Emergence of quantum chaos in finite interacting Fermi systems

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We study the level spacing statistics \(P(s)\) in many-body Fermi systems and determine a critical two-body interaction strength \(U_c\) at which a crossover from Poisson to Wigner-Dyson statistics takes place. Near the Fermi level the results allow to find a critical temperature \(T_{ch}\) above which quantum chaos and thermalization set in.

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The Random Matrix Theory (RMT) was developed to explain the general properties of complex energy spectra in many-body interacting systems such as heavy nuclei, many electron atoms and molecules \(^{(3)}\). Later, it has found many other successful applications in different physical systems. Among the most recent of them we can quote models of quantum chaos where RMT appears due to the classically chaotic but deterministic underlying dynamics \(^{(3)}\). One of the most direct indications of the emergence of quantum chaos is the transition of the level spacing statistics \(P(s)\) from Poisson to Wigner-Dyson (WD) distribution. This property has been widely used to detect the transition from integrability to chaos not only in systems with few degrees of freedom \(^{(3)}\) but also in solid-state models with many interacting electrons \(^{(6)}\). It was also applied to determine the delocalization threshold in noninteracting disordered systems \(^{(7)}\).

While the conditions for the appearance of the WD distribution in noninteracting systems is qualitatively well understood the situation is more intricate in presence of interaction. Indeed, in this case the size of the total Hamiltonian matrix grows exponentially with the number of particles and it becomes very sparse as a result of the two-body nature of the interaction. Due to that it was initially not obvious whether switching on the interaction would lead to the WD statistics. To study this problem a two-body random interaction model (TBRIM) had been proposed \(^{(1)}\). This model consists of \(n\) fermions which can occupy \(m\) unperturbed energy orbitals with mean one-particle level spacing \(\Delta\). The multiparticle states are coupled by two-body random transition matrix elements of typical strength \(U\). It was found that a sufficiently strong \(U\) leads to a level mixing and appearance of WD statistics. Very recently the interest for this model has been renewed and its statistical properties were investigated in more details \(^{(2)}\). This raise of interest was stimulated by the understanding that many statistical properties of real physical systems such as the rare-earth Ce atom \(^{(8)}\) and the \(^{28}\)Si nucleus \(^{(9, 10)}\) are well described by the TBRIM. In addition this model is quite similar to the \(s\)-\(d\) shell model used for a description of complex nuclei \(^{(11)}\). Since interaction is generically of two-body nature it is reasonable to assume that this model will be also useful for a description of interacting electrons in clusters \(^{(11)}\) and mesoscopic quantum dots \(^{(12)}\).

While the statistical properties of the TBRIM were studied in some details, surprisingly, the most important question of the critical interaction strength \(U_c\) at which the WD level spacing statistics sets in was omitted. Apparently the reason for this is based on the common lore in nuclear physics that the level density grows exponentially with the number of particles and therefore an exponentially small interaction is sufficient to mix nearby levels \(^{(9, 10)}\). However recent estimates on few-particle models \((n = 2, 3, 4)\) showed that in spite of the high many-body density of states, only an interaction strength comparable to the two-particle level spacings can give a level mixing \(^{(12)}\). Therefore the dependence of \(U_c\) on the number of particles and orbitals as well as the excitation energy should still be determined. This is the main purpose of this paper. The above border in \(U\) is physically very important. Indeed for \(U < U_c\) levels are not mixed by interaction and hence the system is not thermalized. Consequently the occupation numbers are not described by the Fermi-Dirac statistics. On the contrary a sufficiently strong interaction leads to thermalization as it has been seen in numerical simulations \(^{(13)}\).

To study the effect of interaction on the spectral properties of finite Fermi systems we used the TBRIM model described in \(^{(1)}\). It consists of \(n\) particles distributed over \(m\) orbitals with energies \(\epsilon_{m'\prime}\), \(m' = 1, 2, \ldots, m\). These energies are randomly distributed over the interval \([0, m]\) with average spacing \(\Delta = 1\). The total number of multiparticle states is \(N = m!/(n!(m-n)!\). They are coupled by random two-body transition matrix elements distributed in the interval \([-U, U]\). Due to the two-body nature of the interaction, only states differing by at most two one-particle indices are coupled. As a result each multiparticle state is coupled with \(K = 1 + n(m-n) + n(n-1)(m-n)(m-n-1)/4\) states \(^{(7)}\). All these transitions occur inside a two-body energy interval \(B = 2m - 4\) around the energy of an initial multiparticle state. For large \(m\) and \(n\), the number of tran-
dictions \( K \) is much smaller than the size of the matrix \( N \) but is much larger than the number of different two-body matrix elements \( N_2 \approx n^2/2 \). The total energy of the system varies from the ground-state value \( E_g \approx n^2/2 \) to the maximal value \( E_i \approx mn\Delta - E_g \) and the Fermi energy is \( \epsilon_F \approx n\Delta \). The typical level spacing in the middle of the spectrum at \( E_h \approx (E_i + E_g)/2 \) is \( \Delta_n \approx (E_i - E_g)/N \).

Let us first discuss the situation at high energies \( E \sim E_h \) where all \( K \) transitions are energetically allowed. In this case the density of directly coupled states is \( \rho_c \approx K/B \) because all transitions take place inside the two-body energy band \( B \). According to perturbation theory these levels will be mixed when the transition matrix element \( U \) between them becomes of the order of the corresponding spacing \( \Delta \). This determines the critical coupling \( U_c \):

\[
U_c = C \frac{B}{K} \approx \frac{2C}{\rho_2 n^2} \tag{1}
\]

Here, we introduced the two-particle density \( \rho_2 \approx N_2/B \approx n^2/4 \) assuming \( m \gg n \gg 1 \) and a numerical constant \( C \) to be determined. For \( U \ll U_c \) the perturbation theory works, levels are not mixed and \( P(s) \) is close to the Poisson distribution. For \( U > U_c \) we expect a strong mixing of levels not only on a scale \( \Delta \), but on a much smaller scale \( \Delta_n \). There are few arguments in favor of this statement. The first of them is based on the results for few-particle systems \((n = 2, 3, 4)\) [13]. According to [13], the effective transition matrix element between nearby levels in high orders of perturbation theory becomes comparable to \( \Delta_n \) when the first-order transition mixes directly coupled states \((U > U_c)\). Recently the same conclusion was drawn in [14]. The second argument is based on an analogy with superimposed band random matrices (SBRM) with strongly fluctuating diagonal elements [13,15]. There it was shown that for sufficiently large band (number of nonzero diagonals \( 2b + 1 \gg \sqrt{N} \)) the eigenstates are extended over the whole matrix size \( N \) and \( P(s) \) has the WD form if the transition matrix elements are larger than the energy spacing between directly coupled states. This condition is rather similar to the above border [1].

To check the prediction [1], we numerically computed \( P(s) \) in the middle of the spectrum of the TBRIM (keeping only \( \pm 25\% \) of the levels around \( E_h \)) for \( n \leq 8 \) and \( m \leq 80 \) at various interaction strengths \( U \). Up to 5000 different realizations of disorder have been used to obtain the total spacing statistics \( N_s \approx 30000 \). A typical example of the transition from Poisson to WD statistics is shown in Fig. 1. As expected the level repulsion disappears at small \( U \) while for large \( U \) the distribution approaches the WD form. To characterize this transition we computed for each distribution \( P(s) \) the value \( \eta = \int_{s_0}^{s} (P(s) - P_{WD}(s))ds / \int_{s_0}^{s} (P_{P}(s) - P_{WD}(s))ds \). Here \( P_P(s) \) and \( P_{WD}(s) \) are the Poisson and the WD distributions respectively and \( s_0 = 0.4729... \) is their intersection point. In this way \( \eta \) varies from 1 \((P(s) = P_P(s)) \) to 0 \((P(s) = P_{WD}(s)) \). We determined the critical interaction strength \( U_c \) by the condition \( \eta(U_c) = \eta_c = 0.3 \). The choice of \( \eta_c \) influences only the numerical factor \( C \) in (1). We note that this \( \eta \)-value is close to the value \( \eta_A = 0.215 \) corresponding to \( P(s) \) at the Anderson transition in 3d [4] (in [4] a criterion slightly different from ours was used).

The fact that the concrete choice of \( \eta_c \) is not crucial is also confirmed by Fig. 2 which shows the existence of a scaling \( \eta = \eta(U/U_c) \). Indeed the numerical data in a large parameter range demonstrate the existence of one scaling curve (Fig. 2). This scaling is very similar to the one observed in the SBRM models [13,15]. It also clearly shows that the situation in our model is qualitatively different from the \( \eta \)-scaling in the solid-state models with Anderson transition. There, in the limit of large system size, only three values \( \eta = 1 \) (localized phase), \( \eta = 0 \) (delocalized) and \( \eta = \eta_A \) (at the transition) are possible [4]. On the contrary in our case the scaling function varies smoothly from 1 to 0 with the rescaled transition matrix element \( U/U_c \) for different system sizes \( N \) which varied over more than two orders of magnitude. We relate this qualitative difference between the two models to the fact that in the TBRIM all orbitals are coupled by direct transitions whereas in the Anderson model, the hopping couples only nearby sites. Due to that the TBRIM is more similar to the SBRM models with broad band where many states are directly coupled.
The condition for the critical \( U_c \) \((\eta_c = 0.3)\) allows to check the theoretical prediction (1). The numerical data for which the number of direct transitions varies over more than two orders of magnitude are presented in Fig. 3. They give a clear confirmation of the estimate (1) giving \( C \approx 0.58 \). The results of Figs. 1-3 show that for \( U > U_c \) from (1) all nearby levels are mixed by two-body interaction and \( P(s) \) converges to the RMT result with WD distribution. We stress that for large \( m \) and \( n \), the value of \( U_c \) remains parametrically much larger than the multiparticle spacing \( \Delta_n \).

So far the results were obtained in the middle of the energy spectrum \( E_g \) where all \( K \) direct transitions are energetically allowed and effectively work. The situation becomes quite different close to the Fermi level. There, the estimate (1) should be modified in the following way.

First we should take into account that the density of effectively coupled two-particle states \( \rho_{2e,f} \) becomes energy-dependent so that \( \rho_{2e,f}(\epsilon) \sim \epsilon/\Delta^2 \). Secondly the number of effectively interacting particles is also changed close to the Fermi level. Indeed as it is well known, at a temperature \( T \), only \( \delta n \sim T n/\epsilon_F \sim T/\Delta > 1 \) particles interact near the Fermi surface. At this excitation energy \( \epsilon \sim T < \epsilon_F \), the density of two-particle states is \( \rho_{2e,f} \sim T/\Delta^2 \). By replacing in (1) \( n \) by \( \delta n \) and \( \rho_2 \) by \( \rho_{2e,f} \) we obtain that at a given interaction strength the levels become mixed and \( P(s) \) takes the WD form at a temperature higher than the critical \( T_{ch} \) given by

\[
T_{ch} \approx C_1 \Delta(\Delta/U)^{1/3}
\]

where \( C_1 \) is a numerical constant. The conditions of validity of this equation are \( T n > \Delta \) \((\delta n > 1)\) and \( T_{ch} < \epsilon_F = n \Delta \) that corresponds to \( n^{-3} < U/\Delta < 1 \). It is also assumed that the WD statistics implies thermalization with Fermi-Dirac statistics. Such a conjecture looks quite natural, since the quantum chaos should be related with excitation of many unperturbed modes and mixing. Also without mixing of nearby levels and WD statistics the thermalization is not possible since generally the Poisson distribution indicates an existence of uncoupled parts in the whole system. As a result the thermalization does not exist below \( T_{ch} \).

Since near the Fermi level the total system energy counted from \( E_g \) is \( \delta E = E - E_g \approx T \delta n \), the relation (2) implies that the thermalization takes place only for eigenstates with eigenenergies \( E_x = E_g + \delta E \) so that

\[
\delta E > \delta E_{ch} \approx C_1^2 \Delta(\Delta/U)^{2/3}
\]

The above restriction for \( U \) requires \( 1 < \delta E/\Delta < n^2 \). This result shows that the \( \eta \)-parameter should depend on the excitation energy. Indeed, our numerical data, extracted from \( P(s) \) computed in a small energy interval near a fixed \( \delta E \), clearly show that \( \eta \) decreases with increasing excitation energy \( \delta E \) (Fig. 4). Using the relation (2) we can determine for a given \( \delta E \) an effective \( U_c \) value being \( U_c = C_1^2 \Delta(\delta E)^{3/2} \). The condition \( \eta(\delta E) = \eta_c = 0.3 \) for the data of Fig. 4 at \( n = 6, m = 12, U/\Delta = 0.147 \) gives \( C_1 \approx 1.08 \). With the value \( C_1 = 1.08 \) and the above dependence of \( U_c \) on \( \delta E \) we can check if the data of Fig. 4 will follow the general scaling law of Fig. 2. For that in Fig. 2 we plot the \( \eta \)-values of Fig. 4 vs. the ratio \( U/U_c \) with \( U_c = 1.26(\delta E)^{-3/2} \), \( C_1 = 1.08 \) and \( \Delta = 1 \) (open circles). The fact that these data follow the scaling curve confirms the theoretical estimates (2), (3) for the thermalization
border. The direct check of the dependence of $\delta E_{ch}$ on $U$ (insert in Fig.4) also confirms the prediction (3).

**FIG. 4. Dependence of $\eta$ on the rescaled excitation energy $\delta E/\Delta$ for $n = 6, m = 12$ and $U/\Delta = 0.147$ (o). The straight line marks $\eta = \eta_c = 0.3$. Insert gives the numerically found dependence of $\delta E_{ch}$ with $\eta = \eta_c = 0.3$ on $U$ (diamonds), the straight line shows the theory (3) with $C_1 = 1.08$.**

The obtained estimates for the quantum chaos border (3) can be applied to different finite interacting Fermi systems such as complex nuclei with residual interaction, atoms and molecules, clusters and quantum dots. Here we briefly discuss the case of metallic quantum dots. Fermi systems such as complex nuclei with residual interaction, atoms and molecules, clusters and quantum dots. Further investigation of this crossover in real systems is highly desirable.

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