10). In such chaotic eigenstates any external weak perturbation is exponentially enhanced. The enhancement factor can be estimated as $\sqrt{N_{pc}} \sim 1 / \sqrt{D}$, see Ref. [23]. This huge enhancement have been observed in experiments when studying the parity violation in compound nuclei (see, for example, review [24]). In what follows, we discuss the dynamics of the model above this threshold of chaos.

B. Fidelity

We start now with the expression for the fidelity (9) at small times. According to the perturbation theory, one can easily get,

$$W_0(t) \approx 1 - \Delta_E^2 t^2$$

(13)

where $\Delta_E$ is the width of the strength function (SF) in the energy space determined as

$$\Delta_E^2 = \sum_{m \neq k_0} V_{m,k_0}^2$$

(14)

The second moment $\Delta_E^2$ of the SF for the TBRI model can be found explicitly [7],

$$\Delta_E^2 = \frac{1}{4} V_0^2 N_p(N_p - 1)(M - N_p)(M - N_p + 3)$$

(15)

where $V_0^2$ is the variance of the off-diagonal matrix elements of the two-body interaction $V$. It is interesting that for Fermi-particles the width $\Delta_E$ turns out to be independent of a specific basis state $|k_0\rangle$.

The expressions (13) and (14) are universal, they are correct for any kind of the perturbation $V$. Thus, the quadratic time dependence of the fidelity on a small time scale occurs independently on whether the dynamics is chaotic or regular. This is understandable since the difference between periodic and chaotic motion can be detected on a large time scale only (in principle, for $t \to \infty$).

The situation is much more complicated for large times. In order to understand how strong the decrease of the fidelity on a large time scale, one needs to know the form of the strength function in the energy space. For a long time it was assumed that the SF has generically the Breit-Wigner form (or, the same, the Lorentzian form). On the other hand, recently it was understood that in many physical applications the form of the SF can be quite close to the Gaussian form (see, e.g. [25]). This is because in contrast to full random matrices, physical interactions $V$ always have a finite width in the basis of $H_0$. This point was the reason for Wigner to introduce the so-called Band Random Matrices (BRM) with a finite width. Therefore, one more control parameter arises which is the energy associated with the width of perturbation, in addition to the width of the Lorentzian (see, for example, Ref. [25] and references therein). Full analytical treatment of the form of the SF for the BRM is given in Ref. [26]. Specifically, it was shown that with an increase of the perturbation the form of the SF changes from the Lorentzian to the Gaussian (apart from extremely strong perturbation, when the non-physical semicircle form arises).
Similar transition from the Lorentzian to the Gaussian has been analytically found for the TBRI model discussed above [27], although the analytical expression in the closed form is not known. In order to evaluate the fidelity, in Ref. [19] the following phenomenological expression has been suggested,

\[ P(E) = B \exp \left[ \frac{- (E - E_0)^2}{2\sigma^2} \right] \frac{1}{(E - E_0)^2 + \Gamma^2 / 4} \]  

(16)

where \( E_0 \) is the energy that corresponds to the basis state \(|k_0\rangle\). Strictly speaking, this formula is valid near the center of the energy spectrum that has the Gaussian form, otherwise one should take into account additional distortion effects [7]. Due to the normalization conditions, \( \int P(E) dE = 1 \) and \( \int E^2 P(E) dE = \Delta_E^2 \), only one of three parameters \( B, \Gamma \) and \( \sigma \) is free. The relations between these parameters are:

\[ \frac{1}{B} = 2 \left[ 1 - \Phi \left( \frac{\Gamma}{\sigma \sqrt{8}} \right) \right] \pi \exp \left( \frac{\Gamma^2}{8\sigma^2} \right) \]  

(17)

and

\[ \Delta_E^2 = B \left\{ \sigma \sqrt{2\pi} - \frac{\pi \Gamma}{2} \exp \left( \frac{\Gamma^2}{8\sigma^2} \right) \left[ 1 - \Phi \left( \frac{\Gamma}{\sigma \sqrt{8}} \right) \right] \right\} \]  

(18)

where \( \Phi(z) \) is the error function.

In the case of a relatively small (but non-perturbative) interaction, the form of \( P(E) \) is close to the Lorentzian. In this case \( \Gamma \ll \sigma \) and \( \Gamma \) plays the role of the half-width \( \Gamma_0 \) of the Lorentzian, \( \Gamma \approx \Gamma_0 \). On the other hand, for a strong perturbation the SF has the Gaussian form with \( \sigma \approx \Delta_E \) and formally \( \Gamma \gg \sigma \). The value of \( \Gamma_0 \) for the TBRI model is determined by the Fermi golden rule,

\[ \Gamma_0(E) \approx 2\pi|V_{k_0f}|^2 \rho_f(E) \]  

(19)

where \( \rho_f(E) \) is the density of states directly coupled to the basis state \(|k_0\rangle\) by the two-body interaction \( V \).

In the case of a relatively weak interaction (the Lorentzian form of the SF) for large time, \( t \gg t_c = 1/\sigma \), the evaluation of the fidelity gives,

\[ W_0(t) \approx \exp \left( \frac{1}{\pi} \frac{\Gamma_0^2}{\Delta_E^2} - \Gamma_0 t \right) \approx \exp (-\Gamma_0 t) \]  

(20)

where the correction term \( \frac{1}{\pi} \frac{\Gamma_0^2}{\Delta_E^2} \approx \frac{2\pi}{\sigma \sqrt{2\pi}} \) is small.

In the other limit case of a strong interaction (the Gaussian form of the SF), \( \Gamma \gg \sigma \approx \Delta_E \), we have \( t_c \sim \frac{\Gamma}{\sigma} \gg \frac{1}{\sigma} \). Therefore, the leading dependence of \( W_0(t) \) is the Gaussian,

\[ W_0(t) \approx \exp (-\Delta_E^2 t^2), \]  

(21)

and only for a very long time \( t \gg \frac{\Gamma}{\Delta_E} \) it becomes the exponential function [19],

\[ W_0(t) \approx \frac{\pi^2 \Gamma^2}{8\Delta_E^2} \exp \left( \frac{1}{4} \frac{\Gamma^2}{\Delta_E^2} - \Gamma t \right) \]  

(22)

It is important to note that in this case the return probability \( W_0(t) \) has large correction factor \( \exp \left( \frac{1}{4} \frac{\Gamma^2}{\Delta_E^2} \right) \), in addition to the standard decay law \( W_0(t) = \exp (-\Gamma t) \).

C. Shannon entropy

For the Shannon entropy (7) one needs to know the time dependence of all amplitudes \( w_m(t) \), see Eq.(5). In order to find \( w_m(t) \), in Ref. [25] the theory has been developed which is based on the representation of the dynamics of the system as a flow in the Fock space of many-body states. This approach can be compared with that developed in Ref. [28] where the dynamics in the many-particle basis was represented by a flow on the Cayley tree. For the exponential dependence \( W_0(t) = \exp (-\Gamma t) \), the solution for \( w_m(t) \) has simple form,
\[ W_n(t) = \frac{(\Gamma t)^n}{n!} W_0(t). \] (23)

As one can see, the dynamics of the system can be expressed in terms of the return probability \( W_0(t) \) which is a particular case of the fidelity. Note, that the quantity \( \Gamma \) stands here for the effective width of the SF, and can be either the half-width of the Lorentzian \((\Gamma = \Gamma_0)\), or the square root of the variance of the SF, \((\Gamma = \Delta_E)\), depending on its form (Lorentzian or Gaussian).

As a result, the expression for the Shannon entropy reads,

\[ S(t) \approx \Gamma t \ln N_f + \Gamma t - e^{-\Gamma t} \sum_{n=0}^{\infty} \frac{(\Gamma t)^n}{n!} \frac{(\Gamma t)^n}{n!}, \] (24)

where \( N_f \) is the number of basis states directly coupled to the basis state \(|k_0\rangle\). Two last terms in the right-hand-side of Eq.(24) turn out to be smaller than the first one, therefore, one can write,

\[ S(t) \approx \Gamma t \ln N_f \{1 + f(t)\} \approx \Gamma t \ln N_f \] (25)

with some function \( f(t) \ll 1 \) which slowly depends on time. In this estimate for the increase of entropy, the influence of fluctuations of \( w_n \) is not taken into account. It can be shown that for the gaussian fluctuations of the coefficients \( A_m \), with the variance given by their mean-square values, and \( N_{pc}(t) \approx \exp(S(t)) \gg 1 \), the entropy has to be corrected by a small factor of the order of \( \ln 2 \) (see, for example, [29]).

One should note that at small times the expression for the entropy has to be modified since on this time scale the function \( W_0(t) \) has always the form \( W_0(t) = \exp(-\Delta_E^2 t^2) \). To do this, one needs to replace \( \Gamma t \) in Eq.(23) by a more accurate expression, \(-\ln(W_0)\). This gives \( \Delta_E^2 t^2 \) for small times, \( t \ll \Gamma/\Delta_E^2 \), and \( \Gamma t \) for large times, \( t \gg \Gamma/\Delta_E^2 \). Therefore, at small times, \( t \ll \Gamma/\Delta_E^2 \) the entropy is given by the expression [25],

\[ S(t) \approx \Delta_E^2 t^2 \left(1 + \mathcal{O}(\ln(t^2))\right). \] (26)

As one can see, the “exact” expression (24) for the entropy is quite complicated. Instead, in Ref. [25] it was proposed to use the following simple expression which gives good approximation for systems with a small number of particles,

\[ S(t) = -W_0(t) \ln W_0(t) - (1 - W_0(t)) \ln \left( \frac{1 - W_0(t)}{N_{pc}(m)} \right) \] (27)

Here \( N_{pc}(m) \) is the maximal value of the number of principal components after the saturation of the entropy to its maximal value. Quite often, this phenomenological parameter can be estimated independently.

**IV. THE MODEL OF QUANTUM COMPUTATION**

**A. Description of the model**

Let us now apply the above analysis of the fidelity and entropy to the model of quantum computation. This model describes a one-dimensional chain of \( L \) identical 1/2-spins placed in an external magnetic field. For a selective resonant excitation of spins, it is suggested to choose the time independent part \( B^z = B^z(x) \) of a magnetic field with the constant gradient along the \( x \)-direction. This provides different Larmor frequencies for different spins, \( \omega_k = \gamma_n B^2 = \omega_0 + ak \), where \( \gamma_n \) is the spin gyromagnetic ratio and \( ak = x_k \). One can arrange relative directions of the chain with respect to the \( z \)-axis in a way that the dipole-dipole interaction is suppressed, and the main interaction between nuclear spins is due to the Ising-like interaction mediated by the chemical bonds. This model was first proposed in [30] (see also [31–33]) as a simple realization of a solid-state quantum computation.

In order to implement a time-dependent quantum protocol, the spins are assumed to be subjected to a transversal circular polarized magnetic field. Therefore, the total magnetic field has the following form [34,32,33],

\[ \vec{B}(t) = [b^x_p \cos(\nu_pt + \varphi_p), -b^y_p \sin(\nu_pt + \varphi_p), B^z(x)]. \] (28)

In the above expression, \( b^x_p, \nu_p, \) and \( \varphi_p \) are the amplitudes, frequencies and phases of a circular polarized magnetic field, respectively. The latter is given by a sum of \( p = 1, ..., P \) rectangular time-dependent pulses of length \( t_{p+1} - t_p \), rotating in the \((x, y)\)-plane, in order to make selective excitations of specific spins. Thus, the quantum Hamiltonian of the system has the form,
where the “pulse function” \( \Theta_p(t) \) equals 1 during the \( p \)-th pulse, for \( t_p < t \leq t_{p+1} \), otherwise, it is zero. The quantities \( J_{k,n} \) stand for the Ising interaction between two qubits, \( \omega_k \) are the frequencies of spin precession in the \( B^z \)-magnetic field, \( \Omega_p \) is the Rabi frequency of the \( p \)-th pulse, \( I_k^{x,y,z} = (1/2)\sigma_k^{x,y,z} \) as the Pauli matrices, and \( I_k^z = I_k^x + i I_k^y \).

For a specific \( p \)-th pulse, it is convenient to represent the Hamiltonian (29) in the coordinate system that rotates with the frequency \( \nu_p \). Therefore, for the time \( t_p < t \leq t_{p+1} \) of the \( p \)-th pulse our model can be reduced to the stationary Hamiltonian,

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

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

Below we restrict our considerations by the Hamiltonian for a single pulse, by choosing \( \varphi_p = 0 \). We also assume a constant interaction between nearest qubits, \( J_{k,n} = J \delta_{k,k+1} \). Then the Hamiltonian takes the form,

\[
\mathcal{H}^{(p)} = -\sum_{k=0}^{L-1} \left[ -\xi_k I_k^z - 2 J I_k^z I_{k+1}^z \right] - \sum_{k=0}^{L-1} \Omega_p I_k^x.
\]

In the \( z \)-representation the Hamiltonian matrix of size \( 2^L \) is diagonal for \( \Omega_p = 0 \). Therefore, below we define \( \mathcal{H}_0 \) and \( V \) as

\[
\mathcal{H}_0 = -\sum_{k=0}^{L-1} \left[ -\xi_k I_k^z - 2 J I_k^z I_{k+1}^z \right] \quad V = -\sum_{k=0}^{L-1} \Omega_p I_k^z.
\]

where we omitted the index \( p \). The unperturbed basis (in which \( \mathcal{H}_0 \) is diagonal) is reordered according to an increase of the index \( s \) which is written in the binary representation, \( s = i_{L-1}i_{L-2}...i_0 \) (with \( i_s = 0 \) or 1, depending on whether the single-particle state of the \( i \)-th qubit is the ground state or the excited one). The parameter \( \Omega \) thus is responsible for a non-diagonal coupling, determining matrix elements of \( V \) as \( V_{kn} = V_{nk} = -i\Omega/2 \) with \( n \neq k \). As one can see, in contrast with the TBRI model discussed above, in the \( z \)-representation the interaction between particles is absorbed by \( \mathcal{H}_0 \), and \( V \) describes the coupling to the external magnetic field.

There are two regions of the parameters of physical interest. The first one is known as the so-called non-selective regime which is defined by the conditions, \( \Omega \gg \delta \omega_k \gg J \). This inequality provides the simplest way to prepare a homogeneous superposition of \( 2^L \) states needed for the implementation of both Shor and Grover algorithms. The analytical and numerical treatment of the model (32) in this regime has shown [34] that constant gradient magnetic field (with the non-zero value of \( a \)) strongly reduces the effects of quantum chaos. Namely, the chaos border turns out to be independent of the number \( L \) of qubits, in contrast to the models thoroughly studied in Ref. [13]. In particular, it was shown that quantum chaos occurs for a very large coupling \( \Omega = 100 \) and very strong interaction \( J = 100 \) between qubits. For these parameters the Wigner-Dyson distribution between nearest energy levels has been observed, the fact that can serve as a numerical proof of the quantum chaos. The transition to chaos for \( \Omega = 100 \) in dependence on \( J \) can be analytically understood with the use of the transformation to the “mean field basis” in which the Hamiltonian is diagonal in the absence of the inter-qubit interaction, \( J = 0 \). In this basis the term with \( J \neq 0 \) plays the role of the interaction between \( L \) blocks that correspond to quantum numbers, and the structure of the Hamiltonian matrix is similar to that of the TBRI model, see details in Ref [34].

Another region characterized by inequalities \( \Omega \ll J, a \ll \omega_k \), is referred as the selective excitation, see Ref. [32]. In this regime each magnetic pulse acts selectively on a chosen qubit, resulting in a resonant transition. According to the quantum protocol, many such resonant transitions take place for different \( p \) pulses, with different values of \( \nu_p \). The detailed analytical analysis [35] has revealed that in this regime the perturbation theory works very well for many pulses, thus, indicating that there is no any effect of the quantum chaos. Therefore, the implementation of the constant gradient magnetic field is very effective in reducing any kind of decoherence.

### B. Shannon entropy and fidelity

Now we discuss numerical data for the above model of quantum computation, by paying the main attention to the time-dependence \( S(t) \) of the Shannon entropy and fidelity \( F(t) \). As we have discussed, the time-dependence of the
Shannon entropy provides us with the information about the evolution of the wave packets in the unperturbed basis. Since the latter is determined by the Hamiltonian $H_0$ in Eq.(32), the time-dependence of the entropy is directly related to the $\Omega$–dependent term. The main interest is in the role of the interaction $J$, as well as of static random terms which we add to $\Omega$. Specifically, each of non-zero off-diagonal elements is now the sum of two terms, $\Omega \Rightarrow \Omega_0 + \xi_p$ where $\xi_p$ stands for random variables with the zero mean and variance $\sigma_p^2 = \langle \xi_p^2 \rangle$. This kind of randomness corresponds to the imperfections in the Rabi frequencies.

In the first line, we discuss how the Shannon entropy depends on time if the initial state is the basis state chosen, for simplicity, at the center of the energy spectrum. Typical dependencies for $S(t)$ are shown in Fig.1 where we have normalized the entropy to its maximal value $S_{\text{max}}$ determined by the total number of many-body states. The value $S_{\text{max}}$ corresponds to the case when all basis states are equally populated, with the standard normalization that the total probability is one. As one can see from the data, the entropy saturates to its maximal value in two cases. The first one occurs for the dynamical chaos which is due to a large value of the inter-cubit interaction, $J = 100$. In this case there is no difference whether we have disorder $\sigma_p$ or not. Another case is when the disorder is strong, $\sigma_p = 20$. In this situation, the saturation occurs even for $J = 0$. These results are quite instructive since they demonstrate equivalence of the dynamical chaos to a disorder. It should be pointed out that the entropy does not reach the maximal value $S(t) = 1$ (in the saturation) which may be explained by a suppressed chaos for the states with the energies close to the edges of the spectrum. The most important result is that for strong chaos (dynamical or due to the disorder), the system can be well described by statistical methods.

The depth $S_{\text{min}}$ of the first minimum in the time dependence of $S(t)$ can be used as a relative measure of chaos in the system. In Fig.2 the ratio $S_{\text{min}}/S_{\text{max}}$ is plotted against $J$, thus showing the transition to chaos. Surprisingly, the transition turns out to be quite smooth, in contrast to the transition measured in terms of an effective number of components in exact eigenstates [34]. The latter transition has revealed two borders, one is due to the “delocalization” of the eigenstates in the unperturbed basis (for $J \geq 15$), and the second one which is due to the quantum chaos in the eigenstates (for $J \sim 100$, when the level spacing distribution has the Wigner-Dyson form), see details in Ref [34]. Therefore, the Shannon entropy can serve as the indicator of the delocalization, rather than of the quantum chaos. Indeed, one can have a good relaxation even in a completely integrable system, if one uses the basis which is “very far” from the basis corresponding to the total Hamiltonian.

Let us now analyze how good is the correspondence of the above data to the analytical expression (25) obtained
for the TBRI model. This expression gives the linear increase of the entropy before the saturation. The value of $\Gamma$ in Eq. (25) can be expressed via the variance (14), since in our case $V$ is formally large ($\Omega = 100$). Taking into account that in each row of the matrix $V$ there are only $N_f = L$ non-zero elements, one can easily compare the expression (25) with the numerical data, see Fig. 3. One can see that when the disorder is absent or small, $\sigma_p = 0; 15$, the linear slope of $S(t)$ is slightly different from that predicted by Eq. (25). On the other hand, when the disorder is strong, $\sigma_p = 50$, the correspondence between the analytical expression and numerical data is quite good. Thus, the theory developed in the frame of the TBRI model appears to be also valid for the models that are not fully random. Similar effect was also observed in the Bose-Einstein condensate model [20]. Namely, for a relatively strong interaction between bosons, the Shannon entropy of the wave packet which was initially in the condensate, was found to increase linearly with time in a good agreement with the analytical expression (25). This proves an effectiveness of the approach developed in Ref. [34] in application to both dynamical and random systems.

![FIG. 2. The ratio of the entropy in its first minimum, to the maximal value $S_{\text{max}}$ in dependence on $J$ for two values $\sigma_p$ of the disorder.](image1)

![FIG. 3. Small time scale for the Shannon entropy where the linear increase is expected before the saturation. The data are given for $\Omega_0 = 100$, $J = 100$, $\alpha = 1$ and different strengths of the disorder, $\sigma_p = 0; 15; 50$. Open symbols stand for the numerical data, full symbols, for the analytical estimate (25).](image2)

We turn now to the fidelity. Since in our model there is a large off-diagonal part determined by the constant term $\Omega$ and by random terms $\sigma_p$, we introduce an additional random (small) terms $\varepsilon_p$ that can be treated as the perturbation.
In this way we can analyze the dependence of the fidelity on time $t$ and on the perturbation $\varepsilon^2 = \langle \varepsilon_p^2 \rangle$ for different values of $J$ and $\sigma_p$. Typical dependencies for the fidelity $F(t)$ are reported in Fig. 4. First, it is interesting to discuss the data for the dynamical model, when $\sigma_p = 0$. Unexpectedly, for the integrable case ($J = 0$) the fidelity is much less than for the quantum chaos ($J = 100$). This fact may have the same origin that was discovered in Ref [36]. However, we should stress that our model has no classical limit, therefore, we can speak about integrability or chaos without the reference to the classical dynamics. Moreover, in Ref [36] the effect of a stronger stability for chaotic situation occurs mainly on a small time scale. In our case the effect is clearly seen on a large time scale as well. One should not also forget that for $J = 0$ the unperturbed spectrum is highly degenerate, therefore, the observed effect of a stronger stability for larger values of $J$ may be related to the break of the degeneracy.

Another effect is that practically there is no difference for the values $\sigma_p = 15$ and $\sigma_p = 50$. This means that for $\sigma_p \geq 15$ the disorder is quite strong and does not depend on its strength. Indeed, for such a disorder, the difference between integrable ($J = 0$) and chaotic ($J = 100$) cases is not big. Thus, the results given by the fidelity confirm the conclusion drawn from the entropy data: dynamical chaos that is due to a strong interaction $J = 100$ between qubits, and chaos due to a strong disorder $\sigma = 50$ are similar (compare fidelity for $J = 100$, $\sigma_p = 0$ with that for $J = 0, \sigma_p = 50$).

![Fidelity for different inter-qubit interactions](image)

FIG. 4. Fidelity for different inter-qubit interactions $J$ and the disorder $\sigma_p$, with $\Omega_0 = 100$. The time dependence is shown for 3 different values of the perturbation, $\varepsilon = 5$ (squares), $\varepsilon = 10$ (circles), and $\varepsilon = 20$ (triangles).

It is also instructive to analyze more carefully the time-dependence of the fidelity for the dynamical case when $\sigma_p = 0$, see Fig. 5. One can see a very good scaling $F = F(\varepsilon t)$ for the integrable case $J = 0$, in contrast with the chaotic case $J = 100$. Moreover, as is seen from the data in semi-log scale, practically for all values of $F$, apart from very small values, the time dependence is the Gaussian, $F \sim \exp(-C \varepsilon^2 t^2)$. This is in contrast to the chaotic case with $J = 100$ (additional data show that the dependence of $F$ on time is closer to the exponential one rather to the Gaussian one). The origin of a good scaling, together with its Gaussian form is not clear, however, one can expect that it is related to the form of the strength function, as in the case of the TBRI model. To clear up this problem, additional numerical study is needed.
V. CONCLUDING REMARKS

As is mentioned above, there are many studies where the time-dependence of the fidelity is discussed from the viewpoint of quantum chaos. The main attention was paid to a long time scale on which an exponential or Gaussian decay typically occurs. In the case of the exponential decay the question of general interest is about the characteristic parameter of this decay. Specifically, it is widely discussed whether the exponential decrease of the fidelity is governed by the Fermi golden rule (in this case the strength function has the Lorentzian form), or by the classical Lyapunov exponent of the corresponding classical system.

On the other hand, in application to the models of quantum computation the problem of a long-time behavior of the fidelity seems to be irrelevant. Indeed, for a quantum computation one needs to have a very stable regime where the fidelity is close to one. Therefore, in this application one should pay the main attention to the short time scale, where the fidelity differs from 1, say, not more than $10^{-3}$. This is because the time of the quantum computation can be very large, and many pulses of an external magnetic field are needed to implement the quantum protocol. One should expect that in this situation the perturbation theory works well (see Ref. [35]). Let us see what the perturbation theory gives for our model (32) describing the system within a single pulse. In our case the total Hamiltonian $H = H_0 + V$ has both diagonal and off-diagonal parts, and let us assume that the perturbation is described by an additional term $\Sigma$ of the same structure as the $\Omega-$ term in Eq.(32), with the variance $\varepsilon^2$ for its matrix elements. Also, we assume that the interaction part $V$ may have additional terms, see above.

In this case the perturbation theory gives,

$$\mathcal{F}(t) = 1 - \delta_E^2 t^2 - Re(R) t^2$$  \hspace{1cm} (33)

where

$$\delta_E^2 = \sum_{m \neq k_0} \Sigma^2_{m_k} = \varepsilon^2 N_c ; \quad R = H \Sigma - \Sigma H.$$  \hspace{1cm} (34)

with $N_c$ as the number of non-zero matrix elements of $\Sigma$ for a fixed $k_0$. 

FIG. 5. Comparison of the fidelity for the regular, $J = 0$, and chaotic, $J = 100$, cases, with $\Omega_0 = 100$. In both cases the disorder is absent, $\sigma_p = 0$. Different scales are used for the fidelity and $\varepsilon t$, in order to reveal the time-dependence on a large time scale. As in Fig.4, $\varepsilon = 3; 5; 7$ with squares, circles and triangles, respectively.
One can see that when the unperturbed Hamiltonian \( H \) has a diagonal form (for example, when \( V = 0 \)) the terms \( H \) and \( \Sigma \) commute (therefore, \( R = 0 \)) and we come to the previous expression (13) with \( \Delta_{E}^{2} = \delta_{E}^{2} \). Since in our numerical study the perturbation has the same structure as the off-diagonal \( \Omega \) terms, one can get \( R = V \Sigma - \Sigma V = 0 \) (assuming \( \langle \Sigma_{m,k} \rangle = 0 \)) Therefore, for our particular type of the perturbation, there is no influence of the term \( V \).

Our numerical data confirm these findings. The expression (33), however, shows that in a general case the fidelity strongly depends on the type of the perturbation.

In conclusion, we have studied the time dependence of the Shannon entropy and fidelity for the model of a quantum computation, in comparison with analytical predictions obtained for the model with two-body random interaction. In spite of a big difference between these two models (one is the dynamical one and another is random), we have found that in many aspects some properties of the dynamics are quite similar. One of the important results is that global properties of the dynamics look the same both for the dynamical model with strong chaos, and for the model with a strong disorder. In particular, the entropy and fidelity behave in the same way, manifesting the relaxation of the system to a statistical equilibrium. The time scale on which this relaxation occurs can be described by a linear increase of the entropy, with a good correspondence with the simple analytical expression. This fact confirms the expectation that the TBRI model can serve as the base in understanding the properties of quantum many-body chaos.

Specifically, there are many open questions related to the problem of the universal properties of the fidelity. Much depends on the type of the perturbation and on the form of an initial packet, therefore, more extensive studies are needed. As for the application of the fidelity to a quantum computation, one can expect that real interest is restricted by a small time scale where the standard perturbation theory works very well, and there is no influence of the quantum chaos.


