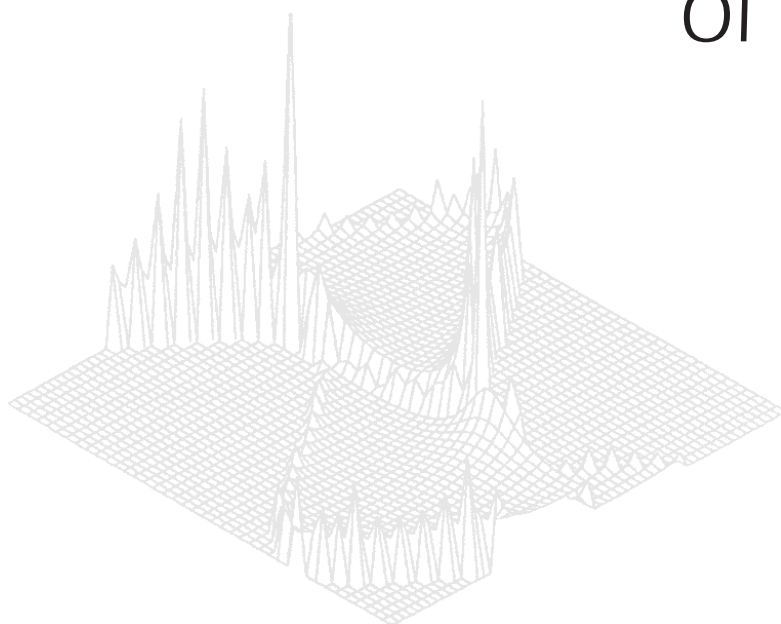

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Time Dynamics in Chaotic Many-body Systems: Can Chaos Destroy a Quantum Computer?*

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Abstract

Highly excited many-particle states in quantum systems (nuclei, atoms, quantum dots, spin systems, quantum computers) can be ‘chaotic’ superpositions of mean-field basis states (Slater determinants, products of spin or qubit states). This is a result of the very high energy level density of many-body states which can be easily mixed by a residual interaction between particles. We consider the time dynamics of wave functions and increase of entropy in such chaotic systems. As an example, we present the time evolution in a closed quantum computer. A time scale for the entropy $S(t)$ increase is $t_c \sim \tau_0/(n \log_2 n)$, where τ_0 is the qubit ‘lifetime’, n is the number of qubits, $S(0) = 0$ and $S(t_c) = 1$. At $t \ll t_c$ the entropy is small: $S \sim n^2 J^2 \log_2(1/t^2 J^2)$, where J is the inter-qubit interaction strength. At $t > t_c$ the number of ‘wrong’ states increases exponentially as $2^{S(t)}$. Therefore, t_c may be interpreted as a maximal time for operation of a quantum computer. At $t \gg t_c$ the system entropy approaches that for chaotic eigenstates.

1. Introduction

Highly excited many-particle states in many-body systems can be presented as ‘chaotic’ superpositions of shell-model basis states—see the recent calculations for complex atoms (Flambaum *et al.* 1994), multicharged ions (Gribakin *et al.* 1999), nuclei (Zelevinsky *et al.* 1996) and spin systems (Georgeot and Shepelyansky 1998). Indeed, the number of combinations to distribute n particles over m orbitals is exponentially large [$m!/n!(m-n)!$ in a Fermi system]. Therefore, the interval between the many-body levels D is exponentially small and residual interaction between the particles mixes a huge number of the mean-field basis states (Slater determinants) when forming eigenstates. The number of principal basis components in an eigenstate can be estimated as $N_p \sim \Gamma/D$, where Γ is the spreading width of a typical component that can be estimated using the Fermi Golden Rule. In such chaotic eigenstates any external weak perturbation is exponentially enhanced. The enhancement factor is $\sim \sqrt{N_p} \propto 1/\sqrt{D}$ (see e.g. Flambaum and Sushkov 1984 and references therein). This huge enhancement has been observed in numerous experiments studying parity violation effects in compound nuclei (see e.g. the review by Mitchell *et al.* 1999 and references therein).

In a recent work (Georgeot and Shepelyansky 1999) the consideration of many-body chaos has been extended to quantum computers (Feynman 1986; Shor 1994; Cirac and Zoller 1995; Monroe *et al.* 1995; Calderbank and Shor 1996; Steane 1996, 1998; Cory *et al.* 1996; Gershenfeld and Chuang 1997; Privman *et al.* 1998; Kane 1998; Loss and Di

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Vincenzo 1998; Nakamura *et al.* 1999; Brennen *et al.* 1999; Jaksch *et al.* 1999). Any model of a quantum computer is somewhat similar to that of a spin system. Georgeot and Shepelyansky (1999) modelled a quantum computer by a random Hamiltonian:

$$H = \sum_i \epsilon_i \sigma_i^z + \sum_{i < j} J_{ij} \sigma_i^x \sigma_j^x, \quad (1)$$

where σ_i are the Pauli matrices for the qubit i and the second sum runs over nearest-neighbour qubit pairs. The energy spacing between the two states of a qubit was represented by ϵ_i which was uniformly distributed in the interval $[0.5\Delta_0, 1.5\Delta_0]$ (in fact the particular form of the ϵ_i distribution is not important). Here ϵ_i can be viewed as the splitting of nuclear spin levels in a local magnetic field, as discussed in recent experimental proposals (Privman *et al.* 1998; Kane 1998). The different values of ϵ_i are needed to prepare a specific initial state by electromagnetic pulses in nuclear magnetic resonance. In this case the couplings J_{ij} will represent the interactions between the spins, which are needed for multi-qubit operations in the quantum computer. The total number of states in this system is $N = 2^n$, and the typical interval between the nearby energies of multiqubit states is $\sim \Delta_0 2^{-n}$.

A rough estimate for the boundary of the chaos in the quantum computer eigenstates is $J_c \sim \Delta_0/qn$, where qn is the number of interacting qubit pairs ($qn = 2n$ in a 2D square array of ‘spins’ with only short-range interactions). This follows from a simple perturbation theory argument: the mixing is strong when the perturbation is larger than the minimal energy interval between the basis states which can be directly mixed by this perturbation (see a detailed discussion of the boundary of chaos in many-body systems in Aberg 1990; Shepelyansky and Sushkov 1997; Altshuler *et al.* 1997; Mirlin and Fyodorov 1997; Weinmann *et al.* 1997; Jacquod and Shepelyansky 1997; Silvestrov 1997, 1998; Flambaum and Izrailev 1997; Flambaum and Izrailev 2000). Numerical simulations in Georgeot and Shepelyansky (1999) have shown that the boundary of the chaos in the quantum computer eigenstates is $J_c \simeq 0.4 \Delta_0/n$. Above this point they observed a transition from Poissonian to Wigner–Dyson statistics for the intervals between the energy levels. For $J < J_c$ one eigenstate is formed by one or few basis states built from the non-interacting qubits (products of ‘up’ and ‘down’ states). For $J > J_c$ a huge number of basis states is required.

Because of the exponential laws it is convenient to study the entropy S of the eigenstates (in many-body systems the entropy is $S \simeq \ln N_p$; see e.g. Flambaum and Izrailev 1997). Georgeot and Shepelyansky (1999) observed a dramatic increase of the eigenstate entropy in the transition from $J < J_c$ to $J > J_c$; in fact, they defined J_c as a point where $S = 1$. This process (Georgeot and Shepelyansky 1999) of the eigenstates becoming chaotic with an increase of J , or number of qubits n , has been termed a ‘melting’ of the quantum computer and has been assumed to lead to destruction of its operability. These authors have stressed that this destruction of operability takes place in an isolated (closed) system without any external decoherence process (one could complement this picture by the $\sqrt{N_p}$ enhancement of any weak external perturbation acting on the quantum computer).

This straightforward conclusion may be misleading. ‘Theoretically’, this picture is similar to that observed in nuclei and atoms. However, the ‘experimental’ situation is very different. In nuclei and atoms, experiments have resolved particular many-body energy levels. Therefore, the description of the systems based on a consideration of the eigen-

states was an adequate one. In quantum computers the energy interval between the eigenstates is extremely small. Georgeot and Shepelyansky (1999) estimated that the average interval between the multi-qubit eigenstates for 1000 qubits, the minimum number for which Shor's (1994) algorithm becomes useful (Steane 1998) is $D \sim 10^{-298}$ K (for a realistic $\Delta_0 \sim 1$ K). Therefore, in the case of a quantum computer it is impossible to resolve multiqubit energy levels. Temperature, or the finite time of the process τ , gives an uncertainty in energy $\delta E \gg D$. In this case the picture with chaotic eigenstates is not an adequate one and we should consider the time evolution of the quantum computer wave function and entropy. Quantum chaos in the eigenstates allows us to apply a statistical approach to this consideration.

2. Time Evolution of the Chaotic Many-Body State

Exact ('compound') eigenstates $|k\rangle$ of the Hamiltonian H can be expressed in terms of simple shell-model basis states $|f\rangle$ in many-body systems or products of qubits in a computer:

$$|k\rangle = \sum_f C_f^{(k)} |f\rangle; \quad |f\rangle = a_{f_1}^+ \dots a_{f_n}^+ |0\rangle. \quad (2)$$

These compound eigenstates $|k\rangle$ are formed by the residual interaction J ; a_s^+ are creation or spin-raising operators (if the ground state $|0\rangle$ corresponds to spins down). The distribution law for the coefficients $C_f^{(k)}$ and the correlations between the different coefficients in chaotic many-body systems have been studied in numerous publications, see e.g. Flambaum *et al.* (1996) and references therein. Consider now the time evolution of the system. Assume that initially ($t=0$) the system basis state $|i\rangle$ (quantum computer in a state with certain spins 'up') which can be presented as a sum over exact eigenstates:

$$|i\rangle = \sum_k C_i^{(k)} |k\rangle. \quad (3)$$

Then the time-dependent wave function is equal to

$$\Psi(t) = \sum_{k,f} C_i^{(k)} C_f^{(k)} |f\rangle \exp(-iE^{(k)}t). \quad (4)$$

The sum is taken over the eigenstates k and basis states f ; we put $\hbar = 1$. The probability $W_i = |A_i|^2 = |\langle i|\Psi(t)\rangle|^2$ to find the initial state in this wave function is determined by the amplitude

$$A_i = \langle i|\exp(-iHt)|i\rangle = \sum_k |C_i^{(k)}|^2 \exp(-iE^{(k)}t) \simeq \int dE P_i(E) \exp(-iEt). \quad (5)$$

In the case where chaos has developed the number of the eigenstates in this sum is very large and the distribution of the coefficients $|C_i^{(k)}|^2$ is smooth. Therefore, we replaced the summation over the eigenstates by the integration over their energies $E \equiv E^{(k)}$ and introduced the 'strength function' $P_i(E)$ which is also known in the literature as the 'local spectral density of states',

$$P_i(E) \equiv \overline{|C_i^{(k)}|^2} \rho(E), \quad (6)$$

where $\rho(E)$ is the density of the eigenstates. In chaotic systems the strength function is given by a Breit–Wigner-type formula (see e.g. Bohr and Mottelson 1969; Flambaum and Izrailev 2000):

$$P_i(E) = \frac{1}{2\pi} \frac{\Gamma_i(E)}{(E_i + \delta_i - E)^2 + (\Gamma_i(E)/2)^2}, \quad (7)$$

$$\Gamma_i(E) \simeq 2\pi \overline{|H_{if}|^2} \rho_f(E) \sim J^2 qn / \Delta_0. \quad (8)$$

Here δ_i is the correction to the unperturbed energy level E_i due to the residual interaction J , $\rho_f(E) \sim qn/\Delta_0$ is the density of the ‘final’ basis states directly connected by the interaction matrix element H_{if} with the initial state $|i\rangle$. We see from the equations above that the time dynamics is determined by the structure of the eigenstates.

It is easy to find $W_i(t)$ for a small time t . Let us separate the energy of the initial state $E_i \equiv H_{ii}$ in the exponent and make a second order expansion in $H - E_i$ or $E - E_i$ in equation (5). The result is

$$A_i = \exp(-iE_i t) [1 - (\Delta E)^2 t^2 / 2], \quad (9)$$

$$W_i(t) = [1 - (\Delta E)^2 t^2], \quad (10)$$

$$(\Delta E)^2 = \sum_{f \neq i} H_{if}^2 = \sum_{i < j} J_{ij}^2 = qn J_r^2. \quad (11)$$

Here $(\Delta E)^2$ is the second moment of the strength function, and J_r is the r.m.s. value of the interaction strength, $J_r^2 \equiv \overline{J_{ij}^2}$. The first moment is equal to $E_i = H_{ii}$ [see e.g. Flambaum and Izrailev (1997) and Flambaum and Izrailev (2000) where one can also find the calculations of $(\Delta E)^2$ and the spreading width $\Gamma(E)$ for many-body systems].

Note that in the special case of a very strong residual interaction, $J \gg \Delta_0$, this short-time dependence can be extended to a longer time using the exact solution for the case of $\Delta_0 = 0$ [in this case it is easy to calculate $\exp(-iHt)$]:

$$A_i = \prod_{i < j} \cos J_{ij} t \simeq \prod_{i < j} [1 - (J_{ij} t)^2 / 2] \simeq \exp[-(\Delta E)^2 t^2 / 2], \quad (12)$$

$$W_i(t) \simeq \exp[-(\Delta E)^2 t^2]. \quad (13)$$

The strength function and density of states in this limit are also described by Gaussian functions with variance $\sigma^2 = (\Delta E)^2$:

$$P_i(E) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-E^2/2\sigma^2), \quad (14)$$

$$\rho(E) = \frac{2^n}{\sqrt{2\pi\sigma^2}} \exp(-E^2/2\sigma^2). \quad (15)$$

The density of states remains Gaussian for $\Delta_0 \neq 0$, with $\sigma^2 = n\overline{\epsilon^2} + (\Delta E)^2$ if there is no gap in the single-qubit spectra (in Georgeot and Shepelyansky 1999 the ‘up’ and ‘down’ spectra were separated by a gap equal to Δ_0). In general the unperturbed density of states ($J = 0$) can be presented as a sum of the Gaussian functions (one should separate classes of

states with a certain number of spins ‘up’). The interaction J in the Hamiltonian (1) mixes these classes and makes the density closer to the single Gaussian function.

The limit at large time in the chaotic case can be obtained by calculation of the integral in equation (5) in the complex E plane. We should close the contour of integration in the bottom part of the complex plane ($\text{Im}(E) < 0$) to provide a vanishing contribution at infinity. The limit at large time t is given by the pole of the strength function (7) closest to the real E axis. If Γ and δ_i do not depend on E the integration gives the usual exponential decay $W_i = \exp(-\Gamma t)$ (Bohr and Mottelson 1969). However, the dependence of the spreading width on energy E is necessary to provide the finite second moment $(\Delta E)^2$ of the strength function. [Note that in many-body systems the dependence $\Gamma(E)$ can be approximated by a Gaussian function, since the density of final states $\rho_f(E_f)$ in equation (8) is usually close to Gaussian (Flambaum and Izrailev 2000).] If $\Gamma < \Delta E$ the closest pole is given by $\tilde{\Gamma} = -2\text{Im}(E_p)$, where E_p is a solution of the equation $E_p = E_i + \delta_i(E_p) - i\Gamma(E_p)/2$ with a minimal imaginary part. If $\Gamma \ll \Delta E$ we have $\tilde{\Gamma} = \Gamma$. As a result we obtain an exponential dependence for large t :

$$W_i(t) \sim \exp(-\tilde{\Gamma}t). \quad (16)$$

It is useful to have a simple extrapolation formula (valid for $\Gamma < \Delta E$) between the cases of the short time equation (10) and the long time equation (16):

$$W_i(t) = \exp\left(\frac{\Gamma^2}{2(\Delta E)^2} - \sqrt{\frac{\Gamma^4}{4(\Delta E)^4} + \Gamma^2 t^2}\right). \quad (17)$$

Now we can estimate the probabilities of the other components W_f . For short time or small interaction J , other components can be populated due to direct transitions from the initial state only:

$$\begin{aligned} W_f &= |\langle f | \exp(-iHt) | i \rangle|^2 \simeq |H_{if}|^2 \left| \int_0^t |A_i(t)| \exp(i\omega_{if}t) dt \right|^2 \\ &\simeq \frac{|H_{if}|^2}{\omega_{if}^2 + \Gamma^2/4} |\exp(i\omega_{if} - \Gamma/2)t - 1|^2. \end{aligned} \quad (18)$$

Here $\omega_{if} = E_f - E_i$. We stress again that this approximate equation does not contain transitions between the small components. For example, it does not contain the width of the state f ; the width Γ is only to indicate some increase of the denominator and to clarify the ‘short time’ condition that should include small $\omega_{if}t$, Γt or $\Delta E t$. For short time we have $W_f = |H_{if}|^2 t^2$. Here H_{if} is equal to one of the J_{ij} that produces a change of the state of a pair of ‘spins’ (qubits), transferring the initial state i to another state f . The result at longer times is different for perturbative and chaotic regimes. In the perturbative regime where $J \ll \Delta_0/qn$, equation (18) is the final one. In the chaotic regime we can find the asymptotic expression for long times. The projection of $\Psi(t)$ in equation (4) to the component f gives

$$W_f(t) = W_f^s + W_f^{\text{fluct}}(t), \quad (19)$$

$$W_f^s = \sum_k |C_i^{(k)}|^2 |C_f^{(k)}|^2 \simeq \int \frac{dE}{\rho(E)} P_i(E) P_f(E) \simeq \frac{1}{2\pi\rho} \frac{\Gamma_t}{(E_i - E_f)^2 + (\Gamma_t/2)^2}. \quad (20)$$

Here $\Gamma_t \simeq \Gamma_i + \Gamma_f \simeq 2\Gamma$ and

$$W_f^{\text{fluct}}(t) = \sum_{k,p; k \neq p} C_i^{(k)} C_f^{(k)} C_i^{(p)} C_f^{(p)} \exp[i(E^{(k)} - E^{(p)})t]. \quad (21)$$

At long time t , the different terms in $W_f^{\text{fluct}}(t)$ rapidly oscillate and we can put $\overline{W_f^{\text{fluct}}(t)} = 0$. Thus, asymptotically, the distribution of the components in the time-dependent wave function is close to that in the chaotic eigenstates [see equations (6) and (7)] with a doubled spreading width.

3. Entropy Increase

It is convenient to define the entropy of a many-body state as a sum over the basis components (a comparison with other definitions can be found in e.g. Flambaum and Izrailev 1997):

$$S = -\sum_s W_s \log_2 W_s = -W_i \log_2 W_i - \sum_{f \neq i} W_f \log_2 W_f. \quad (22)$$

Initially, we have only one component, $W_i = 1$, and the entropy is equal to zero. It is easy to obtain a short-time estimate for the entropy using equations (10), (11) and (18):

$$S \simeq (\Delta E)^2 t^2 \log_2 [qn / (\Delta E)^2 t^2] = qn J_r^2 t^2 \log_2 (1/J_r^2 t^2). \quad (23)$$

We see that the initial increase of the entropy is relatively small ($\sim t^2$), however, it is proportional to the number of qubits n .

The criterion of a quantum computer ‘melting’ used in Georgeot and Shepelyansky (1999) is the entropy $S = 1$. We can extend the short-time consideration to include this point. For a short time we have some decrease of the initial component and population of the components directly coupled to the initial one. The number of such small components is equal to the number of interacting pairs (qn) in the Hamiltonian (1), since each pair can change its state due to interaction and this leads to a different many-body state. Using the normalisation condition $\sum_s W_s = 1$, we obtain an estimate $\overline{W_f} = (1 - W_i)/n_f$, where n_f is the ‘principal’ number of the final components. Initially we have $n_f = qn$. This gives us the following approximate expression for the entropy:

$$\begin{aligned} S &= -W_i \log_2 W_i - \log_2 [(1 - W_i)/n_f] \sum_{f \neq i} W_f \\ &= -W_i \log_2 W_i - (1 - W_i) \log_2 [(1 - W_i)/n_f] \simeq (1 - W_i) \log_2 (n_f). \end{aligned} \quad (24)$$

The last approximate expression is an estimate with logarithmic accuracy, assuming $\log_2(n_f)$ is large.

The condition $S = 1$ combined with equation (17) for $W_i(t)$ and equation (24) for the entropy $S(t)$ gives

$$W_i(t) = \exp \left(\frac{\Gamma^2}{2(\Delta E)^2} - \sqrt{\frac{\Gamma^4}{4(\Delta E)^4} + \Gamma^2 t^2} \right) = 1 - 1/\log_2(n_f). \quad (25)$$

This means that the ‘melting’ happens when the probability to be in the initial state W_i is still close to 1 [since $\log_2(n_f)$ is large]. The loss of operability of the quantum computer is due to the admixture of a large number of the small components (‘wrong’ basis states).

We should note that, strictly speaking, the argument of the \log_2 may differ from $n_f = qn$, since the point t_c can be outside the short time approximation. However, the estimate in equation (25) with $\log_2 n_f \simeq \log_2 n$ is valid with logarithmic accuracy [for example, a more accurate estimate in the case of $\Gamma \ll \Delta E$ is $n_f \simeq qn\Gamma/\Delta_0$; this follows from equation (18)].

Equation (25) allows us to obtain a simple estimate for the maximal operational time t_c :

$$t_c \simeq \frac{\hbar}{\Gamma \log_2(n)} \sqrt{1 + \frac{\Gamma^2 \log_2 n}{(\Delta E)^2}}. \quad (26)$$

In the case of $\Gamma \ll \Delta E$ we have

$$t_c \simeq \frac{\hbar}{\Gamma \log_2(n)} = \frac{\tau_0}{n \log_2(n)}. \quad (27)$$

Here $\tau_0 = \hbar/\Gamma_0$ is the ‘lifetime’ related to a single qubit, $\Gamma_0 = \Gamma/n$; recall that Γ is proportional to the number of qubits n . More accurate results can be obtained numerically using expressions for W_i and W_f presented above.

At this point we can say something about the effects of the environment. These effects lead to ‘depolarisation’ of a qubit, which means a nonzero probability of the opposite spin state. If this probability is small we can speak about the probabilities of the population of n many-qubit basis states. Each admixed basis state in this case has one of the qubit states different from the initial state. To account for this effect one may use a real (experimental) qubit lifetime τ_0 in the estimate (27).

For $t > t_c$ the higher orders in the $H_{if}^2 t^2$ expansion become important and the number of the small components increases exponentially: each state generates qn new states. This corresponds to an approximately linear increase in the entropy. At $t \gg t_c$ we can use the asymptotic form (20) of the component distribution. It is twice as broad ($\Gamma t = 2\Gamma$) as the basis component distribution of chaotic stationary states. This means that the asymptotic number of the principal components is equal to $N_p(t) = 2 N_p^{(k)}$, where $N_p^{(k)} \simeq \Gamma/D$ is the number of principal components in a chaotic eigenstate. It is easy to calculate the entropy in this case. From the normalisation condition $\sum_s W_s = 1$, it follows that $\overline{W_s} = 1/N_p$. Then we get

$$S = -\sum_s W_s \log_2 W_s \simeq \log_2 N_p \sum_s W_s = \log_2 N_p. \quad (28)$$

Thus, the asymptotic value of the entropy is $S(t \gg t_c) = \log_2(2N_p^{(k)}) = S^{(k)} + 1$, where $S^{(k)} = \log_2 N_p^{(k)}$ is the entropy of a chaotic eigenstate. Note that it is smaller than the maximal possible entropy $S_{\max} = \log_2 2^n = n$. This is due to localisation of the wave

function within the energy shell centred at the energy of the initial state E_i with the width 2Γ .

4. Conclusion

The time dependence of the closed quantum computer wave function is different in the non-chaotic and chaotic regimes. In the non-chaotic case $J \ll \Delta_0/n$, the number of principal components $N_p \approx 1$ and the wave function remains localised near the initial state [as pointed out in Georgeot and Shepelyansky (1999) the energy level density of the many-qubit states can be exponentially high even in this case]. An increase in the number of qubits n leads to a transition to a chaotic regime where $J > \Delta_0/n$. In this case one can operate the quantum computer within a limited time $t < t_c = \tau_0/n \log_2 n$, where τ_0 is the ‘lifetime’ of one qubit. For $t > t_c$ it is hardly possible to operate the quantum computer, since in this case one faces a large increase in the entropy $S(t)$ and a very fast exponential increase of the number of ‘wrong’ states $N_p(t) = 2^{S(t)}$. The asymptotic value of the entropy is then close to that for chaotic eigenstates.

A similar picture for the entropy increase is expected in other many-body systems. For example, one can consider a decay of a single-electron wave function in a many-electron quantum dot. In this case we have $t_c \sim \tau/\log_2 n_f$, where n_f is the effective number of final states that contribute to the decay width $\Gamma = \hbar/\tau$. One may also speculate about the ‘entropy’ increase for decay of a single-particle wave function in a chaotic quantum billiard or disordered system using expansion of this wave function in the plane wave basis or the orbital angular momentum basis.

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