Statistical theory of finite Fermi systems based on the structure of chaotic eigenstates

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An approach is developed for the description of isolated Fermi systems with finite numbers of particles, such as complex atoms, nuclei, atomic clusters, etc. It is based on statistical properties of chaotic excited states which are formed by the interaction between particles. A type of ''microcanonical'' partition function is introduced and expressed in terms of the average shape of eigenstates $F(E_k,E)$, where E is the total energy of the system. This partition function plays the same role as the canonical expression $\exp(-E^{(i)}/T)$ for open systems in a thermal bath. The approach allows one to calculate mean values and nondiagonal matrix elements of different operators. In particular, the following problems have been considered: the distribution of occupation numbers and its relevance to the canonical and Fermi-Dirac distributions; criteria of equilibrium and thermalization; the thermodynamical equation of state and the meaning of temperature, entropy and heat capacity; and the increase of effective temperature due to the interaction. The problems of spreading widths and the shape of the eigenstates are also studied. [S1063-651X(97)01811-4]

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I. INTRODUCTION

As is known, quantum statistical laws have been derived for systems with infinite numbers of particles, or for systems in a heat bath; therefore, their applicability to isolated finite systems of a few particles is, at least, questionable. However, the density of many-particle energy levels increases extremely fast (typically, exponentially), both with an increase of number of particles and excitation energy. For this reason, even a weak interaction between particles can lead to a strong mixing between large numbers of simple many-particle states, resulting in so-called *chaotic eigenstates*. If the components of such eigenstates can be treated as random variables (the onset of *quantum chaos*), statistical methods are expected to be valid even for an isolated dynamical system.

One should stress that a statistical description of such isolated systems can be quite different from that based on standard canonical distributions; therefore, application of the famous Fermi-Dirac or Bose-Einstein formulas may give incorrect results. Moreover, for isolated few-particle systems, a serious problem arises in the definition of temperature, or other thermodynamic variables like entropy and specific heat. (This contrasts with infinite systems for which different definitions give the same result.)

The aim of this paper is to develop a statistical theory for finite quantum systems of interacting particles, based on generic statistical properties of chaotic eigenstates (the ''microcanonical'' approach). Typical examples of such systems are compound nuclei, complex atoms, atomic clusters, isolated quantum dots, etc.

The structure of the paper is as follows. In Sec. II, a type of ''microcanonical'' partition function is introduced for finite isolated systems, which is directly related to the average shape of chaotic eigenstates. Based on this partition function, a general expression for the occupation numbers is given which is valid for any number of interacting particles. The relation of this ''microcanonical'' expression (*F distribution*) to that of standard canonical distribution for occupation

numbers is the subject of Sec. III. Also, a form of the canonical distribution is suggested which can be convenient in applications to open systems in thermal equilibrium like quantum dots.

The transition to the standard Fermi-Dirac distribution for large systems is analyzed in Sec. IV. Specific attention is paid to the accuracy of this distribution in applications to isolated systems with few particles.

In Sec. V an analytical derivation of the F distribution of occupation numbers is given. For this, the model of n randomly interacting Fermi-particles distributed over m single-particle levels has been used. An analytical formula for the occupation numbers $n_s(E)$, with E being the total energy of the system, was found to be in excellent agreement with the numerical experiment.

In Sec. VI the influence of the finite width of single-particle states (''quasiparticles'') on the distribution of occupation numbers is considered. An expression for the occupation numbers is discussed which takes into account the finite spreading width of quasiparticles. It is demonstrated that for an isolated system with a fixed total energy E, the incorporation of spreading widths decreases the effective temperature; however, it does not change the occupation numbers.

Section VII deals with the important problem of a thermodynamical description of small systems consisting of finite number of interacting particles. Specifically, different definitions of both temperature and entropy have been analyzed, and the equation of state for finite systems has been derived.

In Sec. VIII we show that statistical effects of the interaction can be imitated by an increase of the effective temperature. This fact allows one to use the standard Fermi-Dirac expression for the occupation numbers (with renormalized parameters) in the application to both isolated and open (in the thermal bath) systems of interacting Fermi particles. This interaction may be strong; however, the assumption of randomness for residual interaction matrix elements is essential.

In Sec. IX the conditions for chaos, equilibrium, and

''thermalization'' have been analyzed for an isolated quantum system with a finite number of particles in terms of the interaction strength, number of particles, and other related parameters. Depending on these conditions, there are four different regions with different distributions of occupation numbers, which are discussed in detail. In this section, the transition to mesoscopic systems is briefly discussed. The question of particular interest is how statistical properties depend on the dimensionality of a system.

Since the approach developed in this paper is entirely related to the structure of chaotic eigenstates, in Appendix A the analytical expression for the average shape of eigenstates is given and discussed in more detail. This expression, which also describes the local spectral density of states (LDOS), essentially depends on two different widths and is valid both for weak and strong interactions between particles. For weak interaction the shape is close to the Lorentzian form, with the half-width given by the Fermi golden rule. For larger interaction the shape is characterized by exponential tails, and by a width which is linear in the interaction strength (contrary to the Fermi golden rule, which gives a quadratic dependence). Transition between these two regimes occurs when the half-width is comparable to the root-mean-square width (the effective bandwidth of the Hamiltonian matrix). In Appendix B the moments of the distributions of the basis components (LDOS) and energy levels are calculated. Finally, in Appendix C, a calculation of the density of final states and spreading widths of the LDOS have been performed using the Fermi golden rule.

II. MICROCANONICAL PARTITION FUNCTION

In this section we derive the partition function for closed (isolated) systems with finite numbers of interacting particles. This function allows one to perform analytical and numerical calculations of statistical mean values of different operators, for example, occupation numbers.

We follow the standard approach which is based on the separation of a total Hamiltonian into two parts,

$$H = H_0 + V = \sum \epsilon_s a_s^\dagger a_s + \frac{1}{2} \sum V_{pqrs} a_p^\dagger a_q^\dagger a_r a_s. \quad (1)$$

The ''unperturbed'' Hamiltonian H_0 should incorporate the effect of a mean field (if any), ϵ_s are the energies of single-particle states (''orbitals'') calculated in this field, $a_s^\dagger$ and a_s are creation-annihilation operators, and V stands for the residual interaction. For simplicity, here we neglect any dynamical effects of the interaction like pairing, collective modes, etc. Instead, we will study the statistical effects of interaction; therefore, in what follows we assume that matrix elements V_{pqrs} of the two-body residual interaction are random variables.

Exact (''compound'') eigenstates $|i\rangle$ of the Hamiltonian H can be expressed in terms of simple ''shell-model basis states'' $|k\rangle$ (eigenstates of H_0):

$$|i\rangle = \sum_k C_k^{(i)} |k\rangle, \quad |k\rangle = a_{k_1}^\dagger \dots a_{k_n}^\dagger |0\rangle. \quad (2)$$

These compound eigenstates $|i\rangle$, characterized by the corresponding energies $E^{(i)}$, are formed by the residual interaction V; in complex systems they typically contain large number $N_{pc} \gg 1$ of the so-called principal components $C_k^{(i)}$ which fluctuate ''randomly'' as a function of indices i and k.

Our main interest is in the occupation numbers n_s of single-particle states (orbitals). They can be represented in terms of components of the exact eigenstates $|i\rangle$,

$$n_s = \langle i|\hat{n}_s|i\rangle = \sum_k |C_k^{(i)}|^2 \langle k|\hat{n}_s|k\rangle. \quad (3)$$

Here $\hat{n}_s = a_s^\dagger a_s$ is the occupation number operator. The knowledge of the distribution of occupation numbers gives the possibility of calculating mean values of any single particle operator $\langle M \rangle = \Sigma_s n_s M_{ss}$. Moreover, the variance of the distribution of nondiagonal elements of M, describing transition amplitudes between ''chaotic'' compound states, can also be expressed through the occupation numbers n_s [1–3].

As one can see from Eq. (3), mean values of occupation numbers depend on the shape of exact eigenstates, given by the ''spreading function'' F (in what follows, the F function),

$$F_k^{(i)} \equiv \overline{|C_k^{(i)}|^2} = F(E_k - E^{(i)}). \quad (4)$$

The last equality in the above expression reflects the fact that the residual interaction V mainly mixes close components k in some energy interval Γ (''spreading width'') nearby the eigenstate energy $E^{(i)}$ (more accurately, nearby the unperturbed energy E_k for $k = i$; see below).

Typically, this spreading function rapidly decreases with an increase of $|E_k - E^{(i)}|$ (since an admixture of distant component is very small). Recently, in numerical studies of the Ce atom [2], the s-d nuclear shell model [4], and random two-body interaction model [3,5], it was found that typical shape F of exact eigenstates practically does not depend on a particular many-body system, and has a universal form which essentially depends on the spreading width Γ. The latter can be expressed in terms of parameters of the model (the intensity V of the residual interaction, the number of particles n, the excitation energy, etc.) and can be calculated analytically (see Appendixes A–C). One can also measure the width of the F function (4) via the number of principal components $N_{pc} \sim \Gamma/D$, where D is the local mean energy spacing for compound states. In many-body systems the value of D exponentially decreases with an increase of the number of ''active'' (valence) particles. As a result, N_{pc} is very large, $\sim 10^4$–10^6 in excited (compound) nuclei and ~ 100 in excited rare-earth or actinide atoms.

The starting point of our approach is an expression for the occupation numbers which stems from Eqs. (3) and (4),

$$n_s(E) = \frac{\Sigma_k n_s^{(k)} F(E_k - E)}{\Sigma_k F(E_k - E)}, \quad (5)$$

where $n_s^{(k)} \equiv \langle k|\hat{n}_s|k\rangle$ equals 0 or 1 for Fermi particles, and the sum in the denominator stands for the normalization. This way of averaging of occupation numbers is a kind of microcanonical averaging, since it is defined for the fixed

total energy E of a system. One can see that, in fact, relation (5) is equivalent to the introduction of a new kind of partition function,

$$Z(E) = \sum_k F(E_k - E), \quad (6)$$

which is entirely determined by the shape of chaotic eigenfunctions. In what follows, we term Eq. (5) the F *distribution*.

The above expression (5) gives insight into the problem of a statistical description of complex systems. Indeed, as was mentioned above, the shape of the F function has universal features and can often be described analytically; therefore, in practice there is no need to diagonalize a huge Hamiltonian matrix of a many-body system in order to find statistical averages. One should stress that the summation in Eq. (5) is carried out over unperturbed energies E_k defined by the mean field, rather than over the energies of exact eigenstates in the standard canonical distribution. As a result, the distribution of occupation numbers can be derived analytically (see Sec. V) even for few interacting particles, in the situation when the standard Fermi-Dirac distribution is not valid.

III. TRANSITION TO THE CANONICAL DISTRIBUTION

It is instructive to compare our F distribution (5) with occupation numbers obtained by making use of the standard canonical distribution

$$n_s(T) = \frac{\sum_i n_s^{(i)} \exp(-E^{(i)}/T)}{\sum_i \exp(-E^{(i)}/T)}, \quad (7)$$

where T is the temperature and the index i stands for exact eigenstates. The important difference between the F distribution (5) and the canonical distribution (7) is that in Eq. (5) the occupation numbers are calculated for a specific energy E of a system unlike the specific temperature T in Eq. (7). However, results of calculations based on Eqs. (7) and (5) can be compared with each other using the relation between the energy E and the temperature T,

$$E = \langle E \rangle_T = \frac{\sum_i E^{(i)} \exp(-E^{(i)}/T)}{\sum_i \exp(-E^{(i)}/T)}. \quad (8)$$

The comparison of Eqs. (7) and (5) also shows that the canonical distribution corresponds to the averaging of the "microcanonical" F distribution over some energy interval Δ_T. To demonstrate this, let us substitute $n_s^{(i)}$ and $\overline{|C_k^{(i)}|^2}$ from Eqs. (3) and (4) into Eq. (7), and replace the summation over i by the integration over $\rho(E^{(i)}) dE^{(i)}$, where $\rho(E^{(i)})$ is the density of exact energy levels,

$$\sum_i n_s^{(i)} \exp(-E^{(i)}/T) \approx \int n_s^{(i)} \Phi_T(E^{(i)}) dE^{(i)}. \quad (9)$$

Here we have introduced the "canonical (thermal) averaging" function

$$\Phi_T(E) = \rho(E) \exp(-E/T), \quad (10)$$

which is discussed below. As a result, we can transform the canonical distribution (7) into a form similar to the F distribution (5),

$$n_s(T) = \frac{\sum_k n_s^{(k)} F(T, E_k)}{\sum_k F(T, E_k)}, \quad (11)$$

where the function $F(T, E_k)$ is the canonical average of $F_k^{(i)}$,

$$F(T, E_k) = \int F_k^{(i)} \Phi_T(E^{(i)}) dE^{(i)}. \quad (12)$$

Note that this form of the canonical distribution can be convenient for a calculation of the occupation numbers and other mean values in quantum dots which are in thermal equilibrium with an environment (with no particle exchange).

In large many-body systems the canonical averaging function $\Phi_T(E)$ has a narrow maximum, since the density of states $\rho(E^{(i)})$ typically grows very fast. The position E_m of its maximum is defined by the expression

$$\frac{d \ln\rho(E)}{dE} = \frac{1}{T}, \quad (13)$$

and the width is given by

$$\Delta_T = \left| \frac{d^2 \ln\rho(E)}{dE^2} \right|^{-1/2}. \quad (14)$$

As an example, let us consider the system of n interacting particles distributed over m orbitals. In Refs. [6,7] it was shown that in the case $m \gg n \gg 1$ the density of states is of the Gaussian form

$$\rho(E) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(E - E_c)^2}{2\sigma^2} \right), \quad (15)$$

where E_c is the center of the spectrum and σ^2 is its variance. According to recent numerical data [5,3], the Gaussian form for the density $\rho(E)$ also occurs for few particles ($n \geq 4$). This fact easily allows us to find the form of $\Phi_T(E)$ which appears to be quite generic,

$$\Phi_T(E) \sim \exp\left(-\frac{(E - E_m)^2}{2\sigma^2} \right), \quad (16)$$

where

$$E_m = E_c - \frac{\sigma^2}{T}. \quad (17)$$

One can see that the width Δ_T of the thermal averaging function equals the root-mean-square (rms) width of the spectrum, $\Delta_T = \sigma$. Now, it is easy to show that the thermal averaging width Δ_T is always larger than the rms width ΔE of the "microcanonical" F function, or the same as the mean width of exact eigenstates in the energy representation. Indeed, there is a simple relation between the widths σ and σ_0 of the energy spectrum with and without interaction, respectively (see Appendix A),

$$\sigma^2 = \sigma_0^2 + (\Delta E)^2; \tag{18}$$

therefore, we have $\Delta_T = \sigma > \Delta E$. One should stress that the latter width ΔE, in fact, is due to statistical effects of interaction. The difference between the widths Δ_T and ΔE is not important when the number of particles n is large. This is because with an increase of n the width σ_0 of the unperturbed spectrum increases as $\sqrt{n}$, unlike the width ΔE, which increases as n. One should also note that in this case both widths Δ_T and ΔE are much smaller than the typical energy interval, $\sigma/|E - E_c| \sim 1/\sqrt{n}$. Therefore, for a large number of particles the function Φ_T can be regarded as the δ function at $E = E_m$, and the F distribution is close to the canonical distribution, see Eq. (12).

To conclude this section, the canonical distribution (7) is not correct when describing isolated systems with a small number of particles; instead, one should use the F distribution (5). This was recently confirmed by numerical experiments with the model of few Fermi particles with a two-body random interaction [5,8].

IV. TRANSITION TO THE FERMI-DIRAC DISTRIBUTION

It is now instructive to show how the standard Fermi-Dirac distribution stems directly from the F distribution (5) in the limit of a large number of particles. By performing explicitly the summation over $n_s = 0$ and 1, expression (5) can be rewritten in the form

$$n_s(E) = \frac{0 + Z_s(n-1, E - \tilde{\epsilon}_s)}{Z_s(n-1, E - \tilde{\epsilon}_s) + Z_s(n, E)} = \frac{1}{1 + \dfrac{Z_s(n, E)}{Z_s(n-1, E - \tilde{\epsilon}_s)}}. \tag{19}$$

Here, two ''partial'' partition functions $Z_s(n, E)$ and $Z_s(n-1, E - \tilde{\epsilon}_s)$ are introduced. In the first one, the summation is taken over all single-particle states of n particles with the orbital s excluded, $Z_s(n, E) = \Sigma'_k F(E_k - E)$. Correspondingly, the sum in $Z_s(n-1, E - \tilde{\epsilon}_s)$ is taken over the states of $n-1$ particles with the orbital s excluded. The latter sum appears from the terms for which the orbital s is filled ($n_s = 1$); thus we should add the energy $\tilde{\epsilon}_s \equiv E_k(n) - E_k(n-1)$ of this orbital to the energy $E_k(n-1)$ of the basis state $|k\rangle$ defined by $n-1$ particles. Since the F function depends on the difference $E_k + \tilde{\epsilon}_s - E$ only, the adding term $\tilde{\epsilon}_s$ to $E_k(n-1)$ is the same as its subtraction from the total energy E. Note that this term is defined by

$$\tilde{\epsilon}_s = \epsilon_s + \sum_{p \neq s} u_{sp} n_p^{(k)}, \tag{20}$$

where ϵ_s is the energy of a single-particle state and u_{sp} is the diagonal matrix element of the two-body residual interaction. By taking $\tilde{\epsilon}_s$ independent of k, we assume that the averaging over the basis states near the energy E is possible; in fact, this is equivalent to a local (at a given energy) mean-field approximation.

One should stress that this approximation is the most important when applying model (1) to realistic systems. For example, for Ce atom there are orbitals from different open subshells (e.g., $4f$ and $6s$) which are quite close in energies;

however, they have very different radii. As a result, the Coulomb interaction between the corresponding electrons is very different [9]. In this case the interaction terms in Eq. (20) depend strongly on the occupation numbers of other particles, which means that there is no good mean-field approximation. As a result, the equilibrium distribution for occupation numbers is very different from the Fermi-Dirac distribution [9]. However, the F distribution (5) for occupation numbers is valid. In other cases like the random two-body interaction model [5,3,8] or nuclear shell model [4], such a local mean-field approximation is quite accurate.

For a large number $n \gg 1$ of particles distributed over $m \gg 1$ orbitals, the dependence of Z_s on n and $\tilde{\epsilon}_s$ is very strong, since the number of terms N in the partition function Z_s is exponentially large, $N = m!/(m-n)!n!$. Therefore, to make the dependence on arguments smooth, one should consider $\ln Z_s$ instead of Z_s. In this case, one can obtain

$$\ln Z_s(n - \Delta n, E - \tilde{\epsilon}_s) \approx \ln Z_s(n, E) - \alpha_s \Delta n - \beta_s \tilde{\epsilon}_s, \tag{21}$$

$$\alpha_s = \frac{\partial \ln Z_s}{\partial n}, \quad \beta_s = \frac{\partial \ln Z_s}{\partial E}, \quad \Delta n = 1.$$

This leads to a distribution of Fermi-Dirac type,

$$n_s = \frac{1}{1 + \exp(\alpha_s + \beta_s \tilde{\epsilon}_s)}. \tag{22}$$

If the number of substantially occupied orbitals in the definition of Z_s is large, the parameters α_s and β_s are not sensitive as to which particular orbital s is excluded from the sum, and one can assume $\alpha_s = \alpha \equiv -\mu/T$ and $\beta_s = \beta \equiv 1/T$ as in the standard Fermi-Dirac distribution. Then the chemical potential μ and temperature T can be found from the conditions of a fixed number of particles and a fixed energy,

$$\sum_s n_s = n, \quad \sum_s \epsilon_s n_s + \sum_{s > p} u_{sp} n_s n_p = \sum_s n_s(\epsilon_s + \tilde{\epsilon}_s)/2 = E. \tag{23}$$

Note that the sums in Eqs. (23) and (20) containing the residual interaction u_{sp} can be substantially reduced by a proper choice of the mean-field basis (for instance, the terms u_{sp} can have different signs in such a basis). In practice, the values ϵ_s and $\tilde{\epsilon}_s$ may be very close. Since in the above expressions (23) the nondiagonal matrix elements of the interaction are not taken into account, one can expect that the distribution of occupation numbers defined by these equations gives a correct result if the interaction is weak enough (the ideal gas approximation). However, we can show (see Sec. VIII) that, in fact, even for strong interaction the Fermi-Dirac distribution can be also valid if the total energy E is corrected in a proper way, by taking into account the increase of the temperature due to statistical effects of interaction.

One should also note that a somewhat similar procedure transforms the canonical distribution (7) into the Fermi-Dirac distribution (see, e.g., Ref. [10]) in the case of many noninteracting particles (ideal gas). It is curious that the Fermi-Dirac distribution is very close to the canonical distribution (7) even for a very small number of particles ($n = 2$), pro-

vided the number of essentially occupied orbitals is large (which happens for $T \gg \epsilon$ or $\mu \gg \epsilon$). In fact, this is a result of a large number of ''principal'' terms in the partition function Z_s which allows us to replace α_s by α in the term $Z_s(n,T)/Z_s(n-1,T) \equiv \exp(\alpha_s + \beta \epsilon_s)$ in the canonical distribution (7) [compare with Eq. (19)].

More accurate consideration shows, however, that the temperature T in the Fermi-Dirac distribution is different from that in the canonical distribution. Indeed, using the expansion $\alpha_s = \alpha(\epsilon_F) + \alpha'(\epsilon_s - \epsilon_F)$, one can obtain the relation between the Fermi-Dirac (β_{FD}) and canonical (β) inverse temperatures, $\beta_{\mathrm{FD}} = \beta + \alpha' \epsilon_F$. Concerning the chemical potential, its definition also changes, $-\mu/T = \alpha(\epsilon_F) - \alpha' \epsilon_F$. This fact is confirmed by our numerical simulations for an isolated system with few interacting Fermi particles [5,3,8]. Namely, for the same total energy E of the system, the canonical and Fermi-Dirac distributions give the same distribution n_s, defined, however, by different temperatures, since they are determined by different equations (8) and (23).

The closeness of these two distributions for any number of particles is not so surprising in the presence of the thermostat, where even one particle is in the equilibrium. On the contrary, for isolated systems with small number of particles the applicability of the Fermi-Dirac distribution is not obvious. To answer this question, one needs to analyze the role of interaction in the creation of an equilibrium distribution.

V. ANALYTICAL CALCULATION OF OCCUPATION NUMBERS IN FINITE SYSTEMS

The advantage of the approach developed in this paper is that if we know the shape of eigenstates in the many-particle basis of noninteracting particles (the F function) and the unperturbed density of states $\rho_0(E)$, one can analytically calculate the distribution of the occupation numbers n_s.

In order to calculate the occupation numbers n_s, we use expression (19) containing two partial partition functions $Z_s(n,E)$ and $Z_s(n-1,E-\epsilon_s)$ which correspond to systems with n and $n-1$ particles, with the orbital s is excluded from the set of single-particle states. The partition function can be found from the relation

$$Z = \sum_k F(E_k - E) \approx \int \rho_0(E_k) F(E_k - E) dE_k. \quad (24)$$

The density of unperturbed states $\rho_0(E_k)$ in a system of n particles distributed over m single-particle states (orbitals) was shown to be close to the Gaussian (see, for example, Refs. [6,7,11]):

$$\rho_0(E_k) = \frac{N}{\sqrt{2\pi\sigma_0^2}} \exp\left(-\frac{(E_k - E_c)^2}{2\sigma_0^2}\right), \quad (25)$$

with E_c as the center of the energy spectrum and N as the total number of states. Let us assume that the shape of eigenstates F is also given by the Gaussian:

$$F(E_k - E) = \frac{1}{\sqrt{2\pi(\Delta E)^2}} \exp\left(-\frac{(E_k - E)^2}{2(\Delta E)^2}\right). \quad (26)$$

Here the variance $(\Delta E)^2$ is defined by Eqs. (55) and (56), and $E = E^{(i)} + \Delta_1^{(i)} = H_{ii}$ (see Appendix A).

As was found, a Gaussian shape of eigenstates (apart from long tails) occurs in realistic systems like the Ce atom [2] and heavy nuclei [4]. Recently, the form of the F function as it depends on the perturbation was studied in detail [12] in the model of Wigner band random matrices, as well as in the random two-body interaction model [8]. In particular, it was discovered that the Gaussian-type shape happens when the interaction is large enough, that is, when the Breit-Wigner width $\Gamma = 2\pi\rho V^2$ is comparable to the root-mean-square width ΔE (an effective bandwidth of a Hamiltonian matrix).

By performing the integration in Eq. (24), one obtains

$$Z(E) = \frac{N}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(E - E_c)^2}{2\sigma^2}\right), \quad (27)$$

where $\sigma^2 = \sigma_0^2 + (\Delta E)^2$ (this coincides with the variance of the perturbed spectrum). In order to calculate the occupation numbers n_s, we use expression (19). For this, one needs to find the partial partition functions $Z_s(n,E)$ and $Z_s(n-1,E-\epsilon_s)$ corresponding to n and $n-1$ particles with the orbital s is excluded from the set of single-particle states. Now we have to calculate the number of states N_s and the center E_{cs} for these truncated systems,

$$N_s(n,m-1) = \frac{(m-1)!}{(m-1-n)!n!},$$

$$N_s(n-1,m-1) = \frac{(m-1)!}{(m-n)!(n-1)!},$$

$$E_{\mathrm{cs}}(n) = \overline{\epsilon_{-s}}n, \quad E_{\mathrm{cs}}(n-1) = (\overline{\epsilon_{-s}})(n-1),$$

$$\overline{\epsilon_{-s}} = \frac{\sum_{p \neq s} \epsilon_p}{m-1},$$

The variance σ_{0s} of the energy distributions can be estimated as

$$\sigma_{0s}^2(n) \approx \sigma_{1s}^2 n, \quad \sigma_{0s}^2(n-1) \approx (\sigma_{1s}^2)(n-1),$$

where σ_{1s}^2 is the variance of the single-particle spectrum with the excluded orbital s. Here, for simplicity, we neglected the Pauli principle, which is valid for $m \gg n$. A more accurate calculation can be easily done with the use of a calculator. As a result, the distribution of occupation numbers has the form

$$\overline{n_s}(E) = \frac{1}{1+R},$$

$$R = \frac{m-n}{n} \frac{\sigma_s(n-1)}{\sigma_s(n)} \exp\left[-\frac{[E - E_{\mathrm{cs}}(n)]^2}{2\sigma_s^2(n)} + \frac{[E - \epsilon_s - E_{\mathrm{cs}}(n-1)]^2}{2\sigma_s^2(n-1)}\right], \quad (28)$$

where $\sigma_s^2 = \sigma_{s0}^2 + (\Delta E)^2$.

It is instructive to compare this result with the Fermi-Dirac distribution which is valid for a large number of par-
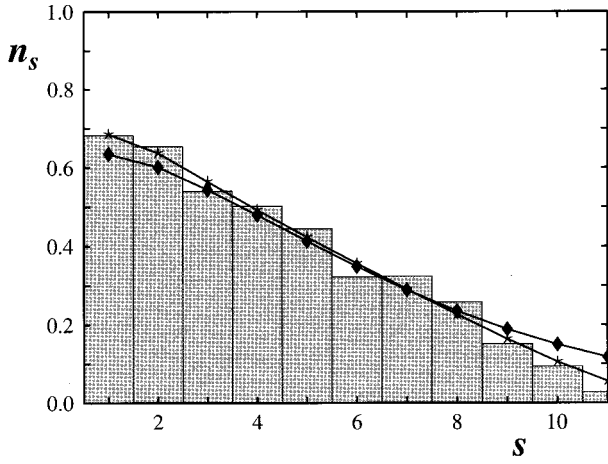
FIG. 1. Analytical description of the occupation numbers. Data are given for the two-body random interaction model (1) of $n=4$ Fermi particles distributed over $m=11$ orbitals with $V=0.20$ and $d_0=1$ in the definition of single-particle energies, $\epsilon_s=d_0[s+(1/s)]$; see Refs. [5,3,8]. The histogram is obtained according to Eq. (3) by the averaging over eigenstates with energies taken from small energy window centered at $E=17.33$ and over 20 Hamiltonian matrices (1) with different realization of the random interaction. Stars represent the analytical expression (28) with σ_{0s} found from single-particle energy spectrum. Diamonds correspond to the Fermi-Dirac distribution with thermodynamical temperature (33) and chemical potential found from the standard condition for the total number of particles, $n=\Sigma_s n_s$.

ticles. In this case $R=\exp[(\epsilon_s-\mu)/T_{th}]$ where $T_{th}=\sigma^2/(E_c-E)$ is the thermodynamic temperature which is discussed below; see Eq. (33). The chemical potential μ in this case should be calculated numerically to fix the total number of particles n. The data are reported in Fig. 1. One can see that Eq. (28) predicts occupation numbers in perfect agreement with the numerical experiment.

Finally, note that the same method can be used to solve another problem: to find the distribution of the occupation numbers $n_s(T)$ in finite systems of interacting particles in the thermal bath with the temperature T. For such a case, it is enough to replace the F function by the canonical average $F(T,E_k)$; see Eq. (12). In fact, this is the method for taking into account the ''random'' interaction in the canonical distribution. The result for the occupation numbers $n_s(T)$ can be obtained from Eq. (28) by replacing $\sigma_s^2 \rightarrow 2\sigma_s^2$ and $E \rightarrow E_m + \Delta_1(E_m)$, where $E_m=E_c-\sigma^2/T$ and Δ_1 is a small correction; see Appendix A.

VI. PARTICLES AND QUASIPARTICLES, ROLE OF SINGLE-PARTICLE SPREADING WIDTH

In previous sections we discussed the distribution of occupation numbers for real particles distributed over given orbitals. At the same time, there exists a traditional approach which is based on the notion of ''quasiparticles.'' It allows us to incorporate the effects of interaction in terms of single-particle states, and goes beyond the mean-field approximation. As is well known, the interaction leads to the spreading width γ_s for single-particle orbitals. It also results in the shift of average energies, $\tilde{\epsilon}_s = \epsilon_s + \delta\epsilon_s$. According to our numeri-

cal data [5] for the random two-body interaction model, the shifts $\delta\epsilon_s$ turn out to be, on average, smaller than γ_s, and for this reason one can take into account the effect of spreading widths γ_s only.

Here we would like to analyze the role of the spreading widths for the distribution of occupation numbers, and compare with our approach where the interaction is taken into account in terms of many-body states. For this, let us average the standard Fermi-Dirac occupation numbers n_s over the energy interval γ_s:

$$n_s = \int_{\epsilon_s-\gamma_s/2}^{\epsilon_s+\gamma_s/2} n(\epsilon)\frac{d\epsilon}{\gamma_s} = 1 - \frac{T}{\gamma_s}\ln\left[\frac{1+\exp\left(\frac{\epsilon_s+\frac{\gamma_s}{2}-\mu}{2T}\right)}{1+\exp\left(\frac{\epsilon_s-\frac{\gamma_s}{2}-\mu}{2T}\right)}\right],$$
(29)

$$n(\epsilon) = \frac{1}{1+\exp\left(\frac{\epsilon-\mu}{T}\right)}.$$
(30)

It seems that this is the simplest form of the Fermi-Dirac distribution for quasiparticles with finite spreading widths. One can check that in the limit $\gamma_s=0$ the Fermi-Dirac expression (30) with $n_s=n(\epsilon_s)$ is recovered.

To test the sensitivity of the occupation numbers to the values of the spreading widths γ_s, we solved equations (23) for chemical potential and temperature (for a given energy of our isolated system) using the standard expression (30), and compared the result with that obtained by using expression (29); see details in Ref. [5]. The data have revealed that the chemical potential practically does not change, while there is a noticeable decrease of the temperature, $T(\gamma\neq0) < T(\gamma=0)$. The striking result is that the two curves for the occupation numbers (29) and (30) coincide with a high accuracy, namely, $n_s(\epsilon_s,\gamma,T) \approx n_s(\epsilon_s,\gamma=0,T+\Delta T) \equiv n_s(\epsilon_s,\tilde{T})$. This means that the temperature mimics the effect of the spreading widths, the phenomenon which is far from being trivial. The shift of the temperature for $\gamma \ll \mu$ can be estimated analytically as $\Delta T \approx \gamma^2/16T$. The above result indicates that one should not worry about the finite width of single-particle orbitals (quasiparticles) when calculating the occupation numbers.

VII. THERMODYNAMICS OF SMALL SYSTEMS

One of the important questions is about thermodynamical description of isolated systems of interacting particles. In any thermodynamical approach one needs to define, in a consistent way, such quantities as entropy, temperature, and the equation of state. Different definitions of the entropy and temperature have recently been discussed [13] in applications to shell models of heavy nuclei. In particular, it was found that for a realistic residual interaction, different definitions of temperatures lead to the same result. Below, we analyze a few definitions of the temperature and entropy, and show that for small number of interacting particles they may give quite different results.

Standard thermodynamical definitions of the entropy S_{th} and temperature are based on the density of states $\rho(E)$,

$$S_{th} = \ln \rho(E) + \text{const}, \tag{31}$$

$$\frac{1}{T_{th}} = \frac{dS_{th}}{dE} = \frac{d \ln \rho}{dE}. \tag{32}$$

In fact, such a definition of the temperature follows from an estimate of the position of maximum of the canonical averaging function $\Phi_T(E)$; see Eqs. (10) and (13). It is usually assumed that the position of its maximum E_m coincides with the energy E of a system. One should stress that in the above definitions $\rho(E)$ is the perturbed density of states; therefore, the interaction is essentially taken into account.

However, for finite isolated systems with a fixed energy E, the definition of the temperature given by the relation $\langle E \rangle_T = E$ [see Eq. (8)] seems to be more natural. Here the averaging is performed over the canonical distribution (7). Since the width Δ_T of the canonical averaging function $\Phi_T(E)$ is not zero, the two definitions of the temperature, Eqs. (32) and (8) give, in principal, different results. Indeed, in the case of the Gaussian form of $\rho(E)$ the value of T_{th} given by Eq. (32) takes the form (see also Ref. [13])

$$T_{th} = \frac{\sigma^2}{E_c - E}, \tag{33}$$

where E_c and σ are the center and the width of the distribution $\rho(E)$.

On the other hand, direct evaluation of relation (8) leads to the following definition of the temperature:

$$T_{can} = \frac{\sigma^2}{E_c - E + \Delta}. \tag{34}$$

Here the shift Δ is given by the expression

$$\Delta = \frac{\sigma}{K} \left[\exp\left(-\frac{(E_{min} - E_m)^2}{2\sigma^2} \right) - \exp\left(-\frac{(E_{max} - E_m)^2}{2\sigma^2} \right) \right], \tag{35}$$

where

$$K = \int_{x_{min}}^{x_{max}} \exp\left(-\frac{x^2}{2} \right) dx \approx \sqrt{2\pi}, \quad x = \frac{E - E_m}{\sigma},$$

$$E_m = E_c - \frac{\sigma^2}{T_{can}}. \tag{36}$$

One can see that the shift Δ itself depends on the temperature and is proportional to the width $\Delta_T = \sigma$ of the function $\Phi_T(E)$. In the above relations, E_{min} and E_{max} are the low and upper borders of the energy spectrum. Note that the relation $\Delta = 0$ occurs at the center of the spectrum; therefore, the temperature in the upper part of the spectrum is negative (it is typical for systems with bounded spectrum, for example, for spin systems). In fact, our model (1) with finite number m of orbitals can be treated as a model of one open shell in atoms, nuclei, clusters, etc. However, in realistic many-body systems there are always higher shells which contribute to the density of states for higher energy. Thus the density of
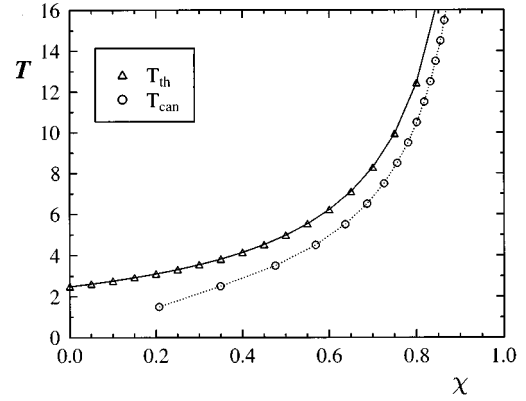

FIG. 2. Different temperatures vs the rescaled energy $\chi = (E - E_{fermi})/(E_c - E_{fermi})$ for the two-body random interaction model with $n = 4$ Fermi particles and $m = 11$ orbitals. Triangles stand for the thermodynamical temperature T_{th} defined by Eq. (33), and should be compared to the canonical temperature T_{can} (circles); see Eq. (34). The width σ of the perturbed density of states is defined by the residual interaction $V = 0.12$ according to Eqs. (18) and (A4), with σ_0 found numerically from the unperturbed many-particle energy spectrum (the mean level spacing d_0 between single-particle levels is set to $d_0 = 1$).

states $\rho(E)$ is a monotonic function which results in positive temperature. For such physical applications, model (1) with finite number of orbitals is reasonable in the lower part of the energy spectrum where the influence of higher shells can be neglected.

One can also see that the difference between the two equations of state $T(E)$ defined by Eqs. (33) and (34) disappears for highly excited eigenstates (for which $E_m - E_{min} \gg \sigma$), or in large systems with $n \gg 1$. Indeed, one can obtain, $E_c - E \sim n\sigma_1$, where σ_1 is the width of the single-particle spectrum. On the other hand, according to the central limit theorem, the variance of the total-energy spectrum can be estimated as $\sigma_0^2 \approx \Sigma_n \sigma_1^2 = n\sigma_1^2$; therefore, the ratio $\sigma/(E_c - E) \sim 1/\sqrt{n}$ tends to zero at $n \to \infty$. Note that, in finite systems (atom, nucleus, etc.) the number of valence particles (particles in an open shell) is not large. For example, for the Ce atom we have $n = 4$ [2] and, in the nuclear shell model [4], $n = 12$, therefore, the corrections to the thermodynamical temperature (32) can be significant, especially for low energies. Here we do not take into account particles from deep closed shells since their excitation energy is high, and they do not contribute to the thermodynamical and statistical properties of systems [though they renormalize parameters of the Hamiltonian (1) describing the interaction between valence particles].

The energy dependence of temperatures T_{th} and T_{can} is shown in Fig. 2. The data are given for the model of $n = 4$ interacting Fermi particles distributed over $m = 11$ orbitals. The two-body interaction is taken to be completely random, given by the Gaussian distribution of two-body matrix elements with $V = 0.12$; this value should be compared with the mean energy distance $d_0 = 1$ between the orbitals (single-particle energies), see details in Refs. [5,3,8]. The comparison of the thermodynamical temperature T_{th} defined by Eq. (33) with the "canonical" temperature (34) reveals quite strong difference in all the range of the rescaled energy χ

$=(E-E_{\text{fermi}})/(E_c-E_{\text{fermi}})$. To test our analytical expression for the canonical temperature T_{can}, we performed a direct numerical calculation of the temperature according to Eq. (8) with the actual spectrum $E^{(i)}$ of the two-body random interaction [instead of the Gaussian approximation of $\rho(E)$]. Numerical results well agree with the analytical expression (34).

The knowledge of the equation of state $E(T)$ gives the possibility to examine heat capacity of closed systems with finite number of interacting particles,

$$C = \frac{dE}{dT} = \frac{\sigma^2}{T^2}\left(1 + \frac{\partial\Delta}{\partial E_m}\right). \qquad (37)$$

The second term in the above expression is a correction which vanishes for highly excited states or in large systems; however, it may be important in other situations.

Following Ref. [13], we can also compare different definitions of entropy. A natural definition of the entropy in isolated systems can be directly related to the number of principal components N_{pc} in exact eigenfunctions.,

$$S_{EF} = \ln N_{\text{pc}}. \qquad (38)$$

In such a definition the entropy characterizes the complexity of a system (note, that for unperturbed ''simple'' states $N_{\text{pc}} = 1$ and $S_{EF} = 0$). There are several definitions of N_{pc}, one of which is the so-called ''entropy localization length'' defined via the information entropy S_{inf} of eigenstates,

$$N_{\text{pc}} = \exp(S_{\text{inf}}), \qquad (39)$$

where

$$S_{\text{inf}}(E) = -\sum_k F_k(E)\ln F_k(E)$$

$$\approx -\int dE_k \rho(E_k) F(E_k-E)\ln F(E_k-E). \qquad (40)$$

Here we used the F function instead of $|C_k^{(i)}|^2$ in order to have a smooth dependence of the entropy S_{inf} on the energy E. Another possibility is to find N_{pc} from the ''inverse participation ratio,''

$$N_{\text{pc}}^{-1} = \sum_k (F_k(E))^2. \qquad (41)$$

One more definition is $N_{\text{pc}}^{-1} = \max[F_k(E)] \approx F(E_k=E)$ which was used in Ref. [2]. The difference between the above definitions of N_{pc} depends on a specific shape of $F_k(E)$; however, the values of N_{pc} differ from each other by some coefficient which is typically close to 1.

On the other hand, the estimate for N_{pc} can be obtained simply from the relation

$$N_{\text{pc}} \approx \frac{\Gamma}{D} = \Gamma\rho(E), \qquad (42)$$

where Γ is the spreading width of the function $F_k(E)$ and D is the local mean spacing between many-particle energy levels. Thus one can directly relate the number of principal components N_{pc} to the density of states $\rho(E)$,
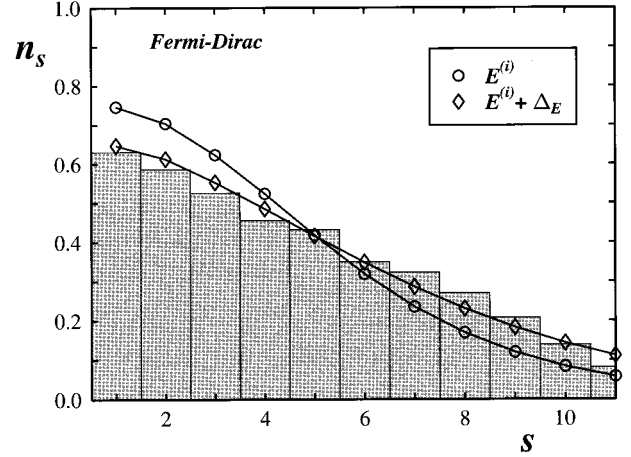

FIG. 3. Fermi-Dirac distribution for strongly interacting particles. The data are given for two-body random interaction model (1) with the parameters of Fig. 1 (the rescaled energy is $\chi = 0.55$). Circles stand for the Fermi-Dirac distribution with the total energy E corresponding to the energy of eigenstates; see Eq. (23). Diamonds correspond to the shifted energy according to expression (47).

$$S_{EF} = \ln N_{\text{pc}} \approx \ln\rho(E) + \ln\Gamma. \qquad (43)$$

One can see that the entropy S_{EF} found from exact eigenstates coincides with the thermodynamical entropy S_{th} if the second term in Eq. (43) does not depend on the energy. As is shown in Appendixes A–C, the spreading width Γ only weakly depends on the energy, in contrast to a very strong energy dependence of $\rho(E)$. The fact that the information entropy S_{inf} contains the term $\ln\rho$ was mentioned for the first time in Ref. [13]. One should stress that the above relations (42) and (43) are valid if N_{pc} is smaller than the size N of the many-particle basis, $N_{\text{pc}} < N/2$. One has also to remind that systems under consideration are assumed to be in equilibrium; see the discussion in Sec. IX.

VIII. INCREASE OF EFFECTIVE TEMPERATURE DUE TO STATISTICAL EFFECTS OF INTERACTION

In Sec. IV we showed that in the case of a large number of particles, the distribution of occupation numbers is of the Fermi-Dirac form (22) if the local mean-field approximation is valid. However, if one uses expression (23) in order to find the chemical potential μ and temperature T, one can obtain inaccurate results. To demonstrate this, we computed the distribution of occupation numbers n_s for the two-body random interaction model directly from exact eigenstates of the Hamiltonian matrix (1) defined on the basis of many-particle unperturbed states (see also Refs. [5, 8]). These data for the ''experimental'' values of n_s are shown in Fig. 3 by a histogram which is obtained by the average over a small energy window in order to smooth the fluctuations (also, an additional averaging over different realizations of the random two-body interaction has been done). To compare with the standard Fermi-Dirac distribution, we have numerically solved Eqs. (23) in order to find the temperature and chemical potential. The resulting distribution of the occupation numbers n_s is shown in Fig. 3 by circles. One should

stress that the value of the energy E in Eq. (23) was taken the same as for the exact eigenstates from which actual distribution of n_s was computed, namely, $E \approx E^{(i)}$. The comparison of the actual distribution (histogram) with the theoretical one [see Eq. (23)] reveals a large difference for a chosen (quite strong) perturbation $V = 0.20$.

This discrepancy is due to the fact that the off-diagonal interaction is not taken into account in Eq. (23). In Ref. [5] it was pointed out that one can take into account statistical effects of interaction and to correct the total energy in Eq. (23) in the following way. Let us first consider the thermodynamical temperature T_{th} defined by Eq. (33). As was mentioned above [see Eq. (18)], one can represent the width of perturbed density, of states $\rho(E)$ in the form $\sigma^2 = \sigma_0^2 + \overline{(\Delta E)^2}$, where σ_0 relates to the unperturbed density and ΔE is an increase of the width of the energy spectrum due to the interaction. Thus the temperature at a given energy E increases due to the interaction as follows:

$$T = T_0 + \Delta T \approx \frac{\sigma_0^2}{E_c - E} + \frac{\overline{(\Delta E)^2}}{E_c - E}, \quad (44)$$

resulting in the relation

$$\Delta T / T_0 = \overline{(\Delta E)^2} / \sigma_0^2. \quad (45)$$

The explanation of this increase of the temperature was given in Ref. [8], and reads as follows. Since the density of states rapidly increases with the energy E, the number of higher basis states admixed to an eigenstate by the interaction is larger than the number of lower basis states. An extreme example is the ground eigenstate, which contains basis components of higher energies only. As a result, the mean energy

$$\langle E_k \rangle_i = \sum_k E_k F_k^{(i)} \approx \int E_k F_k^{(i)} \rho_0(E_k) dE_k \quad (46)$$

of the components in an exact eigenstate $|i\rangle$ is higher than the eigenvalue $E^{(i)}$ corresponding to this eigenstate (we consider here eigenstates in the lower part of the spectrum only). There is another effect which gives the increase of $\langle E_k \rangle_i - E^{(i)}$ even if the density of states does not depend on the energy. Due to repulsion between the energy levels, the eigenvalues move down for this part of the spectrum; therefore, the difference between $\langle E_k \rangle_i$ and $E^{(i)}$ increases due to the interaction. This second effect shifts the "center" of the function $F_k^{(i)} = F(E_k - E^{(i)})$. One should stress that all effects leading to the above shift of the energy are automatically taken into account in relation (46). Thus, one can analytically calculate this shift $\Delta_E = \langle E_k \rangle_i - E^{(i)}$ from Eq. (46). For this, one needs to know the unperturbed density of states and the form of the F function. The evaluation of the shift Δ_E was done in Ref. [8] by assuming some form for the F function which is valid in a wide range of the interaction strength V,

$$\Delta_E = \langle E_k \rangle_i - E^{(i)} = \frac{d \ln \rho_0}{dE} \overline{(\Delta E)^2} = \frac{1}{T_0} \overline{(\Delta E)^2}$$
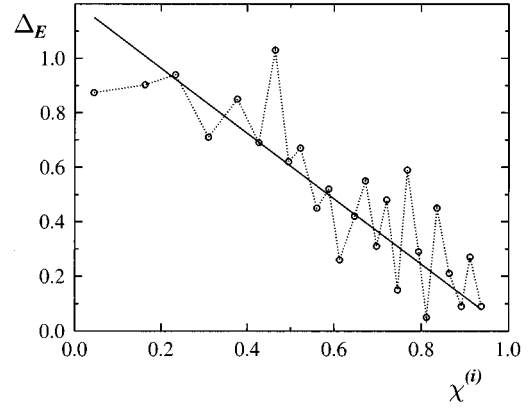

FIG. 4. Shift of the total energy for the corrected Fermi-Dirac distribution. The data are given for model (1) with $n = 4$, $m = 11$, $d_0 = 1$, and $V = 0.12$; see the explanation in the text. The straight line is the analytical expression (47); the dotted line (circles) present a direct computation of the shift based on the diagonalization of Hamiltonian (1) with the following computation of the $\langle E_k \rangle_i$. On the horizontal axes the rescaled energy $\chi^{(i)} = (E^{(i)} - E_{fermi})/(E_c - E_{fermi})$ is plotted.

$$= \frac{\overline{(\Delta E)^2}}{\sigma_0^2} (E_c - E). \quad (47)$$

Now, in order to obtain the corresponding increase of the temperature, one should insert the shifted energy $E \equiv \langle E_k \rangle_i = E^{(i)} + \Delta_E$ into the equation for the temperature,

$$T = T_0 + \Delta T = \frac{\sigma_0^2}{E_c - E^{(i)} - \Delta_E} \approx \frac{\sigma_0^2}{E_c - E^{(i)}} + \frac{\overline{(\Delta E)^2}}{E_c - E^{(i)}}. \quad (48)$$

One can see that Eq. (48) is consistent with Eq. (44) for $\overline{(\Delta E)^2} \ll \sigma_0^2$.

Thus, to find correct values for the occupation numbers in the Fermi-Dirac distribution, we should substitute the increased energy $E = E^{(i)} + \Delta_E = \langle E_k \rangle_i$ into Eqs. (23) for the chemical potential and temperature. The resulting shift of the temperature and chemical potential leads to the distribution of the occupation numbers shown in Fig. 3 by diamonds. As one can see, such a correction gives a quite good correspondence to the numerical data.

To check the analytical prediction (47) for the shift Δ_E, we have calculated this shift directly by comparing the energy $E^{(i)}$ of exact eigenstates with the energy $\langle E_k \rangle_i$. The latter has been computed from the exact relation $\langle E_k \rangle_i = \Sigma_k E_k |C_k^{(i)}|^2$ [compare with Eq. (46)]. The comparison of these data (circles in Fig. 4) with Eq. (47) (straight full line) shows a good agreement, if to neglect strong fluctuations around the global dependence. These fluctuations are due to fluctuations in the components of specific exact eigenstates $|i\rangle$ (note that the presented data correspond to the individual eigenstates, without any additional averaging).

Finally, we would like to note that the described above method can be also used to solve the "canonical" problem of finding the distribution of the occupation numbers for a system of interacting particles in the thermal bath. Indeed,

the distribution $n_s(T)$ for the "ideal" gas is given by the canonical distribution, or, more simply, by the Fermi-Dirac distribution if the number of particles $n \gg 1$ (in practice, $n > 2$ is enough). The increase of "kinetic" energy due to the random residual interaction is given by $\Delta_E = \overline{(\Delta E)^2}/T$; see Eq. (47). Then one can find the effective temperature which corresponds to the same increase of the average "kinetic" energy in the ideal gas. It can be done by the differentiation of $T^{-1} = dS/dE$, where S is the entropy, $S = \ln\rho_0 + $const. The result reads

$$\Delta T = -T \frac{d^2\ln\rho_0}{dE^2} \overline{(\Delta E)^2}. \tag{49}$$

For the Gaussian shape of the level density $\rho_0(E)$, this coincides with Eq. (45). Thus we can use the Fermi-Dirac distribution with the effective temperature $T_{\text{eff}} = T + \Delta T$ in order to describe "randomly" interacting particles (for $\Delta T \ll T$) in the heat bath.

IX. CRITERIA FOR THE ONSET OF CHAOS, EQUILIBRIUM, AND THERMALIZATION

The theory presented above is based on the notion of chaos in terms of statistical properties of compound eigenstates. Typically, the onset of quantum chaos is associated with a large number of components in the eigenstates. However, as we can see below, this condition is not enough for the emergence of equilibrium distributions and, in essence, there are different regimes of "chaos." Here we analyze the conditions under which the possibility of a statistical description of isolated systems of interacting particles can be directly related to statistical properties of eigenstate components.

Let us start with the condition of a large number of principal components N_{pc}, provided there is an equilibrium distribution of the components of eigenstates. For the relatively small interaction, the distribution of the components has the Breit-Wigner form

$$F_k^{(i)} \equiv \overline{|C_k^{(i)}|^2} = \frac{1}{N_{\text{pc}}} \frac{\Gamma_{\text{BW}}^2/4}{(E_k - E^{(i)})^2 + \Gamma_{\text{BW}}^2/4}. \tag{50}$$

Here, the value $N_{\text{pc}} = \pi\Gamma_{\text{BW}}/2D$ is defined by the normalization condition, $D = \rho^{-1}(E)$ is the mean spacing between energy levels, and the spreading width is given by

$$\Gamma_{\text{BW}} = 2\pi \frac{V^2}{d_f}, \tag{51}$$

where V^2 is the mean squared value of matrix elements of the two-body interaction; see Eq. (1). In the denominator, d_f stands for the mean energy spacing of those basis components to which a particular basis state $|k\rangle$ can "decay" due to direct two-body interaction; see details in Appendix C. Thus the condition $N_{\text{pc}} \gg 1$ reads

$$N_{\text{pc}} = \frac{\pi^2 V^2}{d_f D} \gg 1$$

or

$$V \gg \frac{1}{\pi^2} \sqrt{d_f D}. \tag{52}$$

However, as pointed out in Ref. [14] (see further developments in Ref. [15]), there is a phenomenon of "localization in the Fock space" which means that states with different numbers of excited particles do not mix with each other. This situation occurs when $V < d_f$ (with some logarithmic corrections). This means that in order to have an ergodic distribution for the eigenstate coefficients resulting in an equilibrium distribution of occupation numbers for individual eigenstates, one needs both the conditions $V > d_f$ and Eq. (52). Since d_f is typically much larger than D, the condition $V > d_f$ is stronger than Eq. (52).

Let us now discuss the properties of eigenstates and distribution of occupation numbers in dependence on two above parameters, V/d_f and N_{pc}. Since the value of N_{pc} increases with an increase of V, we first start with a very weak interaction for which exact eigenstates have only a few relatively large components ($N_{\text{pc}} \sim 1$). In such a case the eigenstates are strongly localized in the unperturbed basis and, therefore, can be described by conventional perturbation theory. This situation is quite typical for the lowest eigenstates (where the density of states is small) even if for higher energies the eigenstates can be considered very "chaotic" ($N_{\text{pc}} \gg 1$). We term this region (I) a region of strong (perturbative) localization.

The second region (II) is characterized by an "initial chaotization" of exact eigenstates and corresponds to a relatively large $N_{\text{pc}} \gg 1$ number of principal components and $V < d_f$. The latter condition is essential since it results in very strong (non-Gaussian) fluctuation of components $C_k^{(i)}$ [16] for the fixed energy $E^{(i)}$ of compound state $|i\rangle$. Such a type of fluctuation reflects itself in a specific character of eigenstates, namely, they turn out to be "sparsed." As a result, the number of principal components can not be estimated as $N_{\text{pc}} \approx \Gamma/D$, as is typically assumed in the literature. Let us note that the energy width Γ of eigenstates is still close to expression (51).

The above specific properties of compound states can be explained by the perturbation theory in the parameter V/d_f. Indeed, in the zero-order approximation an eigenstate $|i\rangle$ coincides with a basis state $|k_0\rangle$ for which the particles occupy definite orbitals. In first order in V/d_f the eigenstate $|i\rangle$ is constructed by those basis states $|k_1\rangle$ which can be obtained from $|k_0\rangle$ by moving one or two particles (due to the two-body character of the interaction). As a result, the coefficients of the state $|i\rangle$ can be estimated as $C_{k_1}^{(i)} = V_{k_0,k_1}/(E^{(i)} - E_{k_1})$. If the matrix elements V_{k_0,k_1} are Gaussian variables, for the fixed spacing $|E^{(i)} - E_{k_1}|$ the coefficients $C_k^{(i)}$ are also distributed according to the Gaussian.

The situation is completely different in higher orders. For example, in second order we have $C \equiv C_{k_2}^{(i)} = \Sigma_{k_1} V_{k_0,k_1} V_{k_1,k_2}/[(E^{(i)} - E_{k_1})(E^{(i)} - E_{k_2})]$, and the distribution $P(C)$ (for the fixed $|E^{(i)} - E_{k_2}|$) is close to the Lorentzian, namely, $P(C) \sim C_{\text{cr}}/C^2$ for $C_{\text{cr}} < C < 1$ where $C_{\text{cr}} \sim V^2/d_f^2$ [17,16]. Long tails in the distribution $P(C)$ are due to the possibility of small values of the denominator $E^{(i)}$
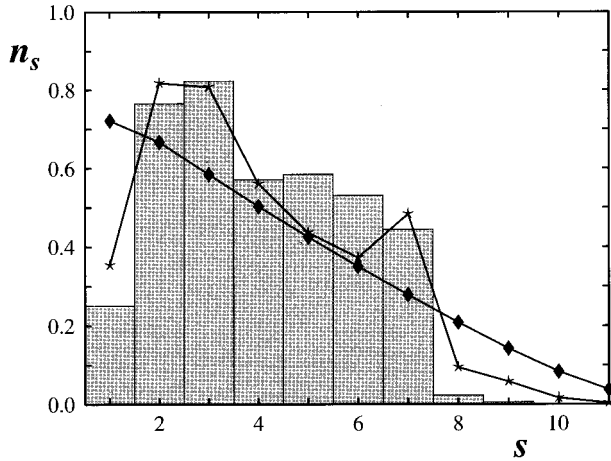
FIG. 5. Distribution of the occupation numbers for small inter-action. The histogram is obtained in the same way as in Figs. 1 and 2, for the very weak interaction $V=0.02$ which corresponds to region II of the "initial chaotization"; see Sec. X. The total energy (center of the small energy window) is $E^{(i)}=17.33$. Diamonds correspond to the theoretical expression (28) which is not valid in this region due to absence of equilibrium. Stars are obtained by direct numerical computation of n_s according to the F distribution (5) with the F function taken in the form of Eq. (A5); see Appendix A and Ref. [8]. The latter values are closer to the "experimental" ones, since we performed the summation over real unperturbed spectrum [instead of the integration with the Gaussian approximation for ρ_0 used to derive Eq. (28)].

$-E_{k_1}$ in intermediate states. The higher orders r of the perturbation theory give stronger fluctuations [with an additional logarithm in $P(C)$] because of the large number of small denominators. Another type of even stronger fluctuations result from very different nature of many-body basis states with close energies. That is, states with nearly the same energy can differ by a large number of moved particles in order to obtain the corresponding states. Therefore, the transition into close (in energies) states appears in different orders of the perturbation. Therefore, the fluctuations of the components C appear to be abnormal, without obeying the standard central limit theorem. In particular, the above effect leads to very large fluctuations in the distribution of the occupation numbers n_s, as a function of the energy E of compound states. Specifically, the fluctuations do not decrease as $N_{pc}^{-1/2}$; for example, if $P(C)\sim 1/C^2$ the fluctuations of $n_s(E)$ do not depend on N_{pc} at all for $N_{pc}<1/C_{cr}$ (see, for example, Ref. [17]).

As an example, one can take the two-body random interaction model (1) with $n=4$ particles and $m=11$ orbitals and very weak perturbation $V/d_0 \approx 0.02$, where d_0 is the mean level spacing between single-particle energy levels; see Fig. 5. One can see that the "experimental" distribution of occupation numbers has nothing to do with the Fermi-Dirac distribution (full diamonds), it turns out to be even the non-monotonic function of the energy ϵ_s of orbitals (see also Ref. [5]). Note that the averaging procedure used in Fig. 5 did not wash out the fluctuations in n_s.

With further increase of the interaction, where $N_{pc} \gg 1$ and $V>d_f$, the region (III) of the equilibrium for the F distribu-

tion (5) emerges. In this region the fluctuations of the eigen-state components $C_k^{(i)}$ are of Gaussian form [16], which leads to small fluctuations of the occupations numbers n_s in accordance with the central limit theorem for the sum (3), $\Delta n_s/n_s \sim N_{pc}^{-1/2} \ll 1$ for $n_s \sim 1$. One should stress that in this region the value of N_{pc} is given by the common estimate $N_{pc} \sim \Gamma/D$. As a result, the distribution of occupation numbers changes slightly when changing the energy of a system. Such a situation can be naturally associated with the onset of thermal equilibrium, though the form of the distribution n_s can be quite different from the Fermi-Dirac distribution. In this case, the F distribution (5) gives a correct description of an actual distribution of occupation numbers in isolated quantum systems of interacting particles. One can see that the equilibrium distribution for the occupation numbers arises for much weaker condition compared to that needed for the Fermi-Dirac distribution. Since the energy interval d_f between two-particle–one-hole energy levels is small, it is enough to have a relatively weak residual interaction $V>d_f$ in order to have the equilibrium distribution (note that the value of d_f decreases rapidly with the excitation energy; see Appendix C).

The next region (IV) is that where the canonical distribution (7) occurs; for this case, in addition to the equilibrium, one needs to have large number of particles, $n \gg 1$. If, also, the condition $\Gamma \ll nd_0$ is fulfilled, the standard Fermi-Dirac distribution is valid, with a proper shift of the total energy due to the interaction; see Sec. VIII. Typically, this region is associated with the onset of the canonical thermalization (see, for example, Ref. [13]).

In practice, condition IV of the canonical thermalization is not easy to satisfy in realistic systems like atoms or nuclei, since n in the above estimates is, in fact, the number of "active" particles (number of particles in a valence shell) rather than the total number of particles. Thus, the description based on the F distribution (5) which does not require the canonical thermalization condition IV, is more accurate.

The above statements are confirmed by a direct numerical study of the two-body random interaction model [5,8], with few particles when changing the interaction strength V/d_0. If, instead, we increase the number of particles keeping the interaction small, $V \ll d_0$, the distribution (5) tends to the Fermi-Dirac, one as is expected for the ideal gas; see Ref. [8].

Finally, we discuss the transition to mesoscopic systems. One can show that the result strongly depends on the dimensionality d of a system. Let us consider the case when the number of particles n is fixed; however, the size l of a system increases. Then the interval between single-particle energy levels decreases as $d_0 \sim l^{-2}$. Since relative interaction between two particles decreases like $V \sim l^{-d}$, one can obtain $V/d_0 \sim l^{-(d-2)}$. Thus for $d=1$ one has $V \gg d_0$, which means that strong mixing (chaos) starts just from the ground state. This is in accordance with the absence of a gap in the distribution of occupation numbers in the one-dimensional (1D) case (the so-called Luttinger liquid). On the contrary, in the 3D case we have $V \ll d_0$; this means that an admixture of the higher states to the ground state can be considered perturbatively, which is consistent with the nonzero gap at $T=0$. One can see that the transition between regular region (region I)

and the equilibrium (region III) in the 3D case occurs for high states when $V \gtrsim d_f$. Recently, the question of this transition was studied in Refs. [14,15].

X. CONCLUSION

In this paper, we have developed a statistical approach to isolated finite systems of interacting particles, which plays the same role as the canonical approach for systems in equilibrium with the thermal bath. It can be applied to complex many-body systems like compound nuclei, rare-earth or actinide atoms, atomic clusters, quantum dots, etc. The key point of this approach is a partition function which is defined as the shape of compound states (F function) in the many-particle basis of a system without residual interaction (Slater determinants). It allows us calculate mean values of different operators as a function of the total energy E of a system. As an example, we calculated the occupation numbers $n_s(E)$, which may be compared with the standard canonical approach, giving $n_s(T)$, where T is the temperature of an open system. In large systems (thermodynamical limit) the distribution of occupation numbers n_s tends to the canonical distribution with the temperature $T^{-1} = d(\ln \rho)/dE$, where $\rho(E)$ is the energy level density.

Another important area of applications of our approach is the calculation of nondiagonal matrix elements (transition amplitudes) between the eigenstates of complex many-body systems. We would like to point out that the approach can also be used for solving the traditional problem of calculations of mean values of operators in open systems of interacting particles in the thermostat.

The suggested approach is entirely based on the statistical properties of chaotic compound states which are due to the two-body interaction between the particles. For a relatively strong interaction the number of components of compound states is typically, large, and these components can be treated as random variables, provided the two-body interaction matrix elements are ''complex'' enough.

The essential question is under which conditions the above approach is valid in systems with two-body random interaction. Note that the randomness of the matrix elements itself is not enough for the onset of the equilibrium in the system, since statistical properties of compound eigenstates essentially depend on such parameters as the relative strength of the interaction, excitation energy, number of particles and orbitals (single-particle states participating in the energy exchange), etc. In particular, even if the number of principal components in compound states is large, for insufficiently strong interactions the statistics of the components can be abnormal, leading to huge (non-Gaussian) fluctuations in the structure of the eigenstates. In such a case, there is no equilibrium in the system, and standard statistical description is not valid. In this regime, our numerical data show that the distribution of the occupation numbers strongly fluctuates when slightly changing the total energy of the system. Therefore, the transition to the statistical equilibrium is far from being trivial in systems with finite numbers of interacting particles. However, for larger interaction the fluctuations of the eigenstate component becomes normal (Gaussian), and equilibrium occurs. In this situation the fluctuations of the occupation numbers $n_s(E)$ are relatively small, and the F

function gives a correct result for the isolated finite systems even for small number of interacting particles (provided the number of principal components in the eigenstates is large).

The advantage of our approach, in comparison with direct calculations of complex quantum systems, is that we do not need to diagonalize huge Hamiltonian matrices in order to perform calculations of observables for excited states. Indeed, for a full statistical description of such systems, one needs to know the average shape of the compound states (rather than the eigenstates themselves) and the unperturbed energy spectrum. Therefore, the problem of an analytical description of the shape of eigenstates is the central point in the technical implementation of the approach. One should note that the average shape of eigenstates is the same as that of the local spectral density of states (LDOS), if the interaction is not extremely strong.

For small interaction the shape of the chaotic eigenstates is known to be well described by the Breit-Wigner form. However, in practice, this region is small if the number of particles is not very large. With an increase of the interaction strength, the average shape of the eigenstates (F function) changes from the Breit-Wigner one to that close to the Gaussian with the exponential tails. As we have found (Appendix A), the correct description of the shape requires two essential parameters. The first one is, in fact, the half-width of the F function which is close to the Breit-Wigner half-width, and for weak interaction is given by the Fermi golden rule. Another parameter is defined by the root-mean-square width of the F function, (an effective bandwidth of the Hamiltonian matrix in the energy representation).

In this paper we suggest a phenomenological expression for the F function which is valid in a large region of the interaction strength and other parameters. This expression allows for analytical and numerical calculations of different mean values and transition amplitudes. As one example, we derived analytical expression for the distribution of the occupation numbers $n_s(E)$ in isolated systems of n interacting Fermi particles distributed over m orbitals (we used the simple Gaussian approximation of the F function; see Sec. V).

By making use of the F function, we have also studied the validity of the standard Fermi-Dirac distribution for the description of finite systems of interacting Fermi particles. As was found, the Fermi-Dirac distribution can provide a reasonable approximation for both isolated and open (in the thermal bath) systems. However, the parameters of the Fermi-Dirac distribution have to be redefined by taking into account the increase of the effective temperature which is due to the effects of the interaction. We calculated this increase of the temperature analytically, and compared with the numerical experiments for the two-body random interaction model; the data show very good agreement.

One should stress that our approach gives more accurate result for n_s and has much wider region of the applicability, compared to the Fermi-Dirac distribution. Specifically, it is valid even in the region where the Fermi-Dirac distribution fails; for example, due to the small number of particles.

To conclude, we would like to point out that a similar approach may be also used for classical chaotic systems. Indeed, let us consider the system described by the Hamil-

tonian $H = H_0 + V$, where H_0 is the unperturbed ("simple") Hamiltonian and V stands for "complex" interaction between particles. Assume that we know the distribution for some variable in the system described by H_0, for example, the statistical average for the energy distribution of a single particle $n(\epsilon, E_0)$, where ϵ is the energy of the particle and E_0 is the total energy of the system. Then one can calculate the effect of the interaction V by averaging $n(\epsilon, E_0)$ over the unperturbed energy E_0 using the F function, $n(\epsilon, E) = \int n(\epsilon, E_0) F(E, E_0) dE_0$. Here $F(E, E_0)$ gives the probability of different values of E_0 for a given value of E. As indicated in Ref. [20] and checked numerically in Refs. [21, 22], this classical F distribution coincides with the shape of quantum eigenstates in the semiclassical region which turns out to be very wide. Thus a knowledge of the shape of quantum eigenstates can be used for the classical calculations, and vice versa.

ACKNOWLEDGMENTS

APPENDIX A: STRUCTURE OF CHAOTIC EIGENSTATES AND SPREADING FUNCTION

For practical implementation of the above approach, one needs to know the average shape of compound eigenstates (the F function). One should stress that there is no simple analytical expression valid in a large range on the interaction strength V. For example, the popular Breit-Wigner expression (Lorentzian) is not good for obvious reasons: it has an infinite second moment. The question of an appropriate description of chaotic eigenstates in realistic many-body systems has been studied in detail for a Ce atom [2]. In particular, it was found that good correspondence to the numerical data is given by two phenomenological expressions. The first one is $F(x) \sim \exp(-\sqrt{1 + 4x^2})$, where $x = (E_k - E)/\Gamma$, with E_k as the energy of a basis state $|k\rangle$ and Γ as the effective width of the distribution. This expression is close to the Gaussian at the central part and is exponential in the tails (see similar conclusions in Ref. [13], where a nuclear shell model was studied).

Another expression, which is more convenient for the analytical study, is the so-called "squared" Lorentzian [2]

$$F(E_k - E) \sim \frac{1}{\left[(E_k - E)^2 + \dfrac{\Gamma^2}{4}\right]^2}, \quad E = E^{(i)} + \Delta_1^{(i)}. \tag{A1}$$

Here $\Delta_1^{(i)} \ll \Gamma$ is some small shift (see below) which in the zero approximation can be neglected, and E_k is defined by

$$E_k = H_{kk} = \sum_s n_s^{(k)} \epsilon_s + \sum_{s > p} u_{sp} n_s^{(k)} n_p^{(k)}. \tag{A2}$$

Since the "resonant" dependence $E_k - E^{(i)}$ of the spreading function $F_k^{(i)}$ for not extremely strong interaction is symmetric in indexes i and k, the value of $\Gamma = 2\sqrt{(\Delta E)^2}$ can be expressed in terms of the second moment of F using the following exact relation for the basis components (see Appendix B)

$$(\Delta E)^2 \equiv \sum_i |C_k^{(i)}|^2 (E_k - E^{(i)})^2 = \sum_{p \neq k} H_{kp}^2 \tag{A3}$$

with H_{kp} standing for nondiagonal Hamiltonian matrix elements defined by the residual interaction V. This allows us to find the second moment of the spreading function $F(E)$. For example, in the case of n particles distributed over m orbitals, we have [3]

$$\left(\frac{\Gamma}{2}\right)^2 = \overline{(\Delta E)^2} = \frac{V^2}{4} n(n-1)(m-n)(3+m-n). \tag{A4}$$

Here $V^2 = \overline{|V_{st \to pq}|^2}$ is the mean-squared value of nondiagonal matrix elements of the two-body residual interaction.

Our detailed study of the two-body random interaction model [3,5,8] has revealed that the shape of the eigenfunctions (as well as the local spectral density of states) strongly depends on the relative strength of the interaction. That is, with an increase of the interaction V, the shape of the F function changes its form from the Breit-Wigner one to the nearly Gaussian (see also Ref. [12]). It was found that for small residual interaction the shape of eigenstates has a more complicated form, compared to Eq. (A1), and should be characterized by two different widths. Indeed, the half-width of the F distribution is given by the Fermi golden rule $\Gamma_{BW} = 2\pi v^2/d_f$, where v is the matrix element of the residual interaction coupling a particular basis component with other basis states $|f\rangle$ directly coupled by the two-body interaction, and d_f is the energy spacing between these basis states (see details in Appendix C). On the other hand, there is relation (A4) which defines another width $\Gamma = 2\sqrt{(\Delta E)^2}$ via the second moment. One should stress that these two widths are parametrically different in the interaction, $\Gamma_{BW} \sim V^2$, and $\Gamma \sim V$. There is also the "nonresonant" energy dependence $F \propto \rho^{-1}$ [a slow variation of the F function due to the change of the density of states $\rho(E)$] which should be taken into account. This dependence follows from the estimate $F_{max} \sim N_{pc}^{-1} \sim \Gamma\rho$.

The above arguments allow us to find more universal expression for the spreading function F when $\Gamma_{BW} < \Gamma$ [8],

$$F_k^{(i)} \sim \frac{(\rho_0(E_k)\rho(E^{(i)}))^{-1/2}}{\left[(E_k - E)^2 + \dfrac{\Gamma_1^2}{4}\right]\left[(E_k - E)^2 + \dfrac{\Gamma_2^2}{4}\right]}. \tag{A5}$$

Here we take into account the shift of the maximum of the F function by the relation $E = E^{(i)} + \Delta_1^{(i)}$. The two parameters, Γ_1 and Γ_2 are directly related to the above two widths, $\Gamma_1 = \Gamma_{BW}$ and $\Gamma_2 = \Gamma^2/\Gamma_1$. The value of Γ_2 is found from the

relation $\Sigma_i F_k^{(i)}(E^{(i)}-E_k)^2=\overline{(\Delta E)^2}=\Gamma^2/4$ [see Eq. (A4) and Appendix B] by integration of Eq. (A5) in the approximation $\rho=$const. Here and below we assume that the F function is normalized, $Z=1$. In expression (A4), $\rho_0(E_k)$ is the density of basis (unperturbed) states and $\rho(E^{(i)})$ is the density of compound states. We assume they are smooth functions of the energy, and that this energy dependence is slow in comparison with the ''resonant'' energy dependence on the scale Γ. Symmetric dependence on ρ_0 and ρ has been chosen in order to keep symmetry in indexes k and i in the F function.

For very small V we have $\Gamma_1 \ll \Gamma_2$ (also $\Delta_1^{(i)} \ll \Gamma_1$; see below), therefore, in the central part the F distribution (A5) has the Breit-Wigner shape with the width Γ_{BW}. Concerning the meaning of Γ_2, it is the effective energy band width of the Hamiltonian matrix H, which is due to the two-body nature of the interaction. Indeed, the expression for Γ_2 is given by the estimate

$$\Gamma_2=\frac{\Gamma^2}{\Gamma_{BW}}\approx\frac{d_f}{2\pi}n(n-1)(m-n)(m-n+3)\approx d_0(m-n),$$
$$(A6)$$

which is independent of the interaction strength V. Here we used expression (A5) and the estimate of the average value $d_f \equiv d_0/M_f$ for high excited states (M_f here is the normalized density of those basis states which are directly connected to the chosen state; see details in Appendix C). On the other hand, the typical bandwidth $\Delta_H \equiv 2bd_0$ of the two-body interaction Hamiltonian matrix is about four times, $\Delta_H \approx 4(m-n)d_0$, of the energy needed to transfer the particle from the Fermi level $\epsilon_F=nd_0$ to the highest available orbital $\epsilon_m=md_0$. Therefore, the estimate for Γ_2 reads as $\Gamma_2 \approx \Delta_H/4$.

Now, we can easily explain the form of the F function (A5) using the perturbation theory in the interaction V. First, let us consider the energy interval $\Gamma_{BW}<|E_k-E^{(i)}|<\Delta_H$. Within this interval, the basis state $|k\rangle$ can be coupled to the principal components of the state $|i\rangle$ in the first order of V, $|C_k^{(i)}|^2 \sim (V_{ik}/E_k-E^{(i)})^2$. This quadratic decay agrees with the Breit-Wigner shape of the F function. Outside the energy band Δ_H, for $\Delta_H<|E_k-E^{(i)}|<2\Delta_H$, the basis state $|k\rangle$ can be coupled to the principal components of the state $|i\rangle$ in the second order of V, resulting in the dependence $|C_k^{(i)}|^2 \sim (V_{ik}/E_k-E^{(i)})^4$. This corresponds to the tails of the squared Lorentzian shape (A5). Therefore, our expression (A5) seems to be good in a large energy interval, and the second moment is finite which is important for applications. Finally, longer tails are described by higher orders $\nu = |E_k-E^{(i)}|/\Delta_H$ of the perturbation theory,

$$|C_k^{(i)}|^2 \sim \left(\frac{V_{ik}}{E_k-E^{(i)}}\right)^{2\nu}=\exp\left(-\frac{2|E_k-E^{(i)}|}{\Delta_H}\ln\left(\frac{|E_k-E^{(i)}|}{V}\right)\right).$$
$$(A7)$$

This explains the exponential tails of the F function, see details in Ref. [2].

Numerical calculations [2,4,13,12] demonstrate that, for stronger interaction V, the width of the spreading function F rapidly becomes linear in V (instead of the quadratic depen-

dence in Γ_{BW}), and it is better to use Eq. (A1). One can write the extrapolation expression both for small and large values of V (see also Ref. [13]):

$$\Gamma_1=\frac{\Gamma_{BW}\Gamma}{\Gamma_{BW}+\Gamma}.$$
$$(A8)$$

As a result, for small V, we have $\Gamma_{BW} \ll \Gamma$ and $\Gamma_1=\Gamma_{BW} \sim V^2$, and for larger values $\Gamma_1 \approx \Gamma_2 \approx \Gamma \sim V \gg \Delta_1^{(i)}$. The critical value for this transition is given by the relation $\Gamma_{BW}=\Gamma=\Gamma_2 \sim \Delta_H$, and reads as $V_{cr} \approx d_f n(m-n)/(2\pi)$; see also Eq. (A4). The estimate of the average value of $d_f \equiv d_0/M_f$ (see Appendix C) far from the ground state gives $V_{cr} \sim d_0/n$. As discussed in Sec. IX, the equilibrium distribution occurs for $V>d_f$; this results in a quite unexpected conclusion. That is, the validity of the standard Breit-Wigner shape turns out to be very strongly limited since the region $1<V/d_f \ll V_{cr}/d_f \approx n(m-n)/(2\pi)$ is practically absent for small number of particles n and orbitals m.

The shift $\Delta_1^{(i)}$ in Eq. (A5) stands due to the level repulsion which forces eigenvalues $E^{(i)}$ in the lower half of the spectrum to move down. The mean-field energies $E_k=H_{kk}$ do not include the nondiagonal interaction which leads to the repulsion; therefore, the ''center'' of the F function is shifted by the value $\Delta_1^{(i)}=H_{ii}-E^{(i)}$, where H_{ii} is the diagonal matrix element of the Hamiltonian matrix. This shift $\Delta_1^{(i)}$ can be estimated from general arguments. Indeed, the shape of the density of states is the same for both interacting and noninteracting particles [6,7], with the same position E_c of the centers of $\rho_0(E)$ and $\rho(E)$ (due to the conservation of the trace of the Hamiltonian H). However, the variances of ρ_0 and ρ are different. This means that one can use the scaling relation ($D \rightarrow KD$) for the energy intervals D, and find the scaling coefficient K from the relation between the variances, $\sigma^2=\sigma_0^2+\overline{(\Delta E)^2}=K^2\sigma_0^2$, where $\overline{(\Delta E)^2}$ is defined by Eq. (A4). Since the center E_c for the energy-level density $\rho(E)$ does not shift, one can obtain the following shift of the levels:

$$\Delta_1^{(i)}=(E_c-E^{(i)})\left[\left(1+\frac{\overline{(\Delta E)^2}}{\sigma_0^2}\right)^{1/2}-1\right].\quad(A9)$$

The value of $\overline{(\Delta E)^2}$ is typically much less than σ_0^2; therefore, one obtains

$$\Delta_1^{(i)}\simeq(E_c-E^{(i)})\frac{\overline{(\Delta E)^2}}{2(\sigma_0)^2}.\quad(A10)$$

Another way to obtain the shift $\Delta_1^{(i)}$ is related to the exact relation for the first moment of F (see Appendix B),

$$E_k=\sum_i E^{(i)}F_k^{(i)}\approx\int F_k^{(i)}\rho(E^{(i)})E^{(i)}dE^{(i)}.\quad(A11)$$

The substitution of the expression (A5) into Eq. (A11) results in the following value of the shift [8]:

$$\Delta_1^{(i)}\simeq\frac{1}{2}\frac{d(\ln\rho)}{dE}\overline{(\Delta E)^2}.\quad(A12)$$

According to Refs. [6,7] (see also Ref. [11]), the shape of the density of states for $m \gg n \gg 1$ is close to the Gaussian both for noninteracting and interacting particles with E_c and σ_0^2 as the center and the variance of the energy distribution $\rho_0(E)$ [respectively, σ^2 for $\rho(E)$]. In this case relation (A12) gives the same estimate (A9) for the shift $\Delta_1^{(i)}$.

The fact that the two different derivations of the shift $\Delta_1^{(i)}$ lead to the same result is far from being trivial, since the assumptions for the two derivations of $\Delta_1^{(i)}$ are different. Indeed, the second derivation of Eq. (A10) is based on the specific dependence of the eigenstate shape on the densities ρ_0 and ρ, unlike the general derivation of Eq. (A9). One should stress that the specific form of the ''resonant'' energy dependence of the F function (the denominator in Eq. (A5) defined by the squared Lorentzian, Gaussian, etc.) is not important for Eq. (A12) provided $\overline{(\Delta E)^2}$ is fixed. The only assumption in the above derivation is the possibility to expand the density $\rho(E)$ near the maximum of the F function. In fact, above we have demonstrated that the nonresonant ''distortion'' factor $\xi \equiv (\rho_0(E_k)\rho(E^{(i)}))^{-1/2}$ in (A5) is necessary.

Thus, the phenomenological expression for the shape of the F function (A5) is self-consistent. Note that one can use other expressions for the F function (see, for example, Ref. [12]); however, it should contain both the resonance term depending on $E_k - E^{(i)}$ and the density distortion factor ξ.

APPENDIX B: MOMENTS OF THE F FUNCTION AND ENERGY SPECTRUM

Here we calculate the first and the second moments of the function $F_k^{(i)}$ over the perturbed spectrum $E^{(i)}$. Note that the dependence of $F_k^{(i)}$ on the energy $E^{(i)}$ is known as the local spectral density of states (LDOS), or the ''strength function.'' On definition,

$$\langle E^{(i)} \rangle_k = \sum_i E^{(i)} F_k^{(i)} \approx \sum_i |\langle k|i \rangle|^2 E^{(i)}$$

$$= \sum_{i,j} \langle k|i \rangle \langle i|H|j \rangle \langle j|k \rangle = H_{kk} = E_k, \quad \text{(B1)}$$

where the relation $\langle i|H|j \rangle = \delta_{ij} \langle i|H|i \rangle$ is used for the exact eigenstates. The variance can be obtained using the matrix elements of H^2,

$$\overline{(\Delta E)_k^2} = \sum_i F_k^{(i)} (E_k - E^{(i)})^2 \approx \sum_i |C_k^{(i)}|^2 (E_k - E^{(i)})^2$$

$$= \sum_{p \neq k} H_{kp}^2. \quad \text{(B2)}$$

For example, in the two-body random interaction model with n particles distributed over m orbitals the sum in Eq. (B2) can be evaluated exactly [see Eq. (A4)].

Now, we calculate the first moment and variance of the energy spectrum. The trace conservation of H gives the first moment,

$$E_c = \frac{1}{N} \sum_k H_{kk} - \left(\frac{1}{N} \sum_k H_{kk} \right)^2.$$

The conservation of $\mathrm{Tr} H^2$ gives

$$\overline{E^2} = \frac{1}{N} \sum_k \langle k|H^2|k \rangle = \frac{1}{N} \sum_{k,p} |H_{kp}|^2,$$

which results in the relation

$$\sigma^2 \equiv \overline{E^2} - E_c^2 = \frac{1}{N} \sum_{p,k} H_{pk} H_{kp} - E_c^2$$

$$= \frac{1}{N} \sum_k H_{kk}^2 + \frac{1}{N} \sum_{p \neq k} H_{pk}^2 - E_c^2$$

$$= \frac{1}{N} \sum_k E_k^2 - E_c^2 + \frac{1}{N} \sum_k \overline{(\Delta E)_k^2} = \sigma_0^2 + \overline{(\Delta E)^2},$$

where σ_0^2 is the variance of the unperturbed spectrum, and we used Eq. (B2).

APPENDIX C: CALCULATIONS OF SPREADING WIDTHS

To start with, we stress that there are different definitions of the spreading widths. One of the natural definitions is $\Gamma_k \equiv 2\sqrt{\overline{(\Delta E)_k^2}}$ where $(\Delta E)_k^2$ is the variance of the distribution of the components $F_k^{(i)}$ [see Eq. (B2)]. In Ref. [3] it was shown that in the model of random two-body interaction this quantity is constant, $\Gamma_k = \Gamma$ [see Eq. (A5)], i.e., it does not depend on a particular basis state (therefore, on excitation energy, number of excited particles n^* corresponding to this state, etc.). Note that it has a linear dependence on the interaction strength V.

Unlike the latter, the commonly used definition of the spreading width is related to the Breit-Wigner distribution, and is defined as its half-width Γ_{BW}. However, this definition is reasonable only for relatively small interaction, when the form of the F function is indeed close to the Breit-Wigner form. In this case, the spreading width is given by the Fermi golden rule

$$\Gamma_{\mathrm{BW}}^{(k)} = 2\pi \frac{\overline{V_{kf}^2}}{d_f}, \quad \text{(C1)}$$

where d_f is the mean spacing between corresponding basis states $|f\rangle$, and V_{kf} is the matrix element of the interaction between the basis states $|k\rangle$ and $|f\rangle$ [18]. As one can see, the spreading width $\Gamma_{\mathrm{BW}}^{(k)}$ is proportional to V^2 and differs from Γ. Note that the second moment of the Breit-Wigner shape diverges; however, its actual form always has a cutoff in the tails which is reflected by the finite value of Γ.

If the interaction V is not small, the form of the F function significantly differs from the Breit-Wigner shape (see Appendix A). The critical value of V for this transition can be estimated from the condition $\Gamma_{\mathrm{BW}}^{(k)} \approx \Gamma_k$.

Contrary to the spreading width Γ, the half-width of the Breit-Wigner shape depends on the basis state $|k\rangle$. Let us start with the estimate of the mean value of the spreading width $\Gamma_{\mathrm{BW}}^{(k)}$. According to definition (C1), one needs to cal-

culate the density of squared transition matrix elements $\overline{V_{kf}^2}/d_f=(\Sigma_f V_{kf}^2)/\Delta$, where the sum is taken over transitions from a given basis state $|k\rangle$ to other basis states $|f\rangle$ in the energy interval Δ. One should stress that the number of "allowed" transitions (due to the two-body interaction) is much less than the total number of basis states in this interval Δ. Let us assume, for simplicity, that the spacings d_0 between single-particle energy levels is constant, and consider a pair of particles which occupy the orbitals s and q. If we move one particle to a higher orbital and another particle to a lower orbital by the same energy interval, the total energy of particles does not change. The total number of such moves is $M\approx[\min(m-s,q)+\min(m-q,s)]/2$, where $m\gg1$ is the number of orbitals. By averaging over all values s and q, one can obtain $M\approx m/3$. The Pauli principle reduces the number of available orbitals; therefore, in the system with n particles we have $M\approx(m-n)/3$. The number of possible pairs is given by $n(n-1)/2$, thus, the total number of basis states $|f\rangle$ which have the same energy and connected with the chosen basis state $|k\rangle$ is defined by

$$M_f\approx(m-n)n(n-1)/6. \tag{C2}$$

Other basis states are separated by, at least, the energy distance d_0. As a result, we obtain

$$\langle\Gamma_{\mathrm{BW}}\rangle\approx2\pi M_f\frac{V^2}{d_0}\approx\frac{\pi}{3}(m-n)n(n-1)\frac{V^2}{d_0}. \tag{C3}$$

It is interesting to note that the simple estimate involving the total strength of transitions $\overline{(\Delta E)^2}$ [see Eq. (A4)] divided by the bandwidth $\Delta\sim d_0(m-n)$ gives a close result. The above estimate (C3) can be used when studying the shape of the F function in the regime of weak interaction. Note that the value of M_f, defining the mean spacing between the "allowed" final states, is

$$d_f=d_0/M_f. \tag{C4}$$

One should stress that the above estimate of M_f has been obtained for the spreading width averaged over all basis states. Near the ground state, the actual value of M_f is much smaller due to the limitation of the available phase space. Also, the spreading width depends on the number of excited particles in the basis state. For example, one can calculate the spreading width Γ_{BW}^1 of the basis states with one excited particle only,

$$M_f=(s-n)^2, \quad \Gamma_{\mathrm{BW}}^1\approx\pi\frac{(s-n)^2 V_0^2}{d_0} \quad \text{for } s\lesssim2n, \tag{C5}$$

$$M_f=n(2s-3n), \quad \Gamma_{\mathrm{BW}}^1\approx\pi\frac{n(2s-3n)V_0^2}{d_0} \quad \text{for } s>2n. \tag{C6}$$

Here s is the position of a particle corresponding to the energy $\epsilon_s\approx sd_0$.

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[18] We would like to point out that an alternative definition involves exact eigenstates $|i\rangle$ (instead of basis state $|f\rangle$) of the Hamiltonian matrix with the excluded basis state $|k\rangle$ (see, for example, Refs. [19,4]); for small interaction, this definition gives the same result.

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