

Distribution of occupation numbers in finite Fermi systems and role of interaction in chaos and thermalization

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A method is developed for calculation of single-particle occupation numbers in finite Fermi systems of interacting particles. It is more accurate than the canonical distribution method and gives the Fermi-Dirac distribution in the limit of large number of particles. It is shown that statistical effects of the interaction are absorbed by an increase of the effective temperature. Criteria for quantum chaos and statistical equilibrium are considered. All results are confirmed by numerical experiments in the two-body random interaction model. [S1063-651X(97)50901-9]

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When studying numerous problems related to many-body compound states one needs to know whether the laws of statistical physics can be used in the description of a particular quantum system with a finite number of interacting particles (nucleus, atom, etc.). The aim of the present work is to develop an accurate method for the calculation of occupation numbers (and other statistical average values) in finite isolated systems and compare the results with the Fermi-Dirac (FD) distribution. The latter is *a priori* valid in infinite systems of noninteracting particles. We show that the accuracy of the FD distribution in finite systems of interacting particles can be improved by introduction of the effective temperature which absorbs statistical effects of the interaction.

For finite systems of interacting Fermi particles the occupation numbers n_s of single-particle orbitals can be found if we know the expansion of exact eigenstates $|i\rangle$ in terms of Slater determinants (“shell model states”)

$$n_s = \langle i | \hat{n}_s | i \rangle = \sum_k |C_k^{(i)}|^2 \langle k | \hat{n}_s | k \rangle, \quad (1)$$

$$|i\rangle = \sum_k C_k^{(i)} |k\rangle, \quad |k\rangle = a_1^\dagger \cdots a_n^\dagger |0\rangle \quad (2)$$

Here, $\hat{n}_s = a_s^\dagger a_s$ is the occupation number operator.

If the residual interaction between the particles is strong enough, the expansion (2) can be treated as a “chaotic” superposition of the basis states $|k\rangle$. In this case mean square values of the expansion coefficients are smooth functions of the energy difference between the energy E_k of the basis state $|k\rangle$ and the energy $E^{(i)}$ of the exact state $|i\rangle$, $|C_k^{(i)}|^2 \equiv F_k^{(i)} = F^{(i)}(E_k - E^{(i)})$.

In numerical studies of the Ce atom [1], the *s-d* nuclear shell model [2] and random two-body interaction model [3,4] it was demonstrated that typical shape of exact eigenstates (“spreading function”) $F_k^{(i)}$ practically does not depend on a particular system and has a universal form characterized by the spreading width Γ . For example, for the Ce atom [1] the squared Breit-Wigner shape of $F_k^{(i)}$ has been found in a good agreement with numerical data, $F_k^{(i)} \propto [(E_k - E^{(i)} - \Delta_1^{(i)})^2 + \Gamma^2/4]^{-2}$, where $\Delta_1^{(i)} \ll \Gamma$ is a small shift (see below), which in the zero approximation can be neglected.

The value of $\Gamma = 2[(\overline{\Delta E})^2]^{1/2}$ can be found using the following relations for the spreading width of basis components:

$$\overline{(\Delta E)_k^2} \equiv \sum_i |C_k^{(i)}|^2 (E_k - E^{(i)})^2 = \sum_{p \neq k} H_{kp}^2, \quad (3)$$

with H_{kp} standing for nondiagonal Hamiltonian matrix elements defined by residual interaction V . For example, in the model of n particles distributed over m orbitals we have [3] $(\Gamma/2)^2 = \overline{(\Delta E)^2} = V_0^2 n(n-1)(m-n)(3+m-n)/4$. Here $V_0^2 = |V_{st \rightarrow pq}|^2$ is the mean square value of two-body residual interaction matrix elements.

Thus, we can rewrite Eq. (1) in the form of the “ F distribution” which gives the actual distribution of occupation numbers in finite Fermi systems,

$$n_s(E) = \frac{\sum_k n_s^{(k)} F(E_k - E)}{\sum_k F(E_k - E)}, \quad (4)$$

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

where $n_s^{(k)} \equiv \langle k | \hat{n}_s | k \rangle$ equals 0 or 1, ϵ_s are the energies of single-particle orbitals, and $u_{sp} = V_{sp \rightarrow sp}$ is the diagonal matrix element of residual interaction. In practice, the second term in the definition of E_k can be substantially reduced by an appropriate choice of the mean field. The denominator in Eq. (4) stands for the normalization of the F distribution. This “microcanonical” distribution is convenient for numerical calculations.

It is instructive to compare the F distribution (4) with occupation numbers obtained by making use of the standard canonical distribution,

$$n_s(T) = \frac{\sum_i n_s^{(i)} \exp(-E^{(i)}/T)}{\sum_i \exp(-E^{(i)}/T)}, \quad (5)$$

where T is the temperature. The difference between Eqs. (4) and (5) is that the summation in Eq. (4) is performed over simple basis states while in the canonical distribution the summation is carried out over exact eigenstates. Another difference is that in Eq. (4) the occupation numbers are calculated for a specific energy E of system unlike specific tem-

perature T in Eq. (5). However, Eqs. (5) and (4) can be compared with each other by setting $E = \langle E \rangle_T$.

It is important to demonstrate that the F distribution (4) tends to the standard FD distribution in the limit of large number of particles. By performing explicitly the summation over $n_s = 0$ and $n_s = 1$, the expression (4) can be written in the form

$$n_s(E) = \frac{0 + Z_s(n-1, E - \tilde{\epsilon}_s)}{Z_s(n-1, E - \tilde{\epsilon}_s) + Z_s(n, E)}. \quad (6)$$

Here, the partition function is introduced, $Z_s(n, E) = \sum_k F(E_k - E)$, where the summation is taken over all states of n particles with the orbital s excluded. 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; this sum appears from the terms for which the orbital s is filled ($n_s = 1$). For such states one can write $E_k(n) = \tilde{\epsilon}_s + E_k(n-1)$, where $E_k(n-1)$ is the energy of the basis state with $n-1$ particles and $\tilde{\epsilon}_s = \epsilon_s + \sum_{p \neq s} u_{sp} n_p^{(k)}$. Note that to add the energy $\tilde{\epsilon}_s$ to $E_k(n-1)$ is the same as to subtract it from E because $F = F(E_k + \tilde{\epsilon}_s - E)$.

By taking $\tilde{\epsilon}_s$ independent of k we assume the averaging over the basis states near the energy E is possible. The number of terms N in the partition function Z_s is exponentially large, $N = m!/(m-n)!n!$, therefore, one should consider $\ln Z_s$, which has slow dependence on n . In the case of a large number of particles one can get $\ln Z_s(n - \Delta n, E - \tilde{\epsilon}_s) = \ln Z_s(n, E) - \alpha_s \Delta n - \beta_s \tilde{\epsilon}_s$, where $\alpha_s = \partial \ln Z_s / \partial n$; $\beta_s = \partial \ln Z_s / \partial E$; $\Delta n = 1$. This leads to the ‘‘FD’’ type of the distribution,

$$n_s = [1 + \exp(\alpha_s + \beta_s \tilde{\epsilon}_s)]^{-1}. \quad (7)$$

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 $\alpha_s = \alpha \equiv -\mu/T$, $\beta_s = \beta \equiv 1/T$. The chemical potential μ and temperature T can be found from the conditions

$$\sum_s n_s = n, \quad \sum_s \epsilon_s n_s + \sum_{s > p} u_{sp} n_s n_p = E. \quad (8)$$

In the case of many noninteracting particles (ideal gas) similar procedure transforms the canonical distribution (5) to the FD distribution (see, e.g., [5]). It is easy to check that the canonical distribution coincides with the FD distribution with a high accuracy even for a very small number of particles, provided the number of effectively occupied orbitals is large (when $T \gg \epsilon$ or $\mu \gg \epsilon$). However, for the fixed total energy E , the temperature T in these two distributions is different. This difference can be explained by the dependence of the parameter α_s on ϵ_s [see Eq. (7)]. Indeed, using expansion $\alpha_s = \alpha(\epsilon_F) + \alpha'(\epsilon_s - \epsilon_F)$ one can obtain the relation between the FD (β_{FD}) and canonical (β) inverse temperatures: $\beta_{\text{FD}} = \beta + \alpha' \epsilon_F$.

Now, we can study the accuracy of the distributions (4), (5), and (7) in the description of realistic quantum systems. As is known, the FD distribution is valid if the gas of particles can be considered as ideal; therefore, when the residual interaction is small enough, $\Gamma \ll \mu \sim n d_0$ or $\Gamma \ll T$ (here d_0 is the mean energy spacing for single-particle states). It is also

assumed that the number of particles is large, $n \gg 1$. However, the equilibrium distribution for occupation numbers arises for much weaker condition, namely, when the number of principal components N_{PC} in exact eigenstates [see Eq. (2)] is large, $N_{\text{PC}} \sim \Gamma/D \gg 1$. In this case the fluctuations of the occupation numbers $\sim N_{\text{PC}}^{-1/2}$. Since the energy interval D for many-body states is exponentially small, it is enough to have relatively weak residual interaction $V_0 \gg D \sim d_0 \exp(-n)$ in order to get the equilibrium distribution.

There are four regions of parameters depending on the strength of interaction and number of particles: (i) ‘‘regular’’ states, $N_{\text{PC}} \approx 1$ for $V_0 < D$; (ii) ‘‘initial chaotization,’’ which is characterized by a relatively large number of ‘‘random’’ principal components, say, $N_{\text{PC}} \sim \Gamma/D \gg 10$; however, the fluctuations are still large, $N_{\text{PC}}^{-1/2} \gg 0.1$; (iii) equilibrium F distribution (4), which is characterized by small fluctuations, $N_{\text{PC}}^{-1/2} \ll 1$ or $N_{\text{PC}} \sim \Gamma/D \gg 100$; in this case components of eigenstates can be treated as random variables with the variance F and the Eq. (4) gives actual distribution of the occupation numbers in quantum systems with interacting particles; (iv) canonical distribution (5), which arises in the case of equilibrium plus large number of particles. If, in addition, the condition $\Gamma \ll n d_0$ is fulfilled, the standard FD distribution is valid.

In practice, the condition (iv) of ‘‘thermalization’’ is not easy to satisfy in realistic systems like atoms or nuclei since n in this estimate is, in fact, the number of ‘‘active’’ particles (number of particles in the valence shell) rather than the total number of particles. Thus, the equilibrium F distribution (4), which does not require the thermalization condition (iv) is more accurate.

To test the above statements we have performed a detailed numerical study of the model of two-body random interaction. This model (see details in [3,4]) is described by few parameters: number n of particles, number m of orbitals, and ratio V_0/d_0 of the two-body interaction strength to the spacing between single-particle levels. For very small interaction the eigenstates are ‘‘regular’’ and the occupation number distribution n_s is a strongly fluctuating function even after averaging over a number of close eigenstates; see Fig. 1. With an increase of the interaction keeping the number of particles small, we obtain equilibrium F distribution, which is different from the FD distribution (see below).

If, instead, we increase the number of particles keeping the interaction small, $V_0 \ll d_0$, the distribution (4) tends to the FD one [Fig. 2(a)]. Finally, when the strength of the interaction is beyond the ideal gas approximation, the equilibrium distribution strongly deviates from the standard FD distribution [Fig. 2(b)]. In fact, the latter result happens for a relatively small interaction $V_0 \sim 0.1 d_0$ which, however, results in the large value of spreading width, $\Gamma > d_0$ since Γ increases with the number of particles very fast.

However, the accuracy of the FD distribution can be improved by renormalizing the temperature. The point is that statistical effects of the interaction can be, at least in part, described by introducing an effective temperature, which is greater than that determined from Eq. (8) at $E = E^{(i)}$. Thus, we showed in Ref. [4] that the interaction between particles, which leads to the spreading widths γ of the single-particle

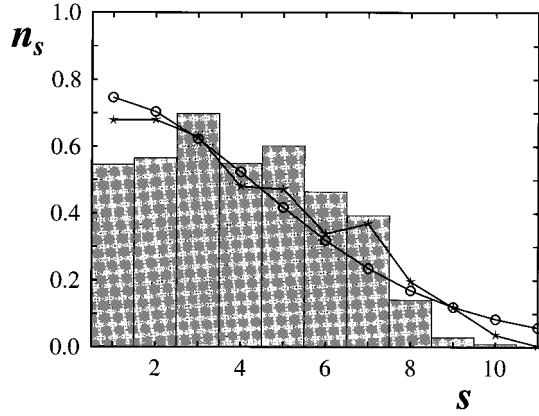


FIG. 1. Distribution of occupation numbers n_s for $n=4$ particles and $m=11$ orbitals for the two-body random interaction model [3,4] with $d_0=1$, weak interaction $V_0=0.04$, and total energy $E=17.33$ (to compare with the ground state energy $E_F \approx 12.1$). Dashed boxes represent numerical data averaged over 20 Hamiltonian matrices of the size $N=330$ with different realization of the random interaction and over the energy range $E \pm \delta E$ with $\delta E=0.25$. Circles correspond to the FD distribution with temperature T and chemical potential μ defined by total number n of particles and total energy E . Stars are given by the F distribution (4) for $n_s(E)$. The number of principal components in exact eigenstates is $N_{\text{PC}} \approx 13$. The latter has been calculated via the inverse participation ratio, $N_{\text{PC}} = [\sum_k F_i^2(E_k - E)]^{-1}$. Large fluctuations $\sim N_{\text{PC}}^{-1/2}$ are seen.

orbitals, can be mimicked by an increase of the temperature, namely, $n_s(\epsilon_s, \gamma, T) \approx n_s(\epsilon_s, \gamma=0, T+\Delta T) \equiv n_s(\epsilon_s, \bar{T})$; for $\gamma \ll T$ one can obtain $\Delta T \approx \gamma^2/48T$. Below we present two stronger arguments. Firstly, we are mainly interested in the eigenstates in the lower half of the spectrum. For them the mean-field energy (8) is substantially higher than the eigenvalue $E^{(i)}$. Indeed, the mean-field energy “does not know” about the effect of level repulsion, which shifts lower eigenvalues downwards (this shift appears in the second-order perturbation theory). Therefore, it is better to estimate E by the unperturbed energy H_{ii} instead of the eigenvalue $E^{(i)}$. Thus, the energy $E = E^{(i)} + \Delta_1^{(i)} \approx H_{ii}$, which is higher than the energy of the eigenstate, should be used in Eq. (8).

Secondly, there is another effect which contributes to the energy shift $\Delta^{(i)}$. The density of states rapidly increases with energy, and the number of higher-energy basis states admitted to the eigenstate is greater than that of the lower-energy basis states (the extreme example is the ground state which is made up of higher basis components only). It is easy to estimate the corresponding increase of the mean-field energy due to this effect if the spreading function $F[E_k - E^{(i)}]$ is symmetric (to separate the two effects we set $\Delta_1^{(i)}=0$ here):

$$\Delta_2^{(i)} = \int F_k^{(i)}(E_k - E^{(i)}) \rho_0(E_k) dE_k \approx \frac{d(\ln \rho_0)}{dE} \overline{(\Delta E)^2}. \quad (9)$$

Here ρ_0 is the unperturbed level density, and $\overline{(\Delta E)^2}$ is given by Eq. (3). According to [7], the shape of the density of states for $m \gg n \gg 1$ is close to Gaussian for both noninteracting and interacting particles, with the center of the spectrum

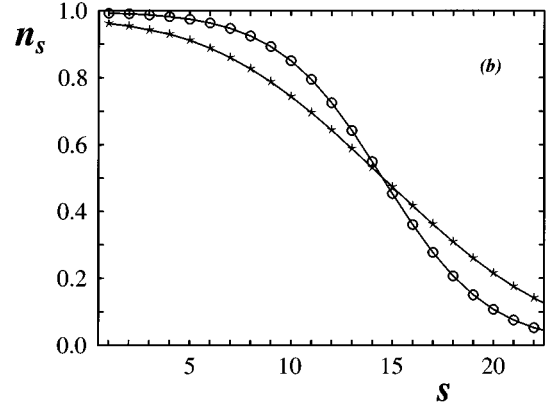
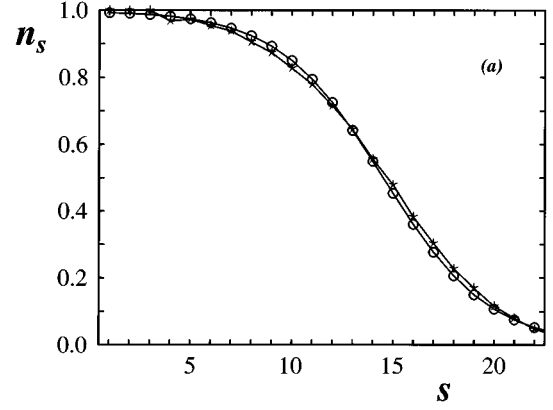


FIG. 2. Distribution of occupation numbers n_s for larger number $n=14$ of particles and $m=28$ of orbitals with the same d_0 and temperature. Direct diagonalization of huge Hamiltonian matrices is not possible in this case. Circles are the FD distribution; stars are the F distribution (4). (a) Weak interaction, $V_0=0.003$, $\Gamma \approx 0.62$, $N_{\text{PC}} \approx 60$. (b) Strong interaction, $V_0=0.08$, $\Gamma \approx 16.6$, $N_{\text{PC}} \approx 11\,000$.

E_c and variances $(\sigma_E)^2$ and $(\tilde{\sigma}_E)^2 = (\sigma_E)^2 + \overline{(\Delta E)^2}$ respectively. Therefore, one can obtain simple estimates of the shifts:

$$\Delta_1^{(i)} \approx (E_c - E^{(i)}) \overline{(\Delta E)^2} / 2(\sigma_E)^2, \quad \Delta_2^{(i)} \approx 2\Delta_1^{(i)}. \quad (10)$$

Taking into account these energy shifts and Eq. (8) one can estimate the increase of the effective temperature of the Fermi gas due to the interaction.

The accurate calculation of this effect requires more detailed knowledge of the spreading function F , including its weak “nonresonant” energy dependence on E_k and $E^{(i)}$. However, the occupation numbers determined by the F distribution (4) are not very sensitive to a particular choice of the spreading function provided the conditions $\sqrt{N_{\text{PC}}} \gg 1$ and Eq. (3) are fulfilled. To check this statement we have considered the form of the spreading function which takes into account important features of the actual distribution $F_k^{(i)}$. If the interaction is small, in the region not very far from the maximum, $F_{\text{max}} \sim D/\Gamma \propto \rho^{-1}$, the spreading function $F_k^{(i)}$ can be described by the Breit-Wigner form with the spreading width $\Gamma_{\text{BW}} = 2\pi V^2/D$ [6]. Also, there is a shift of the maximum due to the repulsion between neighboring levels. These arguments allow us to suggest the improved expression for the spreading function valid for $\Gamma_{\text{BW}} < \Gamma$:

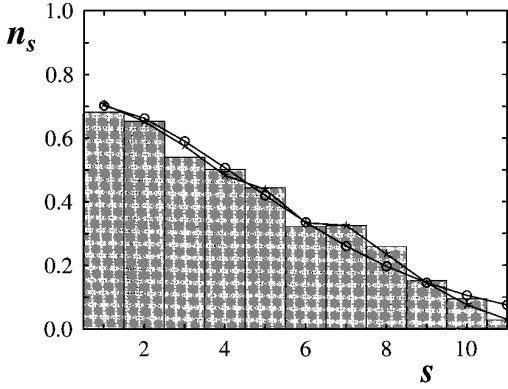


FIG. 3. Distribution of occupation numbers for the Ce atom parameters $n=4, m=11, d_0=1, V_0=0.12, N_{PC} \approx 48$ (boxes) in comparison with the FD distribution, with the corrected temperature (circles) and with the F distribution (stars).

$$F_k^{(i)} \propto \frac{[\rho_0(E_k)\rho(E^{(i)})]^{-1/2}}{\left[(E_k - E)^2 + \frac{\Gamma_1^2}{4} \right] \left[(E_k - E)^2 + \frac{\Gamma_2^2}{4} \right]}, \quad (11)$$

where $E = E^{(i)} + \Delta_1^{(i)}$, $\Gamma_1 = \Gamma_{BW}$, and $\Gamma_2 = \Gamma^2/\Gamma_1$. The value of Γ_2 is found from the exact relation (3). Note that $F_k^{(i)}$ from Eq. (11) automatically satisfies another exact relation, $\sum_i E^{(i)} F_k^{(i)} = E_k$; note that the contribution of the energy shift $\Delta_1^{(i)}$ is compensated by the increase of the level density $\rho(E^{(i)})$.

It follows from Eq. (11) that the energy shift due to the enhanced admixture of higher basis components is two times smaller than in Eq. (9), since the increase of density ρ_0 is partially compensated by the factor $\rho_0^{-1/2}$ in Eq. (11):

$$\Delta_2^{(i)} \approx \frac{d(\ln \sqrt{\rho_0})}{dE} (\Delta E)^2 \approx \Delta_1^{(i)}. \quad (12)$$

Thus, we should substitute the value $E = E^{(i)} + \Delta_1^{(i)} + \Delta_2^{(i)} \approx 2H_{ii} - E^{(i)}$ into Eq. (8). After taking this shift into account the FD expression gives the same result as the F distribution, as shown in Fig. 2(b), where the FD curve (circles) is shifted with respect to that given by stars; both curves also agree with the numerical experiment (Fig. 3).

For small V_0 and a large number of particles we have $\Delta_1^{(i)} \ll \Gamma_1 \ll \Gamma_2$, therefore, in the central part the distribution (11) has the Breit-Wigner shape with the width Γ_{BW} . However, numerical calculations [1,2,8] demonstrate that at larger interaction V_0 the width of the spreading function becomes linear in V_0 and it is better to put $\Gamma_1 = \Gamma_2 = \Gamma$. One

can write the extrapolation expression both for small and large values of V_0 (see also [8]) $\Gamma_1 = \Gamma_{BW}\Gamma/(\Gamma_{BW} + \Gamma)$. We have also checked that for large number N_{PC} of principal components the distribution of the occupation numbers does not depend on Γ_1 ; this fact can be treated as a signature of the equilibrium.

Finally, we discuss the transition to mesoscopic systems. The result depends on the dimensionality d of the system since $d_0 \sim l^{-2}$; $V_0 \sim l^{-d}$, therefore, $V_0/d_0 \sim l^{-(d-2)}$, where l is the size of the system. Thus, for $d=1$ one has $V_0 \gg d_0$, 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 (Luttinger liquid). In the 3D case we have $V_0 \ll d_0$ and the 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 (I) and the initial chaos region II in the 3D case occurs for high states when $V_0 > D \sim d_0 \exp(-n_2^*)$, where $n_2^* \propto E^{1/2}$ is a number of excited particles. On the other hand, the transition from the fluctuating to the equilibrium regime, (II) \rightarrow (III), requires the decrease of D only by one order of magnitude: $n_3^* \approx n_2^* + 2$. This means that such transition in 3D is a very sharp ‘‘phase transition.’’

In conclusion, we developed a method for the calculation of the occupation numbers in finite systems of interacting particles. The method is based on the assumption that exact eigenstates are ‘‘chaotic’’ superpositions of the shell-model basis states, and the smooth spreading function for the eigenstates components can be introduced. This assumption and the results are confirmed by numerical experiments. The ‘‘microcanonical’’ partition function that we have introduced can be used for further studies of statistical and thermodynamic properties of finite systems of interacting particles.

We also demonstrated that occupation numbers in the systems of interacting particles can be reasonably described by Fermi-Dirac distribution with renormalized parameters. As usual, mean field (and possibly other ‘‘regular’’ effects) can be included into single-particle energies $\bar{\epsilon}_s$. Statistical effects of the residual interaction (mainly due to nondiagonal matrix elements of the Hamiltonian matrix) increase effective temperature.

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