Towards a statistical theory of finite Fermi systems and compound states: Random two-body interaction approach

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The model of Fermi particles with random two-body interaction is investigated. This model allows one to study the origin and accuracy of statistical laws in few-body systems, the role of interaction and chaos in thermalization, the Fermi-Dirac distribution for quasiparticles with spreading widths, matrix elements of external fields, and enhancement of weak perturbation in chaotic compound states. [S1063-651X(96)02506-8]

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INTRODUCTION

As is known, excited states in many-body systems such as compound nuclei, rare-earth atoms, molecules, atomic clusters, quantum dots in solids, etc. are very complicated (''chaotic'') and can be described via statistical methods. There are two major approaches. The first is based on random matrix theory (see, e.g., [1]). This approach is very general in nature and therefore it does not describe many important properties of realistic many-body systems, its prediction being limited to level statistics, localization properties of eigenstates, and the like. The other approach is based on direct numerical investigations of the given particular system. For example, the results of direct diagonalization of the Hamiltonian matrix for the rare-earth Ce atom have been compared with statistical theory of compound states [2]. A similar study has been performed for the *s-d* shell model of a complex nucleus [3] where the problem of thermalization has also been considered. Quite obviously with this second approach, it is very hard (e.g., due to the lack of statistics) to draw general conclusions concerning the accuracy of statistical laws in systems with a finite numbers of particles, and the conditions for their applicability.

Here we suggest an ''intermediate'' approach based on a simple mathematical model with random interaction, which, however, takes into account the most important features of many-body systems such as single-particle orbitals, two-body interaction, and the Pauli principle. In our model of random two-body interaction (RTBI) we assume that the system consists of n Fermi particles which can occupy m orbitals with no double occupancy (extension to Bose systems is straightforward). As an example, the energies of orbitals are taken in the form

$$\epsilon_\alpha = d\left(\alpha + \frac{1}{\alpha}\right), \quad \alpha = 1,2,\ldots,m, \tag{1}$$

where the second term is introduced in order to avoid the degeneracy of many-particle states. Matrix elements of the two-body interaction are chosen as random variables distributed according to a Gaussian law with zero mean and the variance V_0. Therefore our model has three independent parameters: n, m, and V_0/d.

STRUCTURE OF THE HAMILTONIAN MATRIX

The basis of our Hamiltonian matrix is chosen to correspond to the products of single-particle orbitals ordered by increasing many-body unperturbed energies. Therefore without interaction the matrix is diagonal, with increasing elements. The size N of the RTBI matrix is given by $N = C_n^m = m!/[n!(m-n)!]$ and is exponentially large for large n and m. Due to the two-body character of the interaction the matrix elements are zero between those basis states which differ by more than two orbitals. Therefore the Hamiltonian matrix is essentially sparse with the sparsity (ratio of nonzero elements to the total number N^2) given by $s = [1 + n(m-n) + n(n-1)(m-n)(m-n-1)/4]/N$. At large n, m the sparsity is exponentially small, $s \sim \exp(-n)$. In fact, the number $N_2 = m^2(m-1)^2/4$ of independent variables (number of pair interactions) in the model is even smaller than the number of nonzero Hamiltonian matrix elements.

There are three types of interactions between many-body states: the diagonal interaction which contains $k_{int} = n(n-1)/2$ two-body terms, the interaction between states which differ by one orbital with $k_{int} = n-1$ terms, and the interaction between states which differ by two orbitals with $k_{int} = 1$. Finally, distant many-body states which differ by more than two orbitals have zero matrix elements. Thus the Hamiltonian matrix H_{ij} has a large and increasing diagonal plus sparse bandlike structure with a decrease of off-diagonal elements as a function of the distance $|i-j|$ from the diagonal.

In what follows we consider a particular case which can be used to describe the Ce atom: $m = 11$, $n = 4$ (therefore $N = 330$), $d = 1, V_0 = 0.12$ (the two last parameters are given in eV). Direct investigation of this atom (see details in [2]) has shown that it can be treated as a very chaotic system.

ENERGY SPECTRUM AND EIGENSTATES

As was found in [4] (see also [5]), for two-body random interaction the density of states (DOS) should be of Gaussian

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type, provided $m \gg n \gg 1$. Our numerical data show that in the RTBI model in spite of the small number of particles the DOS is quite close to a Gaussian with $\langle E \rangle = 25.1$ and $\sigma = 5.7$. Another commonly discussed characteristic of the spectrum is the level spacing distribution; in our model it is well described by the famous Wigner-Dyson law. This fact is also in agreement with old studies [6] of some two-body interaction models (see also references in [5]). However, our interest goes beyond the DOS and spectrum statistics.

A quantity of relevant interest is the so-called spectral local density of states or strength function. It is defined by the weight $w(E,E_j) = |\overline{C_j^2}|$ of a particular basis component $j = 1,2,..,N$ in the eigenstates with an energy close to E, according to the relation

$$\rho(j,E) = \frac{w(E,E_j)}{D} = \left\langle \sum_r |C_j(E_r)|^2 \delta(E - E_r) \right\rangle. \quad (2)$$

Here D is the local mean level spacing. The width of this function in energy E is proportional to the effective number of components in the expansion of an unperturbed basis state in terms of exact eigenstates. In nuclear physics, this function is usually assumed to have the Breit-Wigner form, $\rho(j,E) \sim [(E - E_j)^2 + \Gamma_c^2/4]^{-1}$ (the relevance of this function to ergodicity and chaos is studied in [7]). According to our numerical results, in the center of the spectrum ($j \approx N/2$) the spreading width is equal to $\Gamma_c \approx 1.0$. One should note that close to the edges $j = 1,N$, the symmetric form of the distribution $\rho(j,E)$ is strongly distorted. However, the width of the distribution itself changes slightly. What is more important, the tails of the function $\rho(j,E)$ decay much faster than in the Breit-Wigner law. This is the consequence of the bandlike structure of the Hamiltonian matrix. Both the value of Γ_c and the fast decay of the tails are in agreement with Ce atom calculations [2].

The localization length (number of principal components of the eigenstates) can be defined through the relation $l \sim \exp(\langle S \rangle)$, where S is the statistical entropy of individual eigenstates (see, e.g., [8]). One should note that in spite of the completely random character of the interaction, the lowest states turn out to be quite simple, containing $l \approx 1$ basis components. This can be explained by the low density of states near the ground state. The localization length l is maximal in the center $E \approx \langle E \rangle$ of the energy band and, according to our numerical data, can be well described by the Gaussian function $l = A \exp[-(E - \langle E \rangle)^2/(2\sigma^2)]$ with $A \approx 135$ and $\sigma \approx 5.45$. Thus in the center of the spectrum the number of principle components is about 100, which is again very close to the results of direct calculations for the Ce atom [2].

STATISTICAL TREATMENT OF FINITE FERMI SYSTEMS

As is known, quantum statistical laws are derived for systems with an infinite number of degrees of freedom, or for systems in a thermostat. From this point of view, it is of importance to study how statistical laws appear in systems with a finite number of particles. Below, we show that in the RTBI model one can introduce a reasonably accurate statistical description based on such macroscopic characteristics as the temperature T, the chemical potential μ, and average

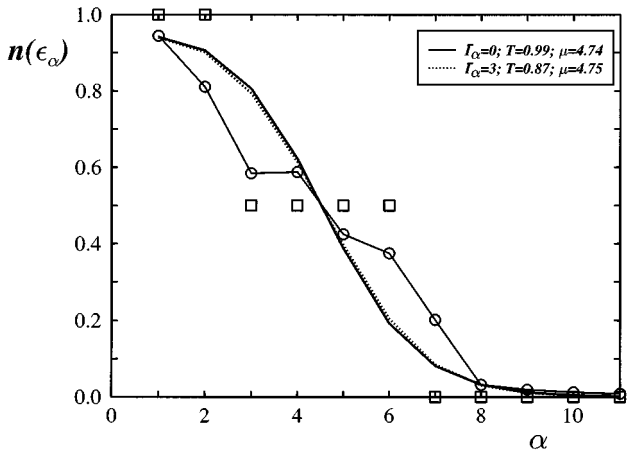

FIG. 1. Distribution of occupation numbers for the excitation energy $\delta E = 1.63$ averaged over an ensemble of five Hamiltonian matrices. The full and dotted lines are numerical solutions of Eqs. (3) and (6) with $\Gamma_\alpha = 0$ and $\Gamma_\alpha = 3$, respectively. The circles and squares give results of the direct computation of average occupation numbers with and without interaction, respectively.

occupation numbers n_i for the orbitals. In the mean-field approximation these quantities can be obtained from the following set of equations:

$$\sum_{\alpha=1}^{m} n_\alpha = n, \quad \sum_{\alpha=1}^{m} \epsilon_\alpha n_\alpha + \left\langle \sum_{\alpha \geqslant \beta}^{m} V_{\alpha\beta} n_\alpha n_\beta \right\rangle = E, \quad (3)$$

$$n_\alpha \equiv n(\epsilon_\alpha) = [1 + \exp(\tilde{\epsilon}_\alpha - \mu)/T]^{-1}, \quad (4)$$

$$\tilde{\epsilon}_\alpha = \epsilon_\alpha + \left\langle \sum_{\beta=1}^{m} V_{\alpha\beta} n_\beta \right\rangle. \quad (5)$$

In our case, the average interaction $\langle V_{\alpha\beta} \rangle$ is zero; therefore we can omit the interaction term in (3) and (5). On the other hand, there exist other important effects of the interaction which appear beyond the mean-field approximation; namely, the interaction leads to a spreading width for the basis states and for the single-particle orbitals (Γ_α). It also results in a shift of average energies, $\tilde{\epsilon}_\alpha = \epsilon_\alpha + \delta\epsilon_\alpha$. According to our numerical data, the magnitudes $\delta\epsilon_\alpha$ are smaller than Γ_α and vanish in the mean ($\delta\epsilon_\alpha < 0$ for low orbitals, $\delta\epsilon_\alpha > 0$ for high orbitals, and $\delta\epsilon_\alpha \approx 0$ near the center). For this reason, we will take into account the effect of the spreading width Γ_α only.

Instead of (4), by averaging the Fermi-Dirac distribution $n(\epsilon)$ over the interval Γ_α:

$$n_\alpha = \int_{\epsilon_\alpha - \Gamma_\alpha/2}^{\epsilon_\alpha + \Gamma_\alpha/2} n(\epsilon) \frac{d\epsilon}{\Gamma_\alpha} = 1 - \frac{T}{\Gamma_\alpha} \ln \left[\frac{1 + \exp[(\epsilon_\alpha + \Gamma_\alpha/2 - \mu)/2T]}{1 + \exp[(\epsilon_\alpha - \Gamma_\alpha/2 - \mu)/2T]} \right], \quad (6)$$

we now introduce the occupation numbers (6) which take into account the finite spreading width of ''quasiparticles.'' In the limit $\Gamma_\alpha = 0$ the expression (4) with $n_\alpha = n(\epsilon_\alpha)$ is recovered. The numerical solution of Eqs. (3) and (6) is presented in Fig. 1. In order to reveal the influence of the

spreading width Γ_α, two curves are given for comparison with $\Gamma_\alpha=0$ and $\Gamma_\alpha=3.0$. The latter value of Γ_α was deliberately taken larger than the spreading width of basic components $\Gamma_c\approx 1.0$ in order to elucidate the effect of Γ_α. The temperature T and chemical potential μ are calculated from the above Eqs. (3) and (6) at fixed excitation energy $\delta E=E-E_{min}$. We found that for small δE the temperature is quite different for different values of Γ_α. Surprisingly, in spite of this, the two ''theoretical'' curves practically coincide. This means that the temperature mimics the statistical effect of the interaction, a phenomenon far from being trivial.

The average occupation numbers directly computed from exact eigenstates are shown in Fig. 1 with circles. One can see that even for four particles the actual distribution of occupation numbers can be approximately described by the statistical Fermi-Dirac distribution. However, there is a clear deviation which indicates that for the chosen parameters the thermalization is not complete. Numerical data show that the deviation disappears with increasing excitation energy δE, while it increases when the perturbation V_0 decreases. The latter effect has also been observed in the s-d nuclear shell model [3] where the relevance of chaos to the thermalization was studied in a different approach. We have to stress that the equilibrium distribution, or ''thermalization,'' in this few-particle system is due to the interaction which ''chaotically'' mixes neighboring basis states with different occupation numbers. To demonstrate this, we plot in Fig. 1 the occupation numbers for the same system with no interaction ($V_0=0$). Their distribution has nothing to do with the Fermi-Dirac distribution: it is singular and for some values of δE even not monotonic.

CORRELATIONS BETWEEN OCCUPATION NUMBERS

In a few body system one could expect quite strong correlations between occupation numbers of different orbitals. We have found, instead, that typically the correlations are weak; even for close orbitals the ratio $\langle\hat{n}_\alpha\rangle\langle\hat{n}_\beta\rangle/\langle\hat{n}_\alpha\hat{n}_\beta\rangle\approx 0.82$. Only when occupation numbers are small can the correlations be very strong.

MATRIX ELEMENTS OF AN EXTERNAL PERTURBATION

The main problem in the compound state theory is the calculation of effects of an external perturbation. Since matrix elements of any single-particle operator can be expressed in terms of elementary density matrix operators $\hat{\rho}_{\alpha\beta}=a^\dagger_\alpha a_\beta$ which transfer the particle from the orbital β to the orbital α, the main interest is in statistical properties of matrix elements $\rho_{\alpha\beta}$. Below, we use a recent approach developed in [9] (see also the study of the Ce atom in [2]) where the following expression for the mean square matrix elements (MSME's) $\xi^{(n_2n_1)}_{\alpha\beta}\equiv\overline{\rho^{(n_2n_1)}_{\alpha\beta}|^2}$ between compound states $\langle n_1|$ and $\langle n_2|$ has been derived:

$$\xi^{(n_2n_1)}_{\alpha\beta}=Q_{\alpha\beta}\sum_r w_{n_1}(E_r+\omega_{\alpha\beta})w_{n_2}(E_r) \qquad (7)$$

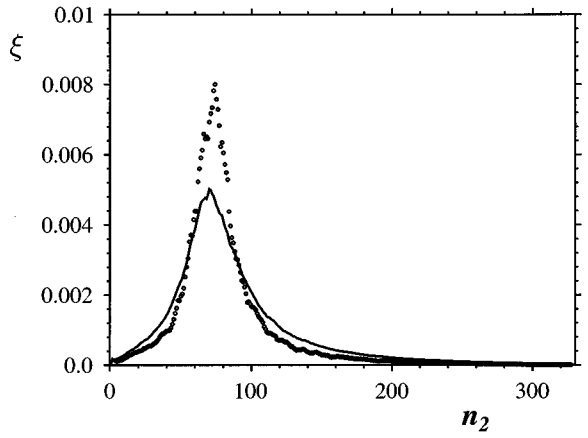

FIG. 2. Mean square matrix element ξ calculated for $n_1=55$, $\alpha=4$, and $\beta=5$ as a function of n_2. Averaging over 100 Hamiltonian matrices with different realizations of random two-body interaction has been made. The dots correspond to the direct numerical computation; the solid line represents the statistical approximation (7).

where $\omega_{\alpha\beta}=\epsilon_\alpha-\epsilon_\beta$ and $Q_{\alpha\beta}=\langle\overline{n_2|\hat{n}_\alpha(1-\hat{n}_\beta)|n_2}\rangle$. Here the sum runs over many-body basis components with w_{n_1} and w_{n_2} being the weights of these components in the states n_1 and n_2 [see Eq. (2)]. If we know the shape of the strength function w, this sum can be replaced by an integral and explicitly evaluated. In particular, when w is of Breit-Wigner type, the final expression for the MSME has also the Breit-Wigner form (see details in [2]).

In order to check the accuracy of the above expression (7) in the RTBI model, we have directly calculated $\xi^{(n_2n_1)}_{\alpha\beta}$ for $\alpha=4$, $\beta=5$ (transition from the ground state to the nearest one), and different values of n_1 and n_2. To reduce fluctuations, an averaging over a number of realizations of the Hamiltonian matrix has been done. The direct comparison with the analytical prediction (7) shows a quite good agreement. In particular, the positions of the maxima as well as the widths of $\xi^{(n_2n_1)}_{\alpha\beta}$ in dependence on n_1 and n_2 are well described by (7). However, quite unexpected deviations have been discovered which were found to be generic in the model. A typical example is given in Fig. 2 where a clear difference is seen between the statistical approximation (7) and numerical data. The absolute difference is maximal at the center of the ξ dependence; however, in the tails the relative difference is even larger. A thorough study of this phenomenon (see details in [10]) has revealed a very intriguing fact: the origin of this effect is in the underlying correlations induced by the two-body nature of the interaction. Similar correlations were observed in the model of random separable interaction [11,12]. Full analytical treatment of the correlations for the RTBI model is given in [10]. In particular, for the tails the contribution of the correlation term ξ_{corr} to the total MSME, $\xi_{total}=\xi_{corr}+\xi_{stat}$, has been estimated as

$$R\equiv\frac{\xi_{corr}}{\xi_{stat}}=-\frac{(n-2)(m-n-1)(m-n+2)}{n(m-n)(m-n+3)} \qquad (8)$$

where ξ_{stat} is very close to that given by the expression (7). In the maximum of ξ, the estimate for $m-n\gg 1$ reads as

$\xi_{total}/\xi_{stat} \approx 2-2m/[n(m-n)]$. The remarkable result is that these correlations do not decrease with an increase of number of particles n and number of orbitals m. Numerical data for larger values of $n=7$ and $m=14$ (with $N=3432$) have confirmed this prediction.

ENHANCEMENT OF A WEAK PERTURBATION IN CHAOTIC MANY-BODY SYSTEMS

The RTBI model allows for the study of a very important effect, namely, the enhancement of a weak perturbation $\hat{W}$, which takes place in systems with chaotic compound states. This effect is proportional to the mixing coefficient $\eta=\langle n_1|\hat{W}|n_2\rangle/\Delta_{12}$ where $\Delta_{12}=E_1-E_2$ is the spacing between the neighboring energy levels of compound states. Since the spacings for strongly excited states of many-body systems are exponentially small, $\Delta_{12}\sim\exp(-n)$, one could expect strong enhancement of the perturbation in comparison with the single-particle mixing defined by $\eta_s=\langle\alpha|\hat{W}|\beta\rangle/(\epsilon_\alpha-\epsilon_\beta)$. The possibility of the enhancement in compound nuclei was pointed out in [13,14] and considered in detail in a recent review [12]. However, such nontrivial effects as repulsion between energy levels and the above discussed correlations may have strong influence on the enhancement. Our preliminary results show that even for four particles the enhancement in the RTBI model does exist.

CONCLUDING REMARKS

In this Brief Report we have analyzed the RTBI model which, unlike conventional random matrix models, allows for the study of many important problems related to the two-body character of the interaction. As an example, the role of interaction for the appearance of the Fermi-Dirac distribution has been investigated for the parameters of Ce atom. It was found that the two-body interaction gives rise to thermalization and that the statistical effect of the interaction can be imitated by an increase of temperature. The study of correlations between occupation numbers has revealed sufficiently weak correlations even for a small number ($n=4$) of particles. This justifies the approximation of independent particles which is typically used in the description of complex compound states. To describe the effect of spreading widths of orbitals, the generalization of the Fermi-Dirac distribution was suggested.

The numerical and analytical treatment has shown that the statistical theory reproduces quite well the global structure of matrix elements of an external perturbation between compound states. On the other hand, underlying correlations have been discovered which are induced by the two-body character of the interaction, even if the latter is completely random. This phenomenon results in serious deviations from the statistical predictions for matrix elements between compound states. At the moment, all consequences of these correlations are still not understood; however, preliminary data [15] show that they can lead to the so-called gross structure (sharp peaks) in a cross section.

In conclusion, our results show that the TBRI model discussed above can be a very useful tool in the study of many important problems of the statistical physics of complex quantum systems.

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