Time dependence of occupation numbers and thermalization time in closed chaotic many-body systems

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We study the time evolution of occupation numbers for interacting Fermi-particles in the situation when exact compound states are “chaotic”. This situation is generic for highly excited many-particles states in heavy nuclei, complex atoms, quantum dots, spin systems and quantum computer models. Numerical data show perfect agreement with a simple theory for the onset of thermalization in close systems of interacting particles.

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It is known that highly excited states can be treated as “chaotic” ones in many-body systems, such as complex atoms [1], multicharged ions [2], nuclei [3], spin systems [4,5] and quantum computer models [6,7]. This happens due to a very high density of many-particle states which strongly increases with an increase of energy. For example, in the case of$n$Fermi-particles occupying the finite number$m$of “orbitals” (single-particle states), the total number$N$of many-body states grows exponentially fast with an increase of number of particles,$N = m!/n!(m-n)! \sim \exp(c_0 n)$. Correspondingly, the density$\rho_f$of those many-body states which are directly coupled by a two-body interaction, also grows very fast. Therefore, even a relatively weak interaction between the particles can lead to a strong mixing between unperturbed many-body states (“basis states”). As a result, an exact (perturbed) eigenstate is represented by a chaotic superposition of a large number of components of basis states [8–10]. The number of principal basis components in such chaotic eigenstates can be estimated as$N_{pc} \sim \Gamma / D$where$\Gamma$is the spreading width of a typical component that can be expressed through the Fermi golden rule, and$D$is the mean interval between the many-body levels.

In this paper we extend the quantum chaos approach to the problem of a time evolution of an initially excited basis state. This initial state may contain one or several excited electrons above other electrons in the ground state of a quantum dot or atom.

Exact many-body eigenstates$|k\rangle$of a Hamiltonian$H = H_0 + V$of interacting Fermi-particles can be expressed in terms of simple shell-model basis states$|f\rangle$of$H_0$,

\[ |k\rangle = \sum_f C_f^{(k)} |f\rangle ; \quad |f\rangle = a_{f_1}^\dagger ... a_{f_n}^\dagger |0\rangle . \]  

Here$|0\rangle$is the ground state,$a_{s}^\dagger$is the creation operator and$C_f^{(k)}$are components of an exact chaotic eigenstate$|k\rangle$in the unperturbed basis, that is formed by a residual interaction$V$.

Below we consider the time evolution of the system, assuming that initially ($t = 0$) the system is in a specific basis state$|i\rangle$. This state can be expressed as a sum over exact eigenstates,

\[ |i\rangle = \sum_k C_i^{(k)} |k\rangle , \]  

therefore, the time-dependent wave function reads as

\[ \Psi(t) = \sum_{k,f} C_i^{(k)} C_f^{(k)} |f\rangle \exp(-iE_k t) . \]  

Here$E_k$are the eigenvalues corresponding to the eigenstates$|k\rangle$. The sum is taken over the eigenstates$|k\rangle >$and basis states$|f\rangle >$(hereafter we assume$h = 1$).

The occupation number$n_{\alpha}$of a single-particles state$\alpha$for the wave function (3) of the system is given by the expression,

\[ n_{\alpha} = \langle \Psi(t) | \hat{\alpha} | \Psi(t) \rangle = \sum_q \langle q | \tilde{\alpha}^\dagger | q \rangle \left( S_q^{(d)} + S_q^{(f)} \right) . \]  

with$\tilde{\alpha}^\dagger = a_{\alpha}^\dagger a_{\alpha}$. Here$S_q^{(d)}$is the diagonal term,

\[ S_q^{(d)} = \sum_k |C_i^{(k)}|^2 |C_q^{(k)}|^2 , \]  

and$S_q^{(f)}$stands for off-diagonal terms,

\[ S_q^{(f)} = \sum_{k \neq p} C_i^{(k)} C_q^{(k)} C_i^{(p)} C_q^{(p)} \exp \left[ i \left( E^{(k)} - E^{(p)} \right) t \right] . \]  

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Since at \( t = 0 \) the only unperturbed basis state \(|i\rangle\) is excited, the occupation numbers \( n_\alpha(t) \) are equal to 0 or 1 (for Fermi systems). For large times, \( t \to \infty \), the terms in the off-diagonal sum \( S_q^{(f)} \) oscillate very rapidly as a function of spacings \( E^{(k)} - E^{(p)} \), therefore, \( S_q^{(f)} \) tends to zero. Thus, the asymptotic distribution \( n_\alpha(\infty) \) of occupation numbers is determined by the diagonal term only.

If the number of principal components in the wave function is large, one can replace \( S_q^{(d)} \) by its average value,

\[
S_q^{(d)} = \bar{F}(E_i, E_q) \approx \sum_k F(E_i, E^{(k)}) F(E_q, E^{(k)}) \approx \int \bar{F}(E_i, E) \rho(E) dE. \tag{8}
\]

Here \( \rho(E) = D^{-1}(E) \) is the density of energy spectrum, and

\[
F(E_i, E^{(k)}) \equiv |C_i^{(k)}|^2 \tag{9}
\]

is the so-called \( F \)-function that characterizes the shape of eigenstates in the unperturbed basis. This \( F \)-function has been studied in details for different models (see, e.g. \[1\]) and the review \[14\]). As was shown in \[3\], in many cases the \( F \)-function can be approximated by the following expression (see also \[16\]),

\[
F(E_i, E) \rho(E) = B \exp \left[ \frac{-\left( \frac{E - E_i}{\Gamma} \right)^2}{2\sigma^2} \right] \tag{10}
\]

In this expression \( B \) is the normalizing constant that can be found from the relation \( \int F(E_i, E) \rho(E) dE = 1 \), and \( \Gamma_i \) is the spreading width of a compound state \(|i\rangle\). The energy \( E_c \) stands for the center of effective energy band \( \sigma \) of the Hamiltonian matrix, and may not coincide with \( E_i \).

If residual interaction \( V \) is not very strong, the spreading width is determined by the standard golden rule, \( \Gamma_i \approx 2\pi |V_{ij}|^2 \rho_f \ll \sigma \). Here \( \rho_f \) is the density of final basis states \(|f\rangle\) that are coupled to \(|i\rangle\) by the interaction \( V \). In the limit \( \Gamma \ll \sigma \) the parameter \( \sigma^2 \) is equal to the variance \( \sigma_f^2 \) of \( \rho_f \). In the opposite limit \( \Gamma \gg \sigma \) the value of \( \sigma^2 \) is approximately the same as the variance \( \Delta^2_E \) of the strength function \( F(E_i, E) \rho(E) \), see Ref. \[1\]. Note also, that \( \Delta^2_E \) is always finite due to a finite range of interaction in the energy representation.

The form of \( F(E_i, E) \) in this limit \( \Gamma \ll \sigma \) has simple Breit-Wigner (BW) shape (apart from long tails that are highly non-universal \[1\]),

\[
F(E_i, E) = \frac{1}{2\pi \rho \left( E - E_i \right)^2 + \Gamma^2/4}, \tag{11}
\]

where \( \Gamma \equiv \Gamma_i \). In this case the function \( \bar{F}(E_i, E_q) \) that gives the final shape of the time-dependent wave function, has also the BW form \[11\] with the width \( \Gamma = 2\Gamma \). Note that fluctuations of the diagonal term \( S_i^{(d)} \) are small, \( S_i^{(d)} = \bar{S}_i^{(d)} + \tilde{S}_i^{(d)} / \sqrt{N_{pc}} \). Thus, for a large number of principal components \( N_{pc} \), the occupation numbers both in compound eigenstates and in large-time asymptotic of the wave function, have the self-average property. As a result, we obtain the following expression for the asymptotic values of occupation numbers,

\[
n_\alpha(\infty) = \sum_q \langle q | \hat{n}_\alpha | q \rangle \bar{F}(E_i, E_q). \tag{12}
\]

In fact, this distribution is very close to the distribution of occupation numbers in compound eigenstates of a system,

\[
\bar{n}_\alpha = \sum_q \langle q | \hat{n}_\alpha | q \rangle F(E_q, E). \tag{13}
\]

The properties of the distribution \[13\] have been studied in details \[1,2,3,12,13\] for different models.

In many cases the two-body random interaction (TBRI) model \[18\], \( s-d \) nuclear shell model \[8\], multiply charged ions \[2\] the \( F \)-distribution \[13\] is very close to the standard Fermi-Dirac distribution for the occupation numbers with a certain temperature \( T(E) \). In these cases the asymptotic distribution \[12\] of the occupation numbers in the time-dependent problem is also given by the Fermi-Dirac distribution. In other cases, like Ce atom \[17\] where the residual interaction between particles on some orbitals is larger than the distance between single-particle energy levels, the \( F \)-distribution \[13\] deviates very strongly from the Fermi-Dirac distribution. This happens since the mean-field approximation is not a “good” one. However, even in this case the distribution of \( n_\alpha \) is close to that obtained from the canonical distribution that takes into account a repulsion between electrons (see details in \[17\]). This canonical distribution is also characterized by some temperature \( T(E) \). Thus, it is natural to term the time evolution of \( n_\alpha(t) \) as the process of thermalization in a closed system.

The natural question is: how fast is this thermalization? To answer this question, one needs to study the evolution of a many-body system taking into account a two-body nature of the interaction between particles. For this, it is convenient to consider the so-called cascade model (see details in \[14\]), that is based on the representation of unperturbed many-body states in the form of “classes”. In this picture, the first class contains those \( N_1 \) basis states that are directly coupled by the two-body interaction \( V_{ij} \). Correspondingly, the second class consists of \( N_2 \) basis states that are coupled with the initial state in the second order of the interaction \( V \) (therefore, the coupling is proportional to \( V_{ik} V_{kj} \), etc.

The analytical expression for time dependence \( W_n(t) \) of a population of the class \( n \) has been obtained in Ref.
The population in the “zero” class is just a probability $W_0(t)$ of the system to remain in an initial state. In the BW case, $\Gamma \ll \sigma$, this probability for large times is $W_0(t) \sim \exp(-\Gamma t)$. In other limiting case, $\Gamma \gtrsim \sigma$, when the form of the $F$-function is close to the Gaussian, the time dependence $W_0(t)$ is more complicated [10]. For example, for $\Gamma \gg \sigma$, it was found to be $W_0(t) = \exp(-\Delta E^2 t^2)$, up to a very long time. In general case it changes from $W_0(t) = \exp(-\Delta E^2 t^2)$ for small times, to $W_0(t) = C \exp(-\Gamma t)$ for large times and saturates near $W_0(t) \approx 3/N_{pc} (\text{here } C > 1 \text{ is the time-independent coefficient, see details in [10]}).$

Let us now consider the thermalization process. Initially, the occupation numbers $n_\alpha(0)$ are equal to 0 or 1. In the BW regime, the first class is populated during the time $\tau \sim 1/\Gamma$ (or, $\tau \sim 1/\Delta E$ in the Gaussian regime, for $\Gamma \gtrsim \sigma$). At that time the occupation numbers $n_\alpha$ already strongly deviate from their initial values since the two-body interaction can move any of two particles to new single-particles levels characterized by the energies $\epsilon_{\alpha}$. Thus, the characteristic time for a thermalization of the occupation numbers is determined by the population time $\tau$ for the first class. Note, that this time is also a characteristic time for the “decay” of the probability $W_0(t)$. To compare with, the population of all $n_c$ classes in a particular system requires a longer time $\tau_{n_c} \sim n_c \tau$ [10]. Thus, in the case of $n_c \gg 1$ (e.g. in a mesoscopic system) the thermalization of the occupation numbers may occur on a smaller time scale than the onset of a complete statistical equilibrium.

This suggests a simple derivation of the time dependence $n_\alpha(t)$ for occupation numbers. From the normalization condition $\sum_{\alpha=0}^{n_c} W_\alpha = 1$ one can find the population of all classes with $s \neq 0$ as $\sum_{s=1}^{n_c} W_s = 1 - W_0$. Now we assume that the thermalization of the occupation numbers occurs on the time scale $\tau$. This assumption leads to a simple expression

$$n_\alpha(t) = n_\alpha(0) W_0(t) + n_\alpha(\infty) (1 - W_0(t)).$$

(14)

Here $n_\alpha(0)$ are initial occupation numbers (0 or 1), and $n_\alpha(\infty)$ determines equilibrium occupation numbers (e.g., the Fermi-Dirac distribution).

In Figs.1-2 we compare numerical data for $n_\alpha(t)$ with the above estimate (14). Two situations are studied, the first (Fig.1) corresponds to the BW regime (weak interaction regime, $\Gamma \ll \sigma$), and in the second (Fig.2) the form of the $F$-function is close to the Gaussian ($\Gamma \gtrsim \sigma$). For numerical simulation, we have used the model with random two-body interaction (see details, in [12]) with $n = 6$ Fermi-particles that occupy $m = 12$ single-particle levels. Since the analytical expression for $W_0(t)$ in general case is quite complicated, in numerical simulations we use the exact value of $W_0(t)$ computed numerically.

Overall, there is an excellent agreement between the theory and numerical data (apart from fluctuations that are neglected in the theory). In order to simplify the picture, we have taken the initial basis state $|i\rangle$ just in the middle of the many-particle spectrum that consists of 924 levels. In this case all final values of the occupation numbers are equal, $n_\alpha(\infty) = n/m = 1/2$ that corresponds to the infinite temperature $T$.

![FIG. 1. Time dependence of occupation numbers $n_\alpha(t)$ for the BW regime (weak interaction ). Thin curves with dots present numerical data, thick smooth curves correspond to the analytical expression (14), see the text. Computations are made for the model with random two-body interaction, with $n = 6$, $m = 12$, $\eta = V^2/D_0^2 \approx 0.003$, $\Gamma \approx 0.50$, $\Delta E \approx 1.16$ (here $D_0$ is the mean spacing between single-particle energies).](image1)

![FIG. 2. Time dependence of occupation numbers $n_\alpha(t)$ for the case when the strength function has the gaussian form: $\eta \equiv V^2/D_0^2 \approx 0.083, \Gamma \approx 10.5, \Delta E \approx 5.8$.](image2)

We would like to point out on an interesting difference between two cases of a weak and strong interaction between the particles. Specifically, for a weak interaction (Fig.1) the transition to equilibrium values of $n_\alpha$ has a
character of damped oscillations. The number of principal components $N_{pc} \sim \Gamma \rho^{-1}$ in this case is not very large, this is why there are considerable fluctuations in $n_\alpha(t)$ even in the equilibrium. To compare with, the case of a strong interaction (Fig.2) shows fast and monotonic transition to thermal values of $n_\alpha(\infty)$ with relatively small fluctuations, see also [19].

Our results demonstrate that actually there are two time scales in the onset of thermalization. The first one is determined by $\tau$. It characterizes an “initial thermalization”, and allows one to use Eq.(14) for a description of the time dependence of occupation numbers. For larger times, damped quantum oscillations (with period $T \sim n_c \tau$) may occur in the transition to a complete equilibrium [16,19].

In conclusion, we present a simple theory for the onset of thermalization in closed systems of interacting particles. The theory allows to describe the time dependence of the occupation numbers, and shows the relaxation to an equilibrium distribution. Numerical data obtained for the model of a random two-body interaction between finite number of Fermi-particles, demonstrate a very good correspondence to the theoretical predictions. Our results can be used in different applications, such as complex atoms, heavy nuclei, atomic clusters, quantum dots, etc.

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