Semiquantal Approach to Finite Systems of Interacting Particles

F. Borgonovi,[1,2] G. Celardo,[2] F. M. Izrailev,[3] and G. Casati[4]
[1]*Dipartimento di Matematica e Fisica and I.N.F.M., via Musei 41, 25121 Brescia, Italy*
[2]*I.N.F.N., Sezione di Pavia, via Bassi 6, 27100 Pavia, Italy*
[3]*Instituto de Física, Universidad Autónoma de Puebla, Apartado Postal J-48, Puebla 72570, México*
[4]*International Centre for the Study of Dynamical Systems and I.N.F.N. and I.N.F.N., 22100 Como, Italy*
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A novel approach is suggested for the statistical description of quantum systems of interacting particles. We show that the occupation numbers for single-particle states can be represented as a convolution of a classical analog of the eigenstate, with the quantum occupation number for noninteracting particles. The latter takes into account the wave function symmetry and depends on the unperturbed energy spectrum only. As a result, the distribution of occupation numbers n_s can be found even for a large number of interacting particles. Using the model of interacting spins, we demonstrate that this approach gives a correct description of n_s even in deep quantum regions with few single-particle orbitals.

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In many physical systems, such as complex atoms, heavy nuclei, and interacting spins, highly excited eigenstates in the unpertured many-particles basis, and for a relatively strong interaction among particles, have a large number of components that can be treated as independent random numbers (see, e.g., [1–3]). This randomness allows for a statistical treatment that takes into account only the symmetry of the Hamiltonian and the type of interaction, e.g., two-body. In Refs. [4,5], for instance, a statistical description of closed systems with a finite number of Fermi particles has been developed. In particular, it was analytically shown that, for a strong enough interaction, a smooth dependence of occupation numbers on the energy occurs, which is directly related to the statistical properties of chaotic eigenstates.

As is known, the direct numerical computation of excited eigenstates is a difficult task for a large number of particles. On the other side, the mean values of occupation numbers turn out to depend on the average shape of chaotic eigenstates in the unperturbed basis, not on exact, specific values of their components [5].

In this Letter, we develop a novel approach to quantum systems with chaotic behavior in the classical limit. This approach takes into account both the chaotic properties of the classical system and the specific features of the unperturbed single-particle spectrum. As a result, one can avoid diagonalization of Hamiltonian matrices of huge size which may be practically unfeasible. This kind of approach can be applied to generic Hamiltonian systems with two-body interaction of the type

$$H = H_0 + V; \qquad H_0 = \sum_{i=1}^{N} h_0^i; \qquad V = \sum_{i=1}^{N} \sum_{j=i+1}^{N} V_{i,j}\,. \tag{1}$$

Here H_0 describes N *noninteracting* particles with h_0^i as single-particle Hamiltonians, and V stands for a long-range two-body interaction between the particles. In what follows, we assume that the single-particle spectrum is determined by a finite number L of single-particle energies ϵ_h, $h = 1, \ldots, L$; however, the approach is valid for more generic systems with an infinite spectrum.

The unperturbed Hamiltonian H_0 determines the many-particle states $|K\rangle = a_{s_1}^\dagger \ldots a_{s_N}^\dagger |0\rangle$ (with $a_{s_j}^\dagger$, a_{s_j} as creation-annihilation operators) that form the basis in which the exact eigenstates of H are represented. As usual, we assume that the basis is ordered according to increasing unperturbed energy values $E_0 = \sum_{h=1}^{L} \epsilon_h n_h$, n_h being the number of particles with energy ϵ_h.

The distribution of occupation numbers (DON) for single-particle states is defined by the relation

$$n_E(h) = \sum_{K=1}^{M} \langle K|\hat{n}_h|K\rangle\, |\psi_K^E|^2, \tag{2}$$

where $\hat{n}_h = a_h^\dagger a_h$ is the occupation number operator giving the occupation numbers $n_h^K = \langle K|\hat{n}_h|K\rangle$ equal to 0 or 1 for Fermi particles, and to $0, 1, 2, \ldots, N$ for Bose particles. These numbers n_h^K indicate how many particles in a many-particle *basis* state $|K\rangle$ occupy a particular single-particle state $|h\rangle$. Correspondingly, the occupation numbers $n_E(h)$ give the probability that one of the N particles in a many-particle *exact* state with the *total* energy E occupies a particular single-particle state $|h\rangle$. The total number M of many-body states equals $M = L!/[N!(L-N)!]$ for Fermi and $M = (N+L-1)!/[N!(L-1)!]$ for Bose particles.

One should note that while, in the above expression for the DON, the components of the eigenfunctions ψ_K^E depend on the total Hamiltonian H, the term n_h^K depends on the unperturbed spectrum only. This fact is crucial for our semiquantal approach. Because of the chaotic structure of exact eigenstates, one can make an average of the DON over a small energy window ΔE around the fixed value E. This averaging procedure is similar to that used in the conventional statistical mechanics developed for systems with

a finite number of particles in contact with a heat bath, or for isolated systems of an *infinite* number of *noninteracting* particles.

Expression (2) for the mean values $n_E(h)$ can be considerably simplified by introducing the so-called *shape of eigenfunctions* (SE) (envelope of eigenstates in energy representation). The form of the SE has been studied in detail both in the model with random two-body interaction [5] and in dynamical models of interacting particles [6–8]. The introduction of the average quantity SE (thus neglecting correlations between different components ψ_K^E) represents the key point of our approach.

We assume that the unperturbed many-body energy spectrum has an intrinsic degeneracy. This situation is typical for spin systems, and is more complicated in comparison with those studied previously [6,7]. Below we show how this difficulty can be overcome. Let us redefine the state $|K\rangle$ by means of an indices pair $|j,l\rangle$, where j labels the "unperturbed energy" E_j^0 of the many-body state, while $l = 1,\ldots,N_j$ labels its degeneracy N_j. If there are N_0 different "unperturbed" energies, one can write $\sum_{K=1}^{M} = \sum_{j=1}^{N_0}\sum_{l=1}^{N_j}$; therefore, one has

$$n_E(h) = \sum_{j=1}^{N_0}\sum_{l=1}^{N_j}\langle j,l|\hat{n}_h|j,l\rangle\,|\psi_{j,l}^E|^2. \tag{3}$$

According to Ref. [7], the SE is given by

$$W_E(E_j^0) = \sum_{l=1}^{N_j}|\psi_{j,l}^E|^2. \tag{4}$$

By substituting $|\psi_{j,l}^E|^2 \simeq \langle|\psi_{j,l}^E|^2\rangle_l = W_E(E_j^0)/N_j$ with $\langle\cdots\rangle_l$ as an average over l, we obtain an approximate expression for the DON in terms of the SE:

$$n_E(h) = \sum_{j=1}^{N_0}\frac{1}{N_j}\sum_{l=1}^{N_j}\langle j,l|\hat{n}_h|j,l\rangle W_E(E_j^0). \tag{5}$$

Needless to say, if an unperturbed spectrum has no degeneracy, Eq. (5) can be written in a similar way by taking an average over a small window of energy around E_j^0.

As one can see, expression (5) depends on two terms of different nature. The first one, $\langle j,l|\hat{n}_h|j,l\rangle$, refers to the unperturbed many-particle spectrum and reflects the specific properties of a single-particle spectrum, as well as quantum features related to Fermi-Dirac or Bose-Einstein statistics. In contrast, the second term, $W_E(E_j^0)$, refers to global properties of eigenstates and describes *interaction* effects. Therefore, the basic idea of our "semiquantal" approach is to substitute the latter term (SE) by its classical analog which can be easily found from classical equations of motion.

Classical analogs of the SE have been studied in different models; see, for example, [6–8]. In practice, one has to derive the distribution $W_E(E_0) = P(H_0 = E_0|H = E)$ for the probability to find the unperturbed energy E_0 for H_0, given the conserved total energy E. This can be obtained by generating many different initial classical configurations on the energy surface $H = E$ or sampling the $H_0(t)$ values generated by one single trajectory onto the energy surface and computing the correspondent distribution of $H_0 = E_0$ [9]. The two procedures have been found to give the same results in the chaotic region [8]. In order to facilitate the comparison with the quantum SE, in our numerical simulations the bin size of E_0 equals the energy distance between neighbor values of E_j^0. In the same way, one can define the classical distribution of occupation numbers, $n_E(h) = P(h_0^i = h|H = E)$ (see also [8]). For the quantum-classical comparison, the bin size of h is taken to be equal to the spacing between close single-particle energy levels ϵ_h.

Let us stress that in this semiquantal approach (SA) it is possible to study specific systems of, for example, 1000 interacting particles occupying 10–20 single-particle levels. Surely, one expects this approach to be valid for highly excited chaotic states. However, by direct numerical simulations, we have found that the SA gives correct results even for energy values close to the ground state.

Our model consists of N 3D interacting spins placed in a magnetic field B directed along the z axis. In order to have a proper many-body operator, one should require a coupling between *all spins* (not only between neighbors). The Hamiltonian thus reads

$$H = B\sum_{i=1}^{N}S_i^z + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}(J_xS_i^xS_j^x + J_yS_i^yS_j^y + J_zS_i^zS_j^z). \tag{6}$$

This model is known in literature as the anisotropic Heisenberg model in a magnetic field with an all-to-all spin interaction (infinite range coupling). The case of nearest neighbor coupling has not been taken into account here since it cannot describe a quantum system with the symmetry or the antisymmetry of the global wave function included.

Using the relations $S_j^{\pm} = S_j^x \pm iS_j^y$ and assuming $J_z = 0$, one can write

$$H = B\sum_{i=1}^{N}S_i^z + \frac{1}{4}(J_x - J_y)\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}[S_i^+S_j^+ + S_i^-S_j^-] + \frac{1}{4}(J_x + J_y)\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}[S_i^+S_j^- + S_i^-S_j^+]. \tag{7}$$

The interaction can be further simplified by the particular choice $J_x = -J_y = J$ and $B = 1$. Thus, our Hamiltonian $H = H_0 + V$ has the following form:

$$H = \sum_{i=1}^{N}S_i^z + \frac{J}{2}\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}[S_i^+S_j^+ + S_i^-S_j^-]. \tag{8}$$

For simplicity, the N classical constants of motion $|\vec{S}_i|$ have been set to 1; therefore, the only free classical parameters are the total conserved energy E and the interaction J. The classical model has been studied in [8] and it was numerically found to be chaotic and exponentially unstable in a wide energy range. More precisely, in order to have strong chaos, one needs the interaction J between particles to be strong enough. A convenient choice is to take the interaction strength $J = 1/N$. One should stress that this situation is the most difficult for theoretical studies; see discussion in [8].

Quantization follows the standard rules: $S_i^2 = \hbar^2 m(m+1)$ and $S_i^z = \hbar s$ with $-m \le s \le m$, and creation and annihilation operators are defined by

$$S_i^{\pm}|\ldots, s_i, \ldots\rangle = \hbar\sqrt{m(m+1) - s_i(s_i \pm 1)} \times |\ldots, s_i \pm 1, \ldots\rangle,$$

where $|s_1, \ldots, s_N\rangle$ are the nonsymmetrized states (first quantization states).

There are $L = 2m + 1$ single-particle energy levels $\epsilon_h = -\hbar h$ with $h = -m, \ldots, m$. Therefore, the unperturbed many-particle energy spectrum consists of a number of degenerate levels with the spacing equal to $\hbar$. Note that both the ground state $E_g = -mN\hbar$ and the upper level $E_u = mN\hbar$ are nondegenerate. The classical limit is recovered when spins are allowed to have any possible orientation, that is, $m \to \infty$ and $\hbar \to 0$.

The choice we have made ($J_x = -J_y = J$) allows us to reduce the dimension of the Hilbert space by, approximately, one-half. This happens because the operator V in Eq. (8) connects only those unperturbed many-body states that are separated by the spacing $2\hbar$. In what follows, we consider the subset of the many-body states containing the ground state. From these states we construct the completely symmetrized states $|s_1, \ldots, s_N\rangle^S = |n_{-m}, \ldots, n_m\rangle$, where the right-hand side refers to their second quantization representation. Note that for the symmetrized states the distribution of occupation numbers is expected to be described, for a large number of particles, by the Bose-Einstein statistics.

In second quantization Eq. (8) can be written as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{V}; \qquad \mathcal{H}_0 = \sum_{h=-m}^{m} \epsilon_h \hat{n}_h, \qquad (9)$$

with

$$\mathcal{V} = \sum_{h=-m}^{m-1} \eta_h \hat{a}_{h+1}^{\dagger}\hat{a}_{h+1}^{\dagger}\hat{a}_h\hat{a}_h + \sum_{h=-m}^{m-2} \xi_h \hat{a}_{h+2}^{\dagger}\hat{a}_h .$$

Here $\hat{n}_h = \hat{a}_h^{\dagger}\hat{a}_h$, with $\hat{a}_h^{\dagger}$ and $\hat{a}_h$ the creation-annihilation operators satisfying the standard relation $[\hat{a}_h, \hat{a}_k^{\dagger}] = \delta_{hk}$. As for the coefficients η_h, ξ_h, they can be easily computed numerically.

The procedure we have used in our numerical simulations consists of the following steps: (i) compute the classical values $n_E(h)$ and $W_E(E_0)$ as described above; (ii) compute the quantum values $n_E(h)$ and $W_E(E_0)$ by diagonalization of the total Hamiltonian (9); (iii) compute $n_E(h)$ and $W_E(E_0)$ by using the semiquantal approximation according to expression (5).

The results for the DON are summarized in Fig. 1. For the sake of comparison, symbols refer to the quantum and SA results, while the classical data are presented as histograms. Note that the energy of each particle belongs to the interval $[-1, 1]$. In order to make the quantum-classical comparison as close as possible, we took the classical bin size equal to $\hbar$. All distributions have been normalized in such a way that $\sum_{h=-m}^{m} n_E(h) = N$. In cases 1(a) and 1(b), we choose the same energy, close to the ground state but two different m values. Instead, in 1(c) and 1(d), we take a higher energy value that corresponds to a more classical situation. One can see that while classical and quantum data disagree only in the *deep* quantum region 1(a) [energy close to the ground state and small m (*big* $\hbar$)], there is a very nice correspondence between quantum and SA data in all cases.

These results confirm our expectation that for excited chaotic states correlations inside eigenstates as well as between the two different terms in Eq. (5) can be indeed neglected. Remarkably, we have found that our approach works well for very low energy states that are definitely nonchaotic. We explain this phenomenon by the fact that in this case most of the probability is concentrated in a single many-body state, and, therefore, correlations are practically absent. On the other side, a problem could arise in an intermediate situation when eigenstates have many components but they are not chaotic. For instance, for $N = 10$,

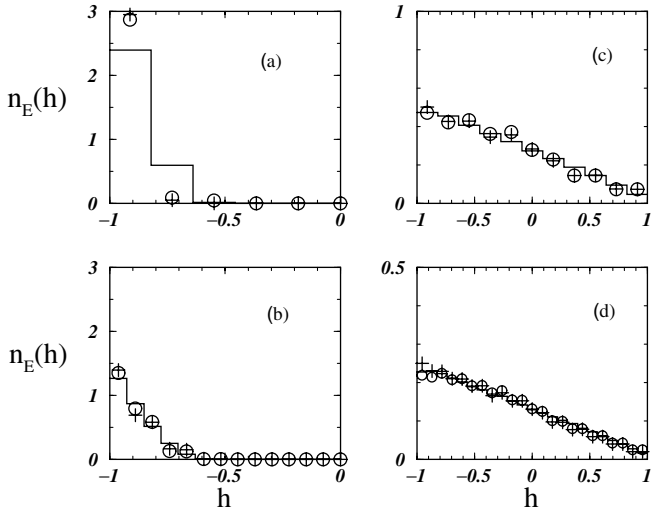

FIG. 1. Occupation number distribution obtained in three different ways. Crosses correspond to the quantum data, open circles stand for the SA approach, and histograms refer to the classical quantities. The data are given for three interacting particles: (a) $E = -2.75$, $\Delta E = 0.15$, $m = 5$; (b) $E = -2.75$, $\Delta E = 0.15$, $m = 13$; (c) $E = -0.91$, $\Delta E = 0.09$, $m = 5$; and (d) $E = -0.91$, $\Delta E = 0.09$, $m = 11$.

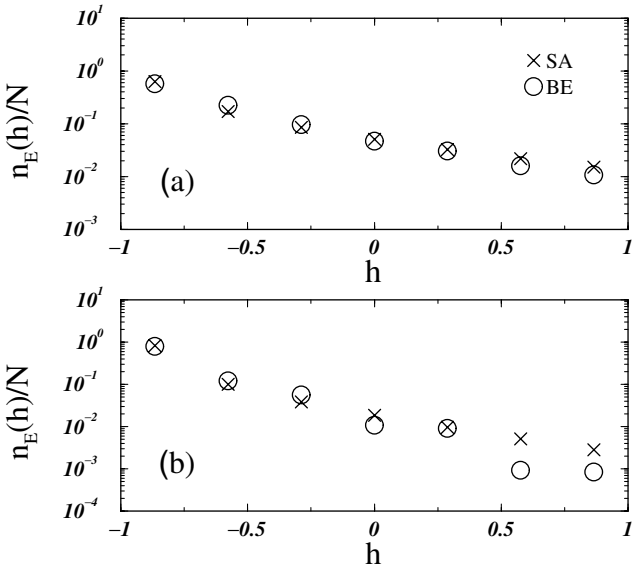

FIG. 2. Distribution of occupation numbers for $N = 10$ particles. Open circles indicate the BE distribution while crosses stand for the SA data: (a) $E = -8$, $\Delta E = 0.2$, $m = 3$; (b) $E = -6.5$, $\Delta E = 0.2$, $m = 13$.

$m = 3$, $J = 0.2$, and $E = -6.5$, the agreement between the SA and quantum data was found to be less accurate than for the ground state.

It is very interesting to explore the occurrence of the Bose-Einstein (BE) distribution in our model. A similar problem has been studied in detail for the model of two-body random interaction [5] where the conditions for the appearance of Fermi-Dirac distribution have been found for few interacting Fermi particles.

By assuming, *a priori,* the validity of the BE distribution $n_E^{\mathrm{BE}}(i) = [e^{\beta(\epsilon_i - \mu)} - 1]^{-1}$ in our closed system, one can find the "temperature" $1/\beta$ and the "chemical potential" μ via the standard relations,

$$\sum_{i=-m}^{m} n_E^{\mathrm{BE}}(i) = N; \qquad \sum_{i=-m}^{m} n_E^{\mathrm{BE}}(i)\epsilon_i = E'. \qquad (10)$$

Here E' is the numerically computed energy obtained from the single-particle quantum distribution (see details in [10]), and N is the number of particles. Notice that, due to interaction, $E' \neq E$.

The comparison between BE and SA distributions is shown in Fig. 2. As one can see, even for relatively small $N = 10$, the distribution $n_E(h)$ is closely approximated by the BE distribution. This confirms the expectation that a strong enough interaction between particles plays the role of an internal heat bath [5]. Therefore, the standard quantum distribution can be used, with a corresponding renormalization of the energy E' (see [5]).

We stress that an exact quantum treatment of the last example calls for a diagonalization of a huge matrix of size 8008×8008, while, with the semiquantal approach, all computations required few minutes on a standard portable personal computer.

In conclusion, we suggest an effective semiquantal approach to closed systems of interacting particles, based on the chaotic structure of eigenstates. In this approach, the computation of the distribution of occupation numbers can be easily performed by making use of the classical analog of the shape of eigenstates in the unperturbed many-particle basis. We demonstrate the effectiveness of this approach using the model of 3D spins with anisotropic Ising interaction. The data show that semiquantal computations give results which are very close to the exact ones.

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