PHYSICAL REVIEW E **80**, 051130 (2009)

Typical state of an isolated quantum system with fixed energy and unrestricted participation of eigenstates

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(Received 2 March 2009; published 30 November 2009)

This work describes the statistics for the occupation numbers of quantum levels in a large isolated quantum system, where all possible superpositions of eigenstates are allowed provided all these superpositions have the same fixed energy. Such a condition is not equivalent to the conventional microcanonical condition because the latter limits the participating eigenstates to a very narrow energy window. The statistics is obtained analytically for both the entire system and its small subsystem. In a significant departure from the Boltzmann-Gibbs statistics, the average occupation numbers of quantum states exhibit in the present case weak algebraic dependence on energy. In the macroscopic limit, this dependence is routinely accompanied by the condensation into the lowest-energy quantum state. This work contains initial numerical tests of the above statistics for finite systems and also reports the following numerical finding: when the basis states of large but finite random matrix Hamiltonians are expanded in terms of eigenstates, the participation of eigenstates in such an expansion obeys the newly obtained statistics. The above statistics might be observable in small quantum systems, but for the macroscopic systems, it rather re-enforces doubts about self-sufficiency of nonrelativistic quantum mechanics for justifying the Boltzmann-Gibbs equilibrium.

DOI: 10.1103/PhysRevE.80.051130 PACS number(s): 05.30.−d, 03.65.Ta

I. INTRODUCTION

It is known empirically since the introduction of quantum hypothesis by Planck that thermal Boltzmann-Gibbs distribution works extremely well for quantum systems. However, purely quantum derivation of this distribution is still not on a satisfactory ground. In a self-contained derivation one should be able to start from a large isolated system and then obtain the statistical distribution for a small subsystem. The conventional derivation of the Boltzmann-Gibbs distribution proceeds by postulating the microcanonical condition. This condition has different status in classical and quantum mechanics. In classical mechanics the microcanonical condition rests on the further assumption of equipartition on the constant energy shell in the phase space, which in turn can be justified by dynamical chaos caused by nonlinear interactions between particles. In this respect, the classical derivation is in a better shape. In contrast, the quantum systems have no phase space, and also they are fundamentally linear. A typical state of an isolated quantum system is not an eigenstate but a superposition of eigenstates:

$$\Psi = \sum_{i=1}^{N} C_i \phi_i, \qquad (1)$$

where Ψ is the wave function of the superposition, ϕ_i is the wave function of the i-th eigenstate, C_i is the corresponding complex amplitude, and N is the total number of eigenstates. Therefore, the straightforward counterpart of the classical microcanonical condition would be to constrain the possible choices of Ψ to the "energy shell" in the Hilbert space:

$$\sum_{i=1}^{N} E_i p_i = E_{\text{av}}, \qquad (2)$$

where $p_i \equiv |\langle \phi_i | \Psi \rangle|^2 = |C_i|^2$ are the occupation numbers of quantum states and E_{av} is the energy of the quantum superposition set externally and referred to below as "average energy."

Condition (2) is, however, different from the conventional microcanonical condition because the latter involves the summation only over the eigenstates inside a very small energy window $E_{\text{av}} \pm \delta E$.

Why the system should limit itself to a small energy window is difficult to justify unless, for example, one assumes that the quantum system is subjected to an external source of decoherence with the subsequent collapse of the density matrix. However, the introduction of collapse would imply that nonrelativistic quantum mechanics is not self-contained when it comes to justifying the Boltzmann-Gibbs equilibrium. [Here and below Boltzmann-Gibbs equilibrium or Boltzmann-Gibbs statistics refers to the density matrices of the form $\rho = \exp(-\mathcal{H}/T)$, where $\mathcal{H}$ is the Hamiltonian of the system and T is temperature in energy units.]

Besides the conceptual issues, there are also practical ones. When a well-isolated quantum system having not too many particles but many quantum levels is shaken in an experiment and then left to itself, the energy window of the participating eigenstates can easily become larger than the temperature, and then the occupations of eigenstates will not change with time. Would such a system end up exhibiting Boltzmann-Gibbs statistics?

It is clear *a priori* that a significant departure from the narrow-energy-window constraint can easily lead to deviations from the Boltzmann-Gibbs statistics [1]. For example, for two sufficiently separated narrow energy windows, the resulting sum of two exponential Boltzmann-Gibbs distributions does not give a single exponential distribution. Still one can hope that somehow the "most probable departure" from the narrow energy window condition would support the Boltzmann-Gibbs equilibrium.

If one is to begin addressing the above issues, the unavoidable limit to consider is the system of $N \gg 1$ quantum levels with constraint (2) and no limit on the energy window, i.e., all quantum superpositions of form (1) satisfying condition (2) are equally probable and, therefore, the probability density as a function of the complex amplitudes C_i is proportional to the volume element on a manifold in the Hilbert space constrained by Eq. (2). Following Ref. [2], I call this condition "quantum microcanonical" (QMC) to contrast it with the conventional microcanonical condition.

The general approach of assigning the probability on the basis of volume in Hilbert space has received a good degree of attention in recent years. Some of the relevant works [3–6] applied this approach to the conventional microcanonical case with small energy window for the participating eigenstates. Other works, however, have looked at the QMC ensemble [2,7–10] and at the quantum canonical ensemble [2,11]. (The latter is related to the OMC ensemble in the same way as the conventional canonical ensemble is related to the conventional microcanonical one.)

In particular, it was found in Ref. [8] for the QMC ensemble in the system of equally spaced energy levels (and confirmed in the present work for the general level structure) that, as $N \to \infty$, the volume of the Hilbert space as function of E_{av} acquires the character of a δ-function with peak located at $E_{\mathrm{av}} = \frac{1}{N}\Sigma_i E_i$. This result, however, does not imply that it is not important to consider the case of E_{av} different from the above value. The situation here is analogous to the conventional microcanonical description when the most probable position of the narrow energy window would correspond to the infinite temperature, but one would still like to know the result for a finite temperature.

In this work, I obtain the QMC-based statistics for the occupation numbers of individual quantum states both for the entire isolated quantum system (Sec. II) and for the density matrix of a small part of it (Sec. III). In technical terms, it amounts to obtaining marginal probability distributions for the individual occupation numbers from the joint probability distribution associated with the QMC ensemble. It is to be shown analytically that the resulting statistics is dramatically different from the Boltzmann-Gibbs statistics: the occupation numbers of quantum states decay with energy algebraically rather than exponentially, and in addition, the macroscopic limit is routinely accompanied by condensation into the lowest-energy state.

Section IV contains preliminary numerical tests of some of the above results for finite systems. This section also reports a numerical finding that the expansion of the basis states of large but finite random matrix Hamiltonians in terms of the eigenstates of these Hamiltonians obeys the statistics found in this work.

The implications of the analytical and numerical results of this work are to be discussed in the concluding remarks (Sec. V).

The notion of chaos does not play any role in the forthcoming derivation, but it will also be touched briefly in the concluding remarks.

Even though the formal treatment below is based essentially on the geometrical analysis of many-dimensional manifolds, it should not escape the readers that the end result is similar to the Boltzmann-Gibbs distribution for grand canonical ensemble—though not for the average values of the occupation numbers $\langle p_i \rangle$, which the Boltzmann-Gibbs distribution aims at predicting but rather for the probabilities of variable p_i to admit different values. In other words, it is an example of superstatistics [12]—consequence of the fact that the occupation numbers p_i, which are interpreted as quantum probabilities, are themselves subject to the probability distribution.

The readers, who would like to get a quick impression of the main results of this work, should familiarize themselves with the definitions of variables and then look at the paragraph preceding Eq. (19) and at Eqs. (19), (21), (33), (43), (46), (64), (69), (70), (73), and (74) and Figs. 2 and 3.

II. STATISTICS FOR THE EIGENSTATES OF AN ISOLATED QUANTUM SYSTEM

A. Formulation of the problem

The Hilbert space of the problem is parametrizable by the absolute values $|C_i|$ and the phases φ_i of complex coefficients $C_i = |C_i| e^{i\varphi_i}$ in Eq. (1). The QMC condition postulates that the joint probability density of variables $|C_i|$ and φ_i is uniform on the manifold in Hilbert space constrained by energy condition (2) and by the normalization condition $\Sigma_i |C_i|^2 = 1$, i.e., this probability density is proportional to the volume element on the above manifold.

Without the energy and the normalization constraints, the volume element in the Hilbert space is given by

$$dV = \prod_i^N |C_i| d\varphi_i d|C_i| = \frac{1}{2}\prod_i^N d\varphi_i d(|C_i|^2). \tag{3}$$

Both the energy and the normalization constraint do not depend on φ_i. Therefore, the marginal distributions of individual phases φ_i are completely uniform and can be integrated out as "not interesting," leaving one only with the subspace of amplitudes $|C_i|$.

One can now change variables from amplitudes $|C_i|$ to "occupation numbers" p_i according to

$$p_i = |C_i|^2 \tag{4}$$

and then re-express the Hilbert-space volume element [Eq. (3)] as

$$dV = \prod_i^N dp_i \tag{5}$$

up to an unimportant prefactor.

The QMC condition now implies that joint probability distribution of variables p_i is uniform on the manifold constrained by energy condition (2), normalization condition

$$\sum_i^N p_i = 1, \tag{6}$$

and positivity condition

$$p_i \geq 0, \quad \forall\ i. \tag{7}$$

The primary goal of the following subsections is to obtain the marginal distribution for individual variables p_k—to be denoted as $P_k(p_k)$—and the associated average values $\langle p_k \rangle$.

Function $P_k(p_k)$ is the probability density for the kth occupation number to have certain value p_k subject to a completely random choice of point $\{p_1,p_2,\ldots,p_k,\ldots,p_N\}$ on the manifold defined by Eqs. (2), (6), and (7). Therefore, $P_k(p_k)$ is proportional to the volume of the intersection of the above $(N-2)$-dimensional manifold with $(N-1)$-dimensional hyperplane corresponding to the fixed value of p_k. The resulting $(N-3)$-dimensional intersection manifold is to be denoted as M_k and its volume as $V_k(p_k)$.

The marginal distribution of p_k is then $P_k(p_k) = V_k(p_k)/[\int_0^1 V_k(p_k')dp_k']$, and the average value of p_k is

$$\langle p_k\rangle = \frac{\int_0^1 p_k' V_k(p_k')dp_k'}{\int_0^1 V_k(p_k')dp_k'}. \tag{8}$$

Everywhere below $V_k(p_k)$ is used as un-normalized probability distribution without $P_k(p_k)$ being explicitly specified.

Let us denote $(N-1)$-dimensional Euclidean space of all variables $\{p_i\}$ with $i\neq k$ as $\{p_i\}_k$. In this space, manifold M_k is constrained by conditions (7) in combination with

$$\sum_{i,i\neq k}^{N} p_i = 1 - p_k, \tag{9}$$

consequence of Eq. (6), and

$$\sum_{i,i\neq k}^{N} (E_i - E_{\text{av}})p_i = -(E_k - E_{\text{av}})p_k. \tag{10}$$

Condition (10), while obviously originating from Eq. (2), requires a preliminary manipulation equivalent to shifting the origin of the energy axis to E_{av}. Namely, E_{av} in the right-hand side of Eq. (2) has to be multiplied by $\Sigma_i^N p_i$ [equal to 1 according to Eq. (6)] and then the result transformed to Eq. (10). Important for the subsequent derivation is the fact that energy hyperplane represented by Eq. (10) crosses the origin of the $\{p_i\}_k$ space when $p_k=0$.

Manifold M_k has the character of $(N-3)$-dimensional polyhedron with flat faces, edges, etc. because all conditions constraining it [Eqs. (7), (9), and (10)] represent hyperplanes in the $\{p_i\}_k$ space. The intersection of Eqs. (7) and (9) forms simplex—a many-dimensional analog of a tetrahedron. Below I call it “Hypertetrahedron” in order both to invoke simple geometrical associations and to label this particular simplex. Hypertetrahedron has dimension $(N-2)$—equal to that of the normalization hyperplane [Eq. (9)] with $(N-1)$ vertices located at the intersections of the $(N-1)$ axes of the $\{p_i\}_k$ space with the hyperplane [Eq. (9)], i.e., in the $\{p_i\}_k$ space, each of the vertices has coordinates of type $(0,0,\ldots,1-p_k,\ldots,0)$, all projections are zero, except for one, which is equal to $1-p_k$. Manifold M_k can now be usefully described as a cross section of the Hypertetrahedron by energy hyperplane [Eq. (10)].

In the following, energies E_i are ordered by their values with the minimum one being $E_{\min}\equiv E_1$ and the maximum one $E_{\max}\equiv E_N$. The zero reference point for the energies is chosen such that

$$\sum_{i}^{N} E_i = 0. \tag{11}$$

[The uniform average of all E_i fixed above to be zero is not to be confused with the quantum-mechanical energy expectation value E_{av} given by Eq. (2).] When not stated otherwise, it will be assumed below that

$$E_{\text{av}} < 0. \tag{12}$$

It is always to be assumed that $N \gg 1$. The notation $O(1/N)$ will refer to terms, which become much smaller than the leading ones as N increases. The order of smallness implied by $O(1/N)$ is, however, *not* necessarily linear in $1/N$.

B. Case of $p_k \ll 1$

I first obtain function $V_k(p_k)$ for $p_k \ll 1$. When p_k is small, the renormalization of the volume $V_k(p_k)$ with respect to $V_k(0)$ can be decomposed into the “normalization factor” F_N due to the nonzero value of p_k in Eq. (9) and the “energy factor” F_E due to the nonzero value of p_k in Eq. (10):

$$V_k(p_k) = V_k(0)F_N F_E. \tag{13}$$

The normalization factor is given exactly by

$$F_N = (1-p_k)^{N-3} \tag{14}$$

for large or small p_k. It is the consequence of the fact that the change in $(1-p_k)$ in the right-hand side of Eq. (9) rescales the distance between any point of the Hypertetrahedron and the origin of the $\{p_i\}_k$ space by factor $(1-p_k)$. Since the energy hyperplane [Eq. (10)] passes through the origin (at $p_k=0$), each of the $(N-3)$ dimensions of the intersection manifold simply undergoes rescaling by factor $(1-p_k)$ thus leading to factor (14).

The calculation of the energy factor F_E requires more effort. The change in $-(E_k-E_{\text{av}})p_k$ in the right-hand side of Eq. (10) shifts the energy hyperplane in the transverse direction, but the resulting change of manifold M_k does not any longer amount to a self-similar rescaling.

The volume V_k of the $(N-3)$-dimensional manifold M_k can in general be presented as a product of $(N-3)$ characteristic linear parameters $\eta_{k\alpha}$:

$$V_k = \prod_{\alpha=1}^{N-3} \eta_{k\alpha}. \tag{15}$$

These parameters can be defined iteratively in the following way: $\eta_{k1}=V_k/V_{k,N-4}$, where $V_{k,N-4}$ is the volume of one of the $(N-4)$-dimensional faces of M_k; $\eta_{k2}=V_{k,N-4}/V_{k,N-5}$, where $V_{k,N-5}$ is the volume of one of the $(N-5)$-dimensional faces of the $(N-4)$-dimensional face selected in the previous step, etc.

After the small shift of the energy hyperplane [Eq. (10)] by $-(E_k-E_{\text{av}})p_k$, each linear parameter $\eta_{k\alpha}$ changes slightly to

$$\eta_{k\alpha}(p_k) = \eta_{k\alpha}(0)[1-\lambda_{k\alpha}(E_k-E_{\text{av}})p_k], \tag{16}$$

where $\lambda_{k\alpha}$ are unknown rescaling coefficients. As a result,

$$F_E = \prod_{\alpha=1}^{N-3} [1 - \lambda_{k\alpha}(E_k - E_{\rm av})p_k] \approx e^{-(N-3)\lambda_k (E_k - E_{\rm av})p_k}, \quad (17)$$

where

$$\lambda_k = \frac{1}{N-3} \sum_{\alpha}^{N-3} \lambda_{k\alpha}. \quad (18)$$

Coefficients $\lambda_{k\alpha}$ are not well differentiable with respect to p_k and $E_{\rm av}$ because the change in p_k and $E_{\rm av}$ is accompanied by the change in the number of vertices of manifold M_k. However, the internal self-consistency of the present treatment indicates that the overall renormalization factor F_E depends on p_k and $E_{\rm av}$ sufficiently weakly and can be efficiently approximated.

Even though each renormalization factor $[1-\lambda_{k\alpha}(E_k - E_{\rm av})p_k]$ in Eq. (17) is very close to 1, the product of the $(N-3)$ of these factors may be significantly smaller than 1 without compromising the validity of small-p_k approximation [Eq. (17)] for F_E alone. Yet, when $p_k \ll 1$, but both F_N and F_E depart significantly from one, one can worry that the effects of shifting the normalization and the energy hyperplanes [Eq. (9) and (10)] do not commute with each other, and therefore, the resulting renormalization is not equal to the product of F_N and F_E. This is, however, not the case because the shift of the normalization hyperplane amounts to a simple rescaling, and after that, the shift of the energy hyperplane always begins from the manifold of the same geometry.

Central to the present work is the result that in the leading order in $1/N$, λ_k is simply independent of k. I denote this independent value as λ without a subscript. It is shown in Appendix A that the linear parameters in Eq. (15) can always be chosen such that all but one summands are equal to each other in the expressions for two different renormalization coefficients $\lambda_k = \frac{1}{N-3}\Sigma_\alpha^{N-3}\lambda_{k\alpha}$ and $\lambda_l = \frac{1}{N-3}\Sigma_\alpha^{N-3}\lambda_{l\alpha}$, i.e., $\lambda_{k\alpha} = \lambda_{l\alpha}$ for all α except for one value α_0. In a typical case, however, $\lambda_{k\alpha_0}$ and $\lambda_{l\alpha_0}$ are much smaller than the rest of their respective sums.

Substituting λ instead of λ_k into Eq. (17) and then combining in Eq. (13) the resulting expression for F_E with F_N from Eq. (14) while keeping only the leading order in N, I obtain

$$V_k(p_k) = V_k(0) e^{-Np_k[1+\lambda(E_k - E_{\rm av})]}. \quad (19)$$

As long as

$$1 + \lambda(E_k - E_{\rm av}) \gg \frac{1}{N}, \quad (20)$$

$V_k(p_k)$ decays almost completely when $p_k \ll 1$, and therefore, expression (19) is sufficient to calculate $\langle p_k \rangle$ from Eq. (8), which gives

$$\langle p_k \rangle = \frac{1}{N[1 + \lambda(E_k - E_{\rm av})]}. \quad (21)$$

The value of λ can now be found numerically from either of the following two conditions originating, respectively, from Eqs. (6) and (2):

$$\sum_{k=1}^{N} \langle p_k \rangle = 1 \quad (22)$$

or

$$\sum_{k=1}^{N} (E_k - E_{\rm av})\langle p_k \rangle = 0. \quad (23)$$

Expression (21) for $\langle p_k \rangle$ has the property that, if the value of λ is found from one of the two conditions [Eq. (22) or Eq. (23)], the other one is fulfilled automatically.

The value of λ thus obtained becomes a function of average energy $\lambda[E_{\rm av}]$. Below I use λ both with and without its argument. In order to distinguish the argument of function $\lambda[E_{\rm av}]$ from the multiplication of λ by an expression in parentheses, the argument of $\lambda[E_{\rm av}]$, if present, will always follow λ in square brackets.

It is useful to present conditions (22) and (23) also in the integral form with the values of $\langle p_k \rangle$ substituted from Eq. (21):

$$\frac{1}{N}\int_{-\infty}^{+\infty} \frac{\nu(E)dE}{1 + \lambda(E - E_{\rm av})} = 1, \quad (24)$$

$$\int_{-\infty}^{+\infty} \frac{(E - E_{\rm av})\nu(E)dE}{1 + \lambda(E - E_{\rm av})} = 0, \quad (25)$$

where $\nu(E)$ is the density of states corresponding to the energy spectrum $\{E_k\}$ and satisfying the condition $\int_{-\infty}^{+\infty}\nu(E) = N$.

C. Meaning of λ

Parameter λ or, more precisely, $N\lambda$ has the meaning of inverse Hilbert-space temperature. This meaning follows from the analogy with the definition of temperature T for classical systems, namely, $1/T = \partial \log V_{\rm cl}(E)/\partial E$, where $V_{\rm cl}(E)$ is the volume of the manifold in classical phase space corresponding to constant energy E, and the Boltzmann coefficient equals 1.

Indeed, parameter λ was introduced to describe the volume change in manifold M_k in the $(N-1)$-dimensional $\{p_i\}_k$ space in response to the change in the right-hand side of the energy constraint, but, in the leading order in $1/N$, it also describes the change of volume $V_{\rm tot}$ of the entire energy manifold constrained by conditions (2), (6), and (7) in the full N-dimensional Hilbert space of the problem as a function of $E_{\rm av}$:

$$\lambda[E_{\rm av}] = \frac{1}{N}\left[\frac{\partial}{\partial E_{\rm av}} \log V_{\rm tot}(E_{\rm av}) + O(1/N)\right]. \quad (26)$$

[The extra dimension would introduce only one extra linear parameter η_0 and one more coefficient $\lambda_{0,\alpha}$ in the sum of $(N-1)$ other comparable coefficients in the early proof that justified the single value of λ for all $\{p_i\}_k$ spaces (see Sec. II B and Appendix A).] As a consequence,

$$V_{\rm tot}(E_{\rm av}) = V_{\rm max} \exp\left[N \int_0^{E_{\rm av}} \lambda(E)dE\right], \quad (27)$$

where $V_{\rm max}$ is the maximum value of $V_{\rm tot}$ corresponding to $E_{\rm av} = 0$, which, in turn, is the average value of all energies in the spectrum as defined by Eq. (11).

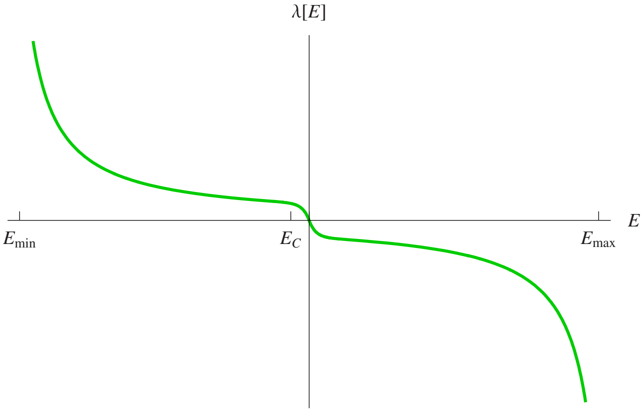

FIG. 1. (Color online) Qualitative sketch of $\lambda[E]$. Here E is the average energy identical with E_{av} in the right-hand side of Eq. (2). Critical average energy E_C is defined by Eq. (32). For $E_C < E_{\text{av}} \leq 0$, the values of $\lambda[E_{\text{av}}]$ are to be found from Eq. (24) or Eq. (25). For $E_{\min} < E_{\text{av}} \leq E_C$, function $\lambda[E_{\text{av}}]$ is well approximated by Eq. (34), but more accurately can be found from the self-consistent solution of Eq. (33).

In order to prove that the maximum of V_{tot} is indeed located at $E_{\text{av}}=0$, one should note that Eq. (26) implies $\lambda=0$ when $\partial V_{\text{tot}}(E_{\text{av}})/\partial E_{\text{av}}=0$. Equation (21) then gives $\langle p_k \rangle = 1/N$, which, according to Eqs. (11) and (23), can only be the case when $E_{\text{av}}=0$. This general result is in agreement with the analysis of Ref. [8] for the special case of equally spaced energy levels.

In principle, the point $E_{\text{av}}=0$ may or may not coincide with the maximum of $\nu(E)$, which is already a significant departure from the conventional statistics predicting the most probable state of the system (zero inverse temperature) always at the maximum of $\nu(E)$.

Another important difference is that even when the maxima of $V_{\text{tot}}(E)$ and $\nu(E)$ coincide, $V_{\text{tot}}(E)$ decays exponentially faster than $\nu(E)$, which has the consequence that the small-p_k condition (20) can be easily violated for the low-lying levels leading to a sort of condensation.

A typical dependence of parameter λ on the value of the average energy is sketched in Fig. 1. One should, in particular, remember that $E_{\text{av}} < 0$ (the default assumption for most of this paper) corresponds to $\lambda > 0$ and vice versa.

D. Beyond small p_k

In general, whether or not the preceding description is sufficient for calculating the occupation of all quantum levels depends on the spectrum of the problem and on the value of E_{av}. One should first try to use Eq. (21) with the value of λ found self-consistently from Eq. (22)or Eq. (23) to see whether $\langle p_k \rangle \ll 1$ for all k. If not, then one should use the following results extended to the case of $\langle p_k \rangle \sim 1$.

Expression (21) has a pole as a function of E_k, which I denote as E_λ:

$$E_\lambda = E_{\text{av}} - \frac{1}{\lambda}. \tag{28}$$

Parameter E_λ in the present treatment is analogous to the chemical potential in conventional thermodynamics. This analogy becomes clear once formula (19) is rewritten as

$$V_k(p_k) = V_k(0)\exp\{-N\lambda(E_k p_k - E_\lambda p_k)\}. \tag{29}$$

One can recall now that $N\lambda$ has the meaning of inverse Hilbert-space temperature, and then consider p_k as if it were a classical number of particles occupying discrete classical state with energy E_k.

Like $\lambda[E_{\text{av}}]$, parameter E_λ is a function of the average energy, $E_\lambda[E_{\text{av}}]$, and, likewise, I will be using square brackets to refer to the argument of this function.

Condition (20) is satisfied for all levels when

$$E_{\min} - E_\lambda \gg \frac{E_{\text{av}} - E_\lambda}{N}, \tag{30}$$

which for all practical purposes translates into

$$E_\lambda < E_{\min} - O(1/N). \tag{31}$$

When λ is positive and small, it corresponds to negative E_{av} sufficiently close to zero, and therefore, the preceding solution is valid. However, it always becomes violated as soon as E_{av} departs significantly from zero. Below I will be using variable E_C to refer to the critical value of E_{av} corresponding to

$$E_\lambda[E_C] = E_{\min} \tag{32}$$

(see Fig. 1).

In order to understand the regime of large p_k, it is necessary to appreciate that once condition (20) or (30) is violated, λ would continue to describe the response of $V_k(p_k)$ to the small shift of the energy hyperplane [Eq. (10)] around $p_k=0$. However, the whole function $V_k(p_k)$ given by Eq. (19) either decays too slowly or increases, and therefore, the linear approximation for the exponent in Eq. (19) becomes insufficient and Eq. (21) is not justified any longer.

It is, however, shown in Appendix B that the derivation of Eq. (19) is amenable to the case of arbitrary p_k. The result is

$$V_k(p_k) = V_k(0)\exp\left\{(N-3)\left[\log(1-p_k) + \int_{E_{\text{av}}}^{E_{\text{av}}-[(E_k-E_{\text{av}})p_k/(1-p_k)]} \lambda[E]dE\right]\right\}, \tag{33}$$

where $\lambda[E]$ is to be determined self-consistently by solving Eq. (22) or Eq. (23), though this time not just for a single value of E_{av} but rather for E_{av} spanning most of the allowed interval $[E_{\min}, E_{\max}]$ as required by the integral in Eq. (33). A possible algorithm of the overall self-consistent solution is discussed in Appendix B. I chose not to approximate $(N-3)$ with N in Eq. (33) because it appears to be an important correction for finite-N systems.

It is possible to anticipate the outcome of the above self-consistent solution qualitatively. Once condition (31) is violated, the average occupation number of the lowest-lying energy levels becomes a significant fraction of one. The overall normalization constraint Eq. (22) then implies that the number of these exceptional levels should be small, certainly much smaller than N. Therefore, as E_{av} continues decreasing beyond E_C, E_λ may increase above $E_{\min}$ but will stay very close to $E_{\min}$. This leads to an important approximation illustrated in Fig. 1. Namely, for $E_{\text{av}} < E_C$,

$$\lambda[E_{\text{av}}] \approx \frac{1}{E_{\text{av}} - E_{\min}}, \tag{34}$$

which one obtains by substituting $E_\lambda \approx E_{\min}$ into Eq. (28).

The value of $|E_C|$ is comparable to $|E_{\min}|$ when N is large but not exponentially large, as might be the case in the numerical studies (see below) and also in nanosized systems having not too large number of particles but very large number of levels. In these cases, the full calculation of the resulting statistics has to be done numerically on the basis of Eq. (33).

However, for a physical system, having macroscopic number of weakly interacting components, further progress can be made analytically.

E. Macroscopic system with nondegenerate ground state

1. Definitions and assumptions about the macroscopic system

As macroscopic, I understand a system consisting of macroscopic number $N_s \sim 10^{23}$ of relatively weakly interacting parts. In a gas, one molecule would constitute such one part. In condensed-matter systems with finite-range interactions, a part would imply a cluster of atoms, whose volume energy is much greater than the surface energy. Each part is assumed to be characterized by a finite Hilbert space. (The limit of large Hilbert space per constituent part is considered in the next subsection.) The total number of levels in such a macroscopic system satisfies inequality:

$$N > 2^{N_s} \gg N_s. \tag{35}$$

Due to the large number of weakly interacting parts, the density of states $\nu(E)$ of this macroscopic system is assumed to have narrow Gaussian peak around $E=0$, which is set by Eq. (11) to be equal to the average of all energies $\{E_i\}$. The mean-squared deviation of $\nu(E)$ from the above peak position is

$$\sigma_s^2 \equiv \frac{1}{N}\sum_{i=1}^{N} E_i^2 \approx N_s \sigma_0^2, \tag{36}$$

where σ_0^2 is the typical mean-squared deviation for a constituent part. The average energy for each constituent part is also to be set to zero. With this convention,

$$|E_{\min}| \sim N_s E_{\min 0} \gg \sigma_s, \tag{37}$$

where $E_{\min 0}$ is the typical minimum energy for a constituent part.

In the conventional microcanonical formulation of statistical physics, the temperature T corresponding to energy E_{av} is defined (with the Boltzmann constant set to 1) by

$$\frac{1}{T} = \left.\frac{d \log \nu(E)}{dE}\right|_{E=E_{\text{av}}}. \tag{38}$$

The substitution of Gaussian approximation for $\nu(E)$ then gives $T = -\sigma_s^2/E_{\text{av}}$. (Positive temperatures correspond to $E_{\text{av}} < 0$.) In a typical situation of physical interest, $T \sim E_0$, where E_0 is a characteristic one-particle energy in the Hamiltonian. Therefore,

$$|E_{\text{av}}| \sim \frac{\sigma_s^2}{T} \gg \sigma_s. \tag{39}$$

Like in Eq. (37), the above inequality is the consequence of $N_s \gg \sqrt{N_s}$. Therefore, it obviously extends to all realistic cases of relatively large constituent parts at temperatures in the range $10^{-5}-10^{5}$ times E_0.

It is shown in Appendix C and further in Appendix D that, under the above conditions, the critical average energy E_C defined by Eq. (32) satisfies inequality

$$|E_C| \ll \sigma_s \ll |E_{\min}|, |E_{\text{av}}|. \tag{40}$$

Finally, important for proving the condensation into a single lowest level is the property

$$E_2 - E_{\min} \gg \frac{|E_{\min}|}{N} \sim \frac{1}{N\lambda[E_{\text{av}}]}, \tag{41}$$

where E_2 is the energy of the second lowest level. This inequality is the consequence of the exponential smallness of N_s in comparison to N in combination with the fact that $E_2 - E_{\min}$ is, crudely speaking, a single-particle property falling on the scale of $|E_{\min}|/N_s$ multiplied, perhaps, by some other factors depending polynomially on N_s. The rightmost expression in Eq. (41) is the consequence of Eq. (34). Inequality (41) is illustrated in Appendix C.

2. Results

It is shown in Appendix D that, when condition (41) is satisfied, E_λ is pinned between $E_{\min}$ and E_2, sufficiently far from E_2, so that

$$N[1 + \lambda(E_2 - E_{\text{av}})] = N\frac{E_2 - E_\lambda}{E_{\text{av}} - E_\lambda} \gg 1. \tag{42}$$

This justifies the approximation $p_k \ll 1$ for $k \geq 2$ and, therefore, the validity of formula (21) for the second lowest level and all levels above it. In this formula the value of λ can then be very accurately approximated by Eq. (34).

As far as the volume $V_1(p_1)$ is concerned, it is narrowly peaked around the maximum, which simultaneously becomes the average value of p_1:

$$\langle p_1 \rangle \approx \frac{E_{\text{av}}}{E_{\min}}. \tag{43}$$

Such a condensation into the lowest-energy state amounts to a significant departure from the result of the conventional microcanonical recipe.

In retrospect, it is also clear that for the case, when the occupation of only one lowest-energy level violates the condition $\langle p_1 \rangle \ll 1$, and therefore formula (19) does not describe $V_1(p_1)$, still formula (21) with the value of λ found self-consistently from Eq. (22) or Eq. (23) amounts to an excellent approximation for all $\langle p_k \rangle$ including $\langle p_1 \rangle$. The reason is that since formula (21) is supposed to describe accurately the occupations of all levels beginning from the second, the occupation of the remaining (first) level is bound by normalization constraint [Eq. (22)] to have the right value. The self-consistent solution using formula (21) would produce E_λ coming as close from below to E_{min} as necessary in order to reproduce value (43). As far as other levels are concerned, for the absolute majority of them, the approximation $E_\lambda \approx E_{\text{min}}$ would remain very accurate independently of whether E_λ is slightly above or slightly below E_{min}. [Here, a few low-lying levels may constitute a possible exception related to the fact that there is some uncertainty in the present derivation about whether E_λ stays much closer to E_{min} than to E_2. If it does, which I suppose is the case, then the above procedure would be very accurate for all levels with $k \geq 2$.]

F. Limit of large number of quantum states per particle

When a macroscopic system consists of particles having translational degrees of freedom, the kinetic energy of the particles can reach very high values before the particles are able to escape from the system. Therefore, the number of quantum states per particle in such a system can be very large.

In order to analyze this limit in the simplest case, one can consider a system of N_s identical noninteracting oscillators having energy levels equally spaced by Ω and the average energy per oscillator $n_e\Omega$, where n_e is a finite number.

Each oscillator can, in turn, be described as a large spin S in magnetic field in the limit $S\to\infty$. The energy of this spin would be $E=\Omega S_z$, where the projection S_z admits $(2S+1)$ values between $-S$ and S.

In this case, the ground-state energy of the whole system is

$$E_{\text{min}} = -N_s S\Omega, \tag{44}$$

while the average energy is

$$E_{\text{av}} = -N_s(S-n_e)\Omega. \tag{45}$$

Therefore, according to formula (43),

$$\langle p_1\rangle \approx \frac{S-n_e}{S} \xrightarrow[S\to\infty]{} 1. \tag{46}$$

In other words, the most probable state of such a system is the ground state with vanishingly small corrections—quite a surprising result.

In order to understand it intuitively, one needs to remember that the exact value of $\langle p_1\rangle$ remains less than one [see Eq. (D16)], and, moreover, $1-\langle p_1\rangle \gg 1/N$. If any eigenstate of the spectrum remains completely unoccupied on average, it means that the corresponding volume in the Hilbert space is zero. Therefore, each of many eigenstates above E_{av} has to have some nonzero average occupation. At the same time, the eigenstates below E_{av} need to have much greater occupation in order to balance in Eq. (23) many more eigenstates above E_{av}. It simply turns out that the volume of the Hilbert space is maximized when almost all (but not all) of the probability weight goes into the ground state.

G. Typical pure state

Even though the statistics derived so far has been obtained through averaging over all possible quantum states subject to the QMC condition, the resulting statistics also describes a typical one among them in the following sense. Once a single state is selected, it will have very large number of eigenstates in each small energy interval between E_{min} and E_{max}. Individually, the occupation numbers of these eigenstates will fluctuate according to the probability distribution proportional to their respective $V_k(p_k)$. That distribution will depend only on the energy of each of these eigenstates, and therefore, within a small energy interval, it will be approximately the same for all of them. Consequently, the average occupation number of eigenstates within any small energy interval will be given by formulas for $\langle p_k\rangle$ obtained above.

III. SMALL SUBSYSTEM WITHIN A LARGE ISOLATED SYSTEM

A. Formulation of the problem

Now I proceed with deriving the energy distribution for a subsystem of an isolated system—subject to the QMC condition. It is assumed that the subsystem and the rest of the system—environment—do not interact with each other. Therefore, the eigenstates of the whole isolated system can now be labeled by two indices as follows:

$$\Phi_{\alpha\beta} = \psi_\alpha \phi_\beta, \tag{47}$$

where indices α and β and the corresponding eigenstates ψ_α and ϕ_β refer to the subsystem and the environment, respectively. The subsystem has N_1 states with energies $E_{S\alpha}$. The environment has N_2 states $(N_2 \gg 1)$ with energies $E_{E\beta}$. The zero reference point for each set of energies is chosen such that

$$\sum_{\alpha=1}^{N_1} E_{S\alpha} = 0 \tag{48}$$

and

$$\sum_{\beta=1}^{N_2} E_{E\beta} = 0. \tag{49}$$

The energy of each eigenstate $\Psi_{\alpha\beta}$ of the whole system is then

$$E_{\alpha\beta} = E_{S\alpha} + E_{E\beta}. \tag{50}$$

General superposition of the eigenstates for the entire system has form

$$\Psi = \sum_{\alpha=1}^{N_1} \sum_{\beta=1}^{N_2} C_{\alpha\beta}\Phi_{\alpha\beta}, \tag{51}$$

where $C_{\alpha\beta}=|C_{\alpha\beta}|\exp^{i\varphi_{\alpha\beta}}$ are expansion coefficients.

Density matrix for the subsystem is then

$$\rho_{S\alpha\alpha'} = \sum_{\beta=1}^{N_2} C^*_{\alpha\beta}C_{\alpha'\beta} = \sum_{\beta=1}^{N_2} |C_{\alpha\beta}||C_{\alpha'\beta}|e^{i(\varphi_{\alpha'\beta}-\varphi_{\alpha\beta})}. \tag{52}$$

The off-diagonal elements of this density matrix are typically negligible in the limit $N_2 \gg 1$. Indeed, each off-diagonal element [Eq. (52)] is the sum of N_2 complex numbers with uncorrelated random phases $(\varphi_{\alpha'\beta} - \varphi_{\alpha\beta})$. It follows from Eq. (21) that the typical absolute value of each of the N_2 terms is $|C_{\alpha\beta}||C_{\alpha'\beta}| \sim 1/N = 1/(N_1 N_2)$. The sum of N_2 of such terms with random relative phases amounts to a random walk in the complex plane. This justifies the estimate $|\rho_{S\alpha\alpha'}| \sim 1/(N_1\sqrt{N_2})$, which is much smaller than $1/N_1$—the average value of diagonal density matrix elements $\rho_{S\alpha\alpha}$.

The above estimate has the following loophole. For the case of macroscopic environment, the condensation into the ground state of the entire system obtained in Sec. II E implies that $|C_{11}| \sim 1$. However, even in this case, sum [Eq. (52)] for each off-diagonal element $\rho_{S1\alpha'}$ contains only one term $|C_{11}||C_{\alpha'1}| \sim 1/\sqrt{N_1 N_2}$, which is still exponentially smaller than $1/N_1$. (In the case of macroscopic environment N_2 is exponentially larger than N_1.)

One can be further concerned with the case of macroscopic environment for a subsystem having a degenerate ground state—e.g., two-fold degenerate. In this case, both $|C_{11}|$ and $|C_{21}|$ become of the order of 1, and, therefore, the off-diagonal element $|\rho_{S12}|$ containing term $|C_{11}||C_{21}| \sim 1$ cannot be neglected.

In general, the rather exceptional cases exhibiting nonnegligible off-diagonal matrix elements $\rho_{S\alpha\alpha'}$ all have the property that a tiny minority of states in the Hilbert space of the entire isolated system have anomalously large occupations. Such situations should be considered on case-by-case basis and are not pursued further in this paper.

The readers should be, finally, reminded that, for $E_{\alpha\beta} \neq E_{\alpha'\beta}$, the phase factors in Eq. (52) have time dependence $\exp[i(\varphi_{\alpha'\beta} - \varphi_{\alpha\beta})] \simeq \exp[i(E_{\alpha\beta} - E_{\alpha'\beta})t]$, which leads to the additional time averaging for the statistical fluctuations of the off-diagonal elements $\rho_{S\alpha\alpha'}$.

The focus of the following subsections is to find the diagonal elements:

$$\rho_{S\alpha\alpha} \equiv \rho_\alpha = \sum_{\beta=1}^{N_2} p_{\alpha\beta}, \tag{53}$$

where $p_{\alpha\beta} = |C_{\alpha\beta}|^2$ is the occupation number of each eigenstate. Here variable ρ_α is introduced just to shorten the notation.

B. General solution

I now relabel the N_2 states contributing to ρ_α with index a, and the remaining $(N_1 - 1)N_2$ states with index b. This results in two new sets of occupation numbers and energies: (p_a, E_a) and (p_b, E_b). Subscripts a and b will play dual role below: as indices and as labels of two different sets. The summation over a implies the first set, and a summation over b implies the second set. When a particular member of each set needs to be specified, it is to be referred to with a "label-and-number" subscript. For example, E_{a2} refers to the second lowest energy of the a set, and $E_{b\,\min}$ refers to the minimum energy of the b set.

The new sets of energies have the average values, respectively,

$$\frac{1}{N_2}\sum_{a=1}^{N_2} E_a = E_{S\alpha}, \tag{54}$$

$$\frac{1}{N_2(N_1 - 1)} \sum_{b=1}^{N_2(N_1-1)} E_b = -\frac{E_{S\alpha}}{N_1 - 1}. \tag{55}$$

The normalization and the energy constraints now have form, respectively,

$$\sum_a p_a + \sum_b p_b = 1 \tag{56}$$

and

$$\sum_a E_a p_a + \sum_b E_b p_b = E_{\text{av}}. \tag{57}$$

Given Eq. (56), condition (57) can be replaced with

$$\sum_a (E_a - E_{\text{av}})p_a + \sum_b (E_b - E_{\text{av}})p_b = 0. \tag{58}$$

The a and the b states can now divide between themselves the occupations and the total energy as follows:

$$\sum_a p_a = \rho_\alpha, \tag{59}$$

$$\sum_a (E_a - E_{\text{av}})p_a = E_A, \tag{60}$$

$$\sum_b p_b = 1 - \rho_\alpha, \tag{61}$$

$$\sum_b (E_b - E_{\text{av}})p_b = -E_A, \tag{62}$$

where E_A is the difference between the energy of the a set and E_{av}. It is an auxiliary parameter to be determined simultaneously with ρ_α.

The goal now is to obtain $\langle\rho_\alpha\rangle$—the average value of ρ_α over all points in the Hilbert space constrained by conditions (56) and (58) in combination with

$$p_a, p_b \geq 0. \tag{63}$$

The probability of each pair of values (ρ_α, E_A) is proportional to the volume in the Hilbert space constrained by conditions (59)–(63). The constraints on a and b states can then be treated independently by analogy with the problem for the whole system that led to Eq. (33). This results in the following expression:

$$V(\rho_\alpha, E_A) = V_0 \exp\Bigg\{ N_2 \log \rho_\alpha + N_2(N_1 - 1)\log(1 - \rho_\alpha) + N_2 \int_{E_{\text{av}}}^{E_{\text{av}} + E_A/\rho_\alpha} \lambda_a[E]\,dE + N_2(N_1 - 1) \int_{E_{\text{av}}}^{E_{\text{av}} - E_A/(1-\rho_\alpha)} \lambda_b[E]\,dE \Bigg\}, \tag{64}$$

where $\lambda_a[E]$ and $\lambda_b[E]$ are the parameters analogous to λ

introduced below for the spectrum of the entire system, but this time defined for the spectra of E_a and E_b separately and V_0 is an unimportant prefactor.

Due to the fact that $N_2 \gg 1$, expression (64) must be very sharply peaked near the maximum of the function in the exponent. Therefore finding $\langle \rho_\alpha \rangle$ is reduced to finding the value of ρ_α at the maximum of this exponent. In order to locate that maximum, I look for the zeros of the partial derivatives of the exponent in Eq. (64) with respect to E_A and ρ_α. Differentiation with respect to E_A gives

$$\frac{N_1 - 1}{1 - \rho_\alpha} \lambda_b \left[E_{\text{av}} - \frac{E_A}{1 - \rho_\alpha} \right] = \frac{\lambda_a \left[E_{\text{av}} + \frac{E_A}{\rho_\alpha} \right]}{\rho_\alpha}. \tag{65}$$

Now, differentiating the exponent in Eq. (64) with respect to ρ_α and also using Eq. (65), I obtain

$$\rho_\alpha (1 - N_1 \rho_\alpha) = E_A \lambda_a \left[E_{\text{av}} + \frac{E_A}{\rho_\alpha} \right]. \tag{66}$$

One can get a useful insight into the solution of Eqs. (65) and (66) by substituting λ_a, λ_b with new variables E_{λ_a}, E_{λ_b}:

$$\lambda_a[E] = \frac{1}{E - E_{\lambda_a}[E]}, \tag{67}$$

$$\lambda_b[E] = \frac{1}{E - E_{\lambda_b}[E]}. \tag{68}$$

Subscripts a and b in variables λ_a, λ_b, E_{λ_a}, and E_{λ_b} are just the labels of the characteristics of the respective energy spectra, i.e., they are not indices running over a set of integer values.

After some manipulations, the above substitution generates two equations equivalent to Eqs. (65) and (66):

$$E_A = \left(\frac{1}{N_1} - \rho_\alpha \right) \left\{ E_{\text{av}} - E_{\lambda_a} \left[E_{\text{av}} + \frac{E_A}{\rho_\alpha} \right] \right\}, \tag{69}$$

$$E_{\lambda_a} \left[E_{\text{av}} + \frac{E_A}{\rho_\alpha} \right] = E_{\lambda_b} \left[E_{\text{av}} - \frac{E_A}{1 - \rho_\alpha} \right]. \tag{70}$$

The latter equation is the key to the following solution for the macroscopic environment.

In general, Eqs. (65) and (66) or equivalently Eqs. (69) and (70) should be solved numerically. It is, however, shown in the next subsection that the system of Eqs. (69) and (70) can be solved analytically in the case of a small subsystem in a macroscopic environment with a realistic value of E_{av} for the entire system (in the sense of Sec. II E).

There is also another analytically solvable limit, which corresponds to the case of high Hilbert-space temperatures, i.e., very small λ_a and λ_b. This limit is not to be considered in this work.

C. Subsystem in a macroscopic environment

The condition of macroscopic environment and a small subsystem amounts formally to the presence of narrow Gaussian-like maximum around $E=0$ in the density of states of the environment $\nu_E(E)$ with the root-mean-squared spread of energies σ_E satisfying the conditions:

$$|E_{E\,\text{min}}|,\ E_{E\,\text{max}},\ |E_{\text{av}}| \gg \sigma_E \gg |E_{S\alpha}|, \quad \forall\ \alpha. \tag{71}$$

In addition, there is a reasonable condition for the differences between two lowest-energy states for the subsystem and the environment:

$$E_{S2} - E_{S\,\text{min}} \gtrsim E_{E2} - E_{E\,\text{min}}. \tag{72}$$

It is shown in Appendix E that, in this case, the occupations of the lowest subsystem state in the leading order of $E_{S\alpha}/E_{E\,\text{min}}$ is

$$\langle \rho_1 \rangle = \frac{E_{\text{av}}}{E_{E\,\text{min}}} + \frac{1}{N_1} \left(1 - \frac{E_{\text{av}}}{E_{E\,\text{min}}} \right), \tag{73}$$

and for the remaining states with $\alpha \geq 2$,

$$\langle \rho_\alpha \rangle = \frac{1}{N_1} \left(1 - \frac{E_{\text{av}}}{E_{E\,\text{min}}} \right), \tag{74}$$

where the right-hand side is obviously independent of α.

It is also possible to obtain more general formulas (see Appendix E):

$$\langle \rho_1 \rangle = \frac{E_{\text{av}} \left(1 - \frac{1}{N_1} \right) + \frac{E_{S\,\text{min}}}{N_1 - 1} + \frac{E_{\text{min}}}{N_1}}{E_{\text{min}} + \frac{E_{S\,\text{min}}}{N_1 - 1}}, \tag{75}$$

and for $\alpha \geq 2$,

$$\langle \rho_\alpha \rangle = \frac{1}{N_1} \frac{E_{\text{av}} - E_{E\,\text{min}}}{E_{S\alpha} - E_{E\,\text{min}}}, \tag{76}$$

where $E_{\text{min}} = E_{S\,\text{min}} + E_{E\,\text{min}}$. Formulas (75) and (76) are certainly valid up to the first order in $E_{S\alpha}/E_{E\,\text{min}}$ but in fact have a broader range of applicability because conditions (71) and (72) are sufficient but not necessary for the validity of approximation (75) and (76). For example, this approximation also describes the case $E_{S\alpha} \sim E_{E\,\text{min}}$ when condition $|E_{S\alpha}| \ll |E_{E\,\text{min}}|$ is replaced by the requirement that $N_1 \gg 1$ and the density of states for energies $E_{S\alpha}$ have a Gaussian-like narrowly peaked shape around $E=0$. Further discussion of the necessary conditions for the validity of approximation (75) and (76) is given in Appendix E.

The basic assumptions leading to the above results contain a loophole of neglecting the interaction between the subsystem and the environment. The same loophole is also present in the conventional microcanonical derivation of the Boltzmann-Gibbs statistics. In principle, given the condensation of the entire system into the lowest-energy state, one should not be surprised that a similar property is exhibited by a subsystem. Yet one can still worry about the validity of the condensation into the single lowest-energy state of the subsystem [Eq. (73)] when the interaction energy with the environment is much greater than the separation between the lowest and the second lowest-energy levels of the subsystem. In this case, the occupation numbers of the subsystem would depend on entanglement properties with the environment in the ground state of the whole system. This loophole potentially opens the window for chaos and nonintegrability to play a role in the resulting statistics. It also cannot be excluded that the result may then reproduce the Boltzmann-Gibbs statistics in the energy range of the order of the subsystem-environment interaction energy. This issue is not addressed further in the present work.

D. Typicality of the pure states of the entire system for the density matrix of a subsystem

The probability distribution of parameters describing the diagonal elements of the density matrix $\rho_{S\alpha\alpha'}$ exhibits exponentially narrow $[O(1/N_2)]$ maxima controlling the average values of these parameters. The off-diagonal elements of $\rho_{S\alpha\alpha'}$ are also suppressed to zero with accuracy $O(1/N_2)$ (except for degenerate ground states—see Sec. III A). Therefore, for a subsystem with nondegenerate ground state, a random choice of QMC-constrained single quantum state would produce a density matrix exponentially close to the average one computed in the previous subsection. This situation is analogous to the "canonical typicality" [4,5] for the conventional microcanonical condition and to the typicality for a broader class of equilibria discussed in Ref. [13].

IV. NUMERICAL RESULTS

The analytical approximations made for the QMC ensemble in this work and the relevance of the QMC ensemble to realistic systems should be checked numerically. Here, I present two numerical results of preliminary nature addressing only the statistics for the entire isolated quantum system.

A. Direct random sampling

The first test is a direct Monte Carlo sampling of the Hilbert space under constraint (2). I have done this sampling directly in the Euclidean space of variables $\{p_i\}$ using the algorithm consisting of the following steps: (i) selection of an orthonormal basis in the $(N-2)$-dimensional hyperplane constrained by Eqs. (2) and (6); (ii) identification in that hyperplane a $(N-2)$-dimensional hypercube, which encloses all the vertices of the intersection manifold; (iii) random sampling of points within that hypercube; and, finally (iv) acceptance of only those random points, which in the original N-dimensional $\{p_i\}$ space have all non-negative coordinates as required by constraint (7).

This algorithm is not very efficient: its acceptance rate at step (iv) decreases by about factor of 10 as N increases by one. Using MATHEMATICA software, I was able to generate statistically significant number of random points for the case of $N=10$ with the spectrum and the average energy shown in Fig. 2.

This figure compares the average occupation numbers obtained numerically with the approximate theoretical values obtained on the basis of Eq. (21), where the value of λ was found by solving Eq. (23) numerically.

The lowest level in Fig. 2(b) violates the condition $\langle p_k\rangle \sim 1/N \ll 1$. However, as discussed at the end of Sec. II E, the overall structure of the more accurate solution guarantees that, for a single level violating the above condition, result (23) would still amount to a very good approximation even though the corresponding Hilbert-space volume $V_1(p_1)$ does not any longer decay exponentially but instead is peaked around $p_1 \approx \langle p_1\rangle$.

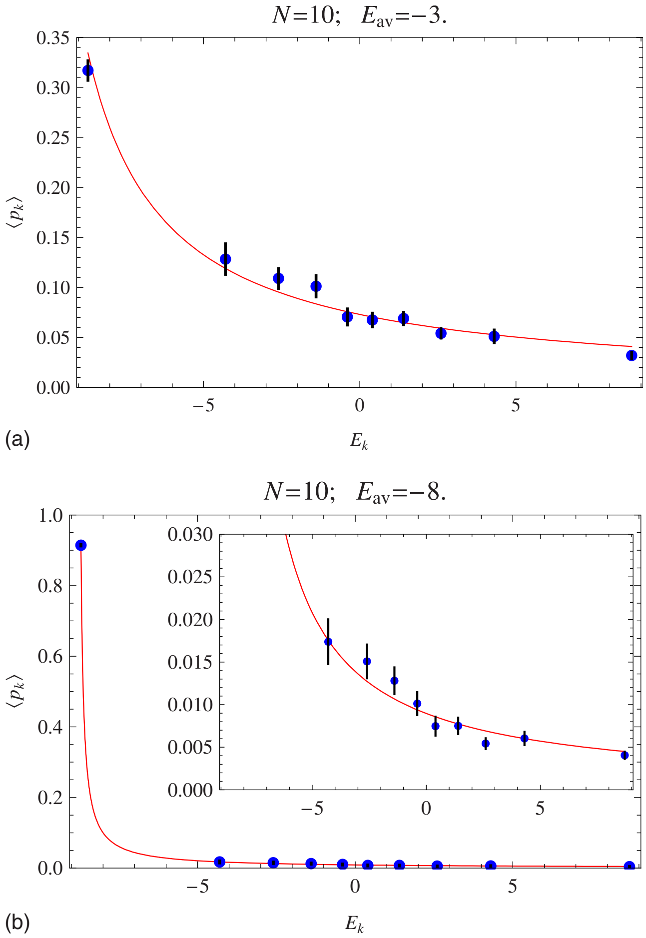

FIG. 2. (Color online) Two results of direct random sampling of quantum states in a system of ten energy levels. Average energies are indicated above the plots. Dots with error bars represent the averages over all sampled states. Solid lines represents the prediction of Eq. (21) with the value of λ obtained numerically from formula (23). The inset in plot (b) magnifies the small $\langle p_k\rangle$ part of the main plot.

Given that $N=10$ barely qualifies as a very large number, the overall agreement exhibited in Fig. 2 is surprisingly good.

B. Random matrices

Now I present a result of a numerical experiment indicating that the QMC-based statistics manifests itself in systems describable by random matrix Hamiltonians. The connection is not self-evident *a priori*. No attempt is to be made in this work to clarify it further.

Let us consider a random matrix Hamiltonian, select one of its basis states and then expand this state in terms of the eigenstates of the Hamiltonian. The basis state selected would have energy expectation value E_{av} equal to the corresponding diagonal element of the random matrix. This imposes constraint (2) on the eigenstates participating in the expansion. The present numerical experiment was based on a guess, successfully confirmed by the end result, that the eigenstates would participate in the expansion of a basis state as if that expansion was done randomly on the basis of the QMC condition.

I took a 4096×4096 matrix, where all diagonal elements and a fraction $\frac{30}{4096}$ of off-diagonal elements were assigned random values picked in the interval $[-1,1]$. The remaining off-diagonal elements were zeros. The Hamiltonian was diagonalized, and then one state of the original basis was chosen and expanded in terms of eigenstates. The weight of individual eigenstates fluctuated as expected from Eq. (19). However, once the spectrum is divided in groups of 64 adjacent eigenstates having approximately the same energy, then the average weight within each group begins converging to the theoretical approximation (21) as discussed in Sec. II G. I further improve the error bars by combining the overall statistics for 34 and 35 noneigenstates with average energies within a narrow energy window $E_{\mathrm{av}}\pm 0.01$, where E_{av} is equal to -0.5 and -0.9 in the two examples shown in Fig. 3. The good agreement is then revealed with the theoretical approximation (21), which uses λ computed numerically from Eq. (23). It should be emphasized that the results presented in Fig. 3 all correspond to a single randomly selected Hamiltonian and not to the ensemble of Hamiltonians.

When the fraction of nonzero off-diagonal elements in the random matrix is increased, the agreement between numerics and the theory continues to hold. In this case, however, the width of the nearly semicircle eigenspectrum increases, while the window for E_{av} determined by the diagonal elements of the Hamiltonian remains the same. As a result, λ becomes small and dependence (21) becomes difficult to distinguish from a linear one. On the other hand, if the fraction of nonzero off-diagonal elements decreases, then the assumption of perfect mixing of eigenstates in each of the original basis states becomes increasingly inadequate as the weights of eigenstates start to peak around $E=E_{\mathrm{av}}$. Such a behavior is natural to expect as this system gradually approaches the limit of small off-diagonal elements in the Hamiltonian (see, e.g., Ref. [14]).

V. CONCLUDING REMARKS

(1) The results presented in this work, indicate that the statistical description of an isolated quantum system subject to a fixed energy constraint and unrestricted participation of eigenstates contradicts (at least in the limits considered) to the Boltzmann-Gibbs statistics derivable on the basis of the conventional microcanonical assumption.

In particular, the resulting energy distributions for both the whole isolated system [Eq. (21)] and a small subsystem of it [Eq. (74)] show algebraic rather than exponential dependence on the energies of participating states as well as routine macroscopic occupancy (condensation) for the lowest-lying energy states [Eqs. (43), (46), and (73)].

One should be mindful though of the loophole associated with the neglected interaction between the subsystem and the environment (see the discussion at the end of Sec. III C).

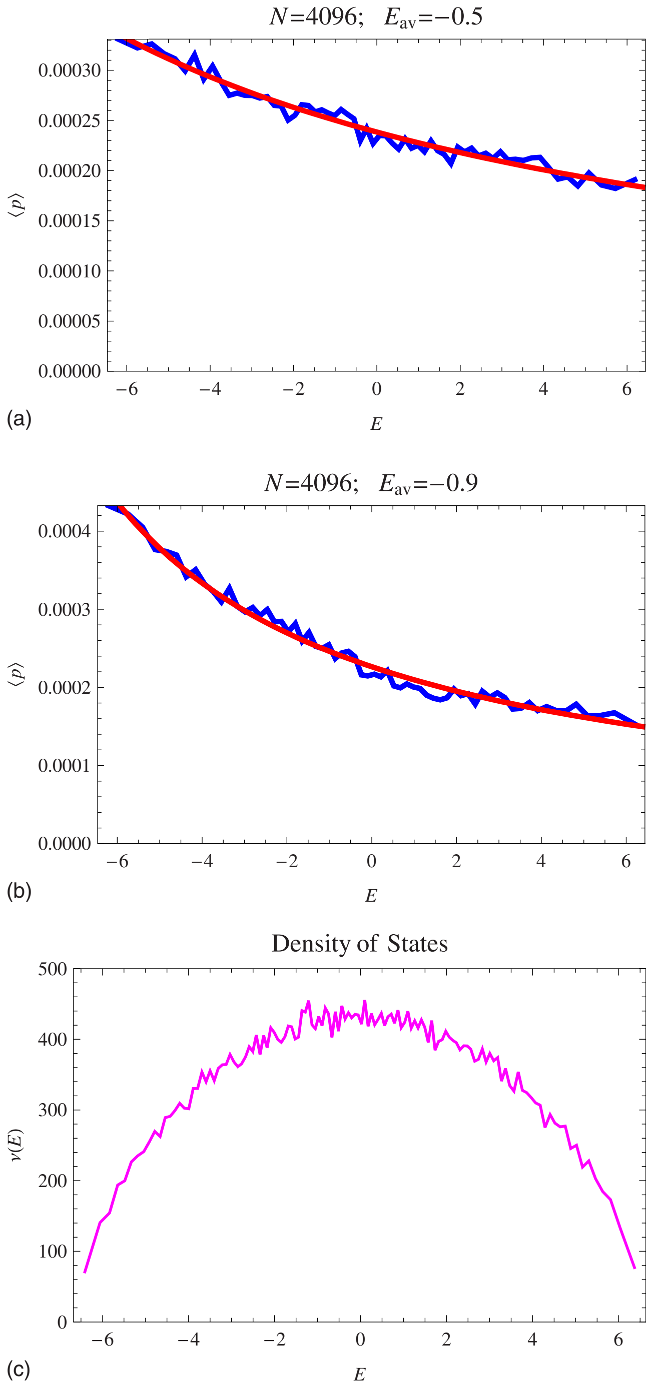

FIG. 3. (Color online) Average occupations of eigenstates $\langle p\rangle$ participating in the expansions of noneigenstates of the initial basis, which (the noneigenstates) are selected from a narrow energy window $E_{\mathrm{av}}\pm 0.01$ around the values indicated above plots (a) and (b). Broken lines in these two plots represent numerical results averaged over groups of 64 adjacent eigenstates. Smooth lines represent the prediction of Eq. (21) with the values of λ obtained numerically from Eq. (23). The density of eigenstates $\nu(E)$ for this system averaged over groups of 32 states is presented in plot (c).

(2) The statistics derived in this work is supported by the numerical findings presented in Sec. IV. Particularly interesting is the finding presented in Sec. IV B that the expansion

of the noneigenstates of the random matrix basis in terms of eigenstates follows this statistics for large but finite random matrices, which are not too sparce.

(3) The finite size version of this statistics might be observable after a strong (and preferably nonintegrable) perturbation of a well-isolated system having a relatively small number of particles but a large number of quantum levels. Nanoscale-limited systems should be good candidates for such a study. For a better control of the total energy after the perturbation, one can proceed in analogy with the "numerical experiment" on a random matrix presented in Sec. IV B. Namely, one can force the system into a single quantum state, e.g., the ground state, before perturbing it.

(4) In systems of bosons, the condensation described in this work into the ground state or a few lowest states may produce an appearance of Bose-Einstein condensation because the ground state is indeed Bose condensed. Yet the nature of the two kinds of condensations is different. The former represents a jump in the occupation of many-particle states, while the latter is a single-particle phenomenon accompanied by the usual exponential statistics for the occupations of all many-particle quantum states.

(5) When it comes to macroscopic systems, the contradiction indicated in remark 1 re-enforces the concern that nonrelativistic quantum mechanics alone is not sufficient to justify the Boltzmann-Gibbs statistics. One needs an assumption of external origin, such as the quantum collapse of the broad distribution of eigenstates into a narrow energy window postulated by the conventional microcanonical description.

If such a collapse happens even once, it appears very difficult if not impossible to realistically perturb a typical macroscopic system containing many weakly interacting parts into a state characterized by a broad energy range of participating eigenstates.

Yet, if this collapse occurs continuously, its description would go beyond the linear quantum mechanics and in particular may imply additional source of energy fluctuations for the entire system.

(6) Even though the statistics obtained in this work appears to contradict to the everyday experience well describable by the Boltzmann-Gibbs statistics, it is still interesting to think what the present statistics might imply if one assumes that the entire universe is describable by a single wave function.

(7) Quite a few researchers including this author (see, e.g., Refs. [15–21]) share the feeling that the elusive notion of quantum chaos plays an important role in the foundations of quantum statistical physics. Chaos, however, plays no role in finding the most probable quantum state both in the present and in the conventional microcanonical formulation. This suggests that the role of chaos is not to determine the equilibrium itself but rather to influence how a subsystem relaxes towards the equilibrium.

Yet, one should not forget about the loophole related to the neglected interaction between the subsystem and environment [see the end of Sec. III C]. In addition, what quantum chaos certainly does is that it strongly suppresses the fluctuations of the number of energy levels within any fixed energy window—consequence of the repulsion of energy levels. Whether and how this property would affect the macroscopic characterization of equilibrium in quantum systems is not clear to this author.

(8) From a broader perspective, the statistics based on simple constraints [Eqs. (2), (6), and (7)] describes a distribution of an essentially positive and limited in the amount quantity p among N agents having characteristics $\{E_k\}$. It is, therefore, tempting to speculate that such a statistics might be applicable beyond the quantum mechanical problems, in particular, to the problems of economics when and if one finds a meaningful interpretation for constraint (2).

ACKNOWLEDGMENTS

The author is grateful to D. Antonov, P. Gaspard, T. Grünewald, A. Komnik, and F. Wegner for discussions related to the content of this work and to W. Wustmann for early computer studies. A significant part of this work was done during author's stay at the University of Tennessee, Knoxville.

APPENDIX A: PROOF THAT ALL VALUES OF λ_k ARE APPROXIMATELY EQUAL

In order to be specific, let us compare the intersection manifolds M_1 and M_2 pertaining, respectively, to λ_1 in the space of all variables p_i excluding p_1 and λ_2 in the space of all variables p_i excluding p_2. Let us also, for this part only, shift the zero point of the energy axis to E_{av}, i.e., the condition $E_{\text{av}}=0$ replaces Eq. (11); and assume that E_1 and E_2 are not necessarily two lowest energies of the spectrum but rather two arbitrary ones.

In the first case, the intersection manifold is defined by

$$p_2, p_3, \ldots, p_N \geq 0, \tag{A1}$$

$$p_2 + p_3 + \cdots + p_N = 1, \tag{A2}$$

$$E_2 p_2 + E_3 p_3 + \cdots + E_N p_N = v, \tag{A3}$$

where $v = -E_1 p_1$.

Parameter λ_1 characterizes the change of volume V_1 of the above manifold in response to small shift v of hyperplane [Eq. (A3)]. Specifically, from Eqs. (15) and (16),

$$\lambda_1 = \left.\frac{1}{V_1}\frac{dV_1}{dv}\right|_{v=0} = \sum_{\alpha=1}^{N-3} \frac{1}{\eta_{1\alpha}}\frac{d\eta_{1\alpha}}{dv} = \sum_{\alpha=1}^{N-3} \lambda_{1\alpha}. \tag{A4}$$

In the second case, the intersection manifold is

$$p_1, p_3, \ldots, p_N \geq 0, \tag{A5}$$

$$p_1 + p_3 + \cdots + p_N = 1, \tag{A6}$$

$$E_1 p_1 + E_3 p_3 + \cdots + E_N p_N = v, \tag{A7}$$

where $v = -E_2 p_2$.

Parameter λ_2 characterizes the change of volume V_2 of the above manifold:

$$\lambda_2 = \left.\frac{1}{V_2}\frac{dV_2}{dv}\right|_{v=0} = \sum_{\alpha=1}^{N-3}\frac{1}{\eta_{2\alpha}}\frac{d\eta_{2\alpha}}{dv} = \sum_{\alpha=1}^{N-3}\lambda_{2\alpha}. \tag{A8}$$

If one changes the variable p_1 to p_2 in Eqs. (A5)–(A7), then one finds that the problems of calculating λ_1 and λ_2 are nearly identical to each other with the only difference that term $E_2 p_2$ in Eq. (A3) has to be replaced with $E_1 p_2$. One can already anticipate the result $\lambda_1 \approx \lambda_2$ from the fact that vectors $\{E_2, E_3, \ldots, E_N\}$ and $\{E_1, E_3, \ldots, E_N\}$ determining the normal directions of the hyperplanes [Eqs. (A3) and (A7)], respectively, are nearly parallel to each other—consequence of the large number of identical components. The proof given below, however, takes a different route.

It is, in fact, possible to show that the sets of characteristic linear parameters $\{\eta_{1\alpha}\}$ and $\{\eta_{2\alpha}\}$ can be chosen such that $\eta_{1\alpha}(v) = \eta_{2\alpha}(v)$ for all but one value of α, and therefore, $N-4$ out of $N-3$ terms contributing to λ_1 and λ_2 in Eqs. (A4) and (A8) are identical to each other. Therefore, in general,

$$\lambda_2 = \lambda_1 + O(1/N). \tag{A9}$$

The proof of the above statement lies in the fact that two $(N-3)$-dimensional manifolds M_1 and M_2 (with the p_1-to-p_2 variable change in the second case) have a common $(N-4)$-dimensional face. This face is defined by condition $p_2 = 0$. Therefore, one can choose the first linear parameter η in each case differently by dividing the volumes V_1 and V_2 by the $(N-4)$-dimensional volume of that face, but then the rest of the parameters can be chosen identically because they will describe the volume renormalization for the same face.

I now describe the above $(N-4)$-dimensional face in more detail and, in particular show, that the $(N-1)$-dimensional hyperplane $p_2 = 0$ contains more than $N-3$ vertices of M_1 or M_2—a necessary condition to form a $(N-4)$-dimensional face.

All the vertices of either manifold M_1 or M_2 are obtained by the intersection of the linear edges of the normalization hypertetrahedron (defined in Sec. II B) with the energy hyperplane. In turn, all of these edges have form $p_i = 1 - p_j$, $(0 \leq p_i, p_j \leq 1)$ in the two-dimensional plane defined by condition $p_k = 0, \forall k \neq i, j$.

The energy hyperplane (with $v = 0$) intersects such an edge only in the case, when E_i and E_j have opposite signs. (Here and everywhere below I ignore the nongeneric case of E_i or E_j equal to zero.) Therefore, if there are K quantum states with $E_i > 0$ $[E_i > E_{\mathrm{av}}]$ and $L = N - 1 - K$ with $E_i < 0$ $[E_i < E_{\mathrm{av}}]$, then the intersection manifold has KL vertices.

Among these KL vertices, only those originating from the edges involving p_2 change between the manifolds M_1 and M_2 (shift or disappear): if $E_1, E_2 > 0$, then L vertices shift, possibly significantly; if $E_1, E_2 < 0$, then K vertices shift; if E_1 and E_2 have opposite signs, then L vertices in one case are replaced by K vertices in the other case.

All other vertices remain identical. They all lie in the hyperplane $p_2 = 0$. Their number is greater than $KL - (N-1)$, which, in turn is greater (normally, much greater) than $(N-3)$ when $K, L > 2$. Therefore this number is sufficient to form an $(N-4)$-dimensional face.

One can further show that the above vertices do not fall into a lower dimensional subspace but instead can be used to form $(N-4)$ linearly independent vectors. The coordinates of these vectors can have $(N-2)$ projections in the original Hilbert space: $p_3, p_4, \ldots, p_N$. Let us further assume that $E_3 < 0$ and $E_4 > 0$. Therefore, there will be one vertex in the $\{p_3, p_4\}$ two-dimensional plane. I denote this vertex as w_{34}. In addition, there will be K' vertices in $\{p_3, p_i\}$ planes, such that $i \geq 5$ and $E_i > 0$; and L' vertices in $\{p_4, p_j\}$ planes, such that $j \geq 5$ and $E_j < 0$. The total number of vertices in the latter two sets is $K' + L' = N - 4$. One can now form $(N-4)$ vectors by subtracting the coordinates of vertex w_{34} from each of the above $(N-4)$ vertices. The resulting vectors will be linearly independent, because the projections on each of the axes $p_5, p_6, \ldots, p_N$ will be present in this set only once in one of the vectors, and therefore the linear combination with other vectors cannot cancel that projection.

Finally, the above $(N-4)$-dimensional face changes identically under the shift of the energy hyperplanes in the both cases (which includes the possible change in the number of vertices). Indeed, because of the condition $p_2 = 0$, the projected shifts of the energy hyperplanes in both cases are described by identical equation:

$$E_3 p_3 + \cdots + E_N p_N = v. \tag{A10}$$

Therefore, all $(N-4)$ renormalization coefficients describing the volume change of this face with v can be chosen identically.

As indicated in the discussion of manifold vertices, the structures of the two manifolds compared can be very different outside the common face. However, all these differences contribute to a single linear parameter η corresponding to the direction perpendicular to the common face, which changes only weakly under the change of v.

The last step for the complete rigor of the present proof would be to impose the limits on the exceptional cases when the renormalization of a single parameter $\lambda_{k\alpha_0}$ would be comparable with the sum of the rest of $\lambda_{k\alpha}$.

Here, one can be concerned, for example, that the parameter $\lambda_{k\alpha_0}$ is accidentally defined on the basis of an uncharacteristic $(N-4)$-dimensional face (e.g., a face of a small "appendix" to a large polyhedron). Such a case, however, is highly unlikely, because, if, in the proof following Eq. (A9), all vertices of the $(p_2 = 0)$ face are removed from the manifold, the remaining ones will not be enough to form an $(N-3)$-dimensional manifold (when $K > 1$ and $L > 1$).

Another anomalous possibility occurs when the sum of all $\lambda_{k\alpha}$ except for $\lambda_{k\alpha_0}$ accidentally turns to zero even though each term of that sum is comparable to $\lambda_{k\alpha_0}$. However, this would actually mean that the typical λ, as used in the main text, is zero within the accuracy of the present approximation.

The real problematic case corresponding to one $|\lambda_{k\alpha_0}|$ being much greater than all other $|\lambda_{k\alpha}|$ requires one energy level to have an anomalous property as compared with the rest. I was able to identify only one example of this kind, namely, when $E_1 = E_{\min}$, and it is the only energy level below E_{av}, i.e., $L = 1$. However, even in this case, all λ_k except for

λ_1 will have the same large term $\lambda_{k\alpha_0}$ and therefore remain approximately equal. At the same time, the value of λ_1 is irrelevant because it describes the response of $V_1(p_1)$ to small deviation of p_1 from zero, while, as explained in Sec. II D and in Appendix B, $V_1(p_1)$ is narrowly peaked not around $p_1=0$ but around a finite value of p_1. [In fact, in this case, $V_1(p_1)=0$ until p_1 reaches the finite value given by condition $E_{\min}p_1+E_2(1-p_1)=0$. Here E_2 is the second lowest-energy level.]

One can further consider, the cases of L$=2,3,4$, etc. In this case too, the few lowest levels up to $k=L$ may have anomalous values of λ_k, but all these anomalous λ_k are expected to be irrelevant because the corresponding $V_k(p_k)$ are expected to be sharply peaked around $p_k \neq 0$.

The above analysis thus suggests, that, in order to include all anomalous cases, $O(1/N)$ in Eq. (A9) should be replaced by $O(1/\min[K,L])$ but this claim requires further proof.

APPENDIX B: DERIVATION OF GENERAL FORMULA (33) FOR THE HILBERT SPACE VOLUME OF MANIFOLD M_k

The derivation of formula (33) proceeds as follows.

Both sides in each of Eqs. (9) and (10) are divided by $(1-p_k)$ and new variables

$$p_i' = \frac{p_i}{1-p_k} \tag{B1}$$

for $i \neq k$ are introduced. This gives, respectively,

$$\sum_{i,i\neq k}^{N} p_i' = 1, \tag{B2}$$

$$\sum_{i,i\neq k}^{N} (E_i - E_{\mathrm{av}})p_i' = v, \tag{B3}$$

where

$$v = -\frac{(E_k - E_{\mathrm{av}})p_k}{1-p_k} \tag{B4}$$

is not a small number. The above equations in combination with constraints

$$p_i' \geq 0 \tag{B5}$$

describe a manifold M_k' with volume V_k' in the space of variables p_i'. Due to rescaling of axes [Eq. (B1)],

$$V_k = (1-p_k)^{N-3} V_k' \tag{B6}$$

where V_k is the volume of the original manifold M_k defined in Sec. II A and exponent $N-3$ is equal to the dimension of manifolds M_k' and M_k.

Since the set of energy coefficients in the left-hand side of Eq. (B3) for manifold M_k' is the same as the set for the original manifold M_k in Eq. (10), both manifolds are characterized by the identical dependence of the parameter λ on the shift of the energy hyperplanes:

$$\lambda[E_{\mathrm{av}}] = \frac{1}{N-3}\frac{d \log V_k'}{dv} = \frac{1}{N-3}\frac{d \log V_k'}{dE_{\mathrm{av}}} \tag{B7}$$

(see also Appendix A). Therefore,

$$V_k' = V_{k0}' \exp\left\{ (N-3)\int_{E_{\mathrm{av}}}^{E_{\mathrm{av}}+v} \lambda[E]dE \right\}, \tag{B8}$$

where V_{k0}' is the volume of M_k' corresponding to $v=0$, which is simultaneously equal to V_k, when $p_k=0$. Combining Eqs. (B4), (B6), and (B8), I obtain

$$V_k(p_k) = V_k(0)\exp\left\{ (N-3)\left[\log(1-p_k) + \int_{E_{\mathrm{av}}}^{E_{\mathrm{av}}-[(E_k-E_{\mathrm{av}})p_k/(1-p_k)]} \lambda[E]dE \right]\right\}, \tag{B9}$$

the same as Eq. (33) in the main text. This equation has to be solved together with Eq. (23), which requires finding $\lambda[E]$ for most of the allowed interval $[E_{\min},E_{\max}]$. In practice, however, if the purpose is to find $V_k(p_k)$ for a particular value of $E_{\mathrm{av}}<0$, the interval $[E_{\mathrm{av}},0]$ would suffice. This self-consistent solution can proceed as follows:

One first finds the values of $\lambda[E_{\mathrm{av}}]$ in the interval, where approximation (21) is valid, i.e., for E_{av} between 0 and a certain value somewhat below the critical value E_C defined by Eq. (32) and then proceed with reducing E_{av} further in sufficiently small steps and using approximation (21) only for $E_k \geq E_{\mathrm{av}}$, while for $E_k < E_{\mathrm{av}}$ using full formula (B9), where at each step the integral would require only the knowledge of $\lambda[E]$ for $E > E_{\mathrm{av}}$. In principle, that integral may extend to $E>0$, but this corresponds to sufficiently large values of p_k, for which $V_k(p_k)$ is guaranteed to exhibit fast exponential decay. Therefore, a cutoff p_{kC} can be imposed that does not allow the upper integration limit to extend above 0. This cutoff is further discussed in Appendix D.

The general numerical solution of Eq. (B9) is to be described elsewhere [22].

APPENDIX C: SYSTEM OF MANY SPIN 1/2

In order to appreciate certain general aspects of the macroscopic case, it is sufficient to consider an otherwise very artificial example of $N_s \gg 1$ noninteracting spins 1/2 in magnetic field. The number of levels in this system is

$$N = 2^{N_s} \gg N_s. \tag{C1}$$

In the basis of spins quantized along the direction of the magnetic field (z direction), each eigenstate is determined by a set of spin projections $S_{nz} = \pm 1/2$, and the corresponding energy is

$$E = \sum_{n=1}^{N_s} \Omega S_{nz}, \tag{C2}$$

where Ω is the "Larmor energy" associated with the splitting of spin states. The minimum and the maximum energies of this spectrum are, respectively,

$$E_{\text{min}} = -\frac{1}{2}N_s\Omega \tag{C3}$$

and

$$E_{\text{max}} = \frac{1}{2}N_s\Omega. \tag{C4}$$

The average of all energies in the spectrum is zero, and the mean-squared deviation from this average is

$$\sigma_s^2 = \frac{1}{4}N_s\Omega^2. \tag{C5}$$

All energies have form

$$E = E_{\text{min}} + \Omega m, \tag{C6}$$

where m is an integer number between 0 and N_s. The degeneracy D_m of the energy levels corresponding to a given value of m is

$$D_m = \frac{N_s!}{m!\,(N_s - m)!}. \tag{C7}$$

For $m,(N_s-m) \gg 1$, one can use Stirling approximation $m! \approx \sqrt{2\pi m}\exp\{m(\log m - 1)\}$ and likewise for $(N_s-m)!$ and $N_s!$ and then divide the degeneracy D_m by distance between levels Ω to obtain the density of states:

$$\nu(E) = \frac{1}{\Omega}\sqrt{\frac{N_s}{2\pi m(N_s - m)}}e^{N_s \log N_s/(N_s-m) + m \log (N_s-m)/m}, \tag{C8}$$

where $m=(E-E_{\text{min}})/\Omega$—as follows from Eq. (C6). The density of states can be further approximated by Gaussian:

$$\nu(E) = \frac{N}{\sqrt{2\pi}\sigma_s}e^{-E^2/2\sigma_s^2}, \tag{C9}$$

which is the consequence of the central limit theorem. It becomes increasingly inaccurate for $|E| \gg \sigma_s$.

As the most representative physical situation, let us consider the case $T=\Omega$, where T is the usual temperature defined by Eq. (38). In this case, the Gaussian approximation (C9) for $\nu(E)$ would imply $E_{\text{av}}=-\frac{1}{4}\Omega N_s = E_{\text{min}}/2$, i.e.,

$$|E_{\text{av}}| \gg \sigma_s, \tag{C10}$$

with most routine being the case when E_{av} is negative and a finite fraction of E_{min}. [The Gaussian approximation for $\nu(E)$ is not, in fact, very accurate for $E_{\text{av}} \sim E_{\text{min}}$. For example, for $E_{\text{av}}=E_{\text{min}}/2$, the accurate approximation (C8) gives $T=\Omega/\log 3$. However this discrepancy does not invalidate the general estimate [Eq. (C10)].]

Now, I would like to show that condition (31), which guarantees the smallness of all p_k, is violated for the present spin system almost immediately after E_{av} starts decreasing below zero. Let us consider what it takes to satisfy Eq. (25) when condition (31) is fulfilled. The integral in this equation has the character of the average value of $(E-E_{\text{av}})$ under the effective distribution described by a product of a slow varying function $1/[1+\lambda(E-E_{\text{av}})]$ and a sharply peaked symmetric function $\nu(E)$, which for the present purpose is well approximated by the Gaussian [Eq. (C9)]. In the leading order, this effective distribution will remain symmetric but with respect to a maximum, which is slightly shifted relatively to that of $\nu(E)$. Equation(25) can only be satisfied when that maximum coincides with E_{av}. Such a condition gives $\lambda = E_{\text{av}}/\sigma_s^2$. Then requiring that $E_\lambda = E_{\text{min}}$, I obtain the critical value of E_{av} denoted earlier [Eq. (32)] as E_C:

$$E_C = \frac{\sigma_s^2}{E_{\text{min}}} = -\frac{1}{2}\Omega \ll \sigma_s, \tag{C11}$$

which implies that the small-p_k condition (31) is violated at least for some k, when the values of E_{av} fall in the range of primary physical interest [Eq. (C10)].

The analysis in Sec. II E relies on the assumption that, for $N_s \sim 10^{23}$,

$$E_2 - E_{\text{min}} \gg \frac{|E_{\text{min}}|}{N}, \tag{C12}$$

where E_2 is the energy of the second lowest level, E_{av} satisfies Eq. (C10). The above property is obviously true for the present spin system, where $E_2-E_{\text{min}}=\Omega$, but it should also remain valid for any realistic macroscopic system with nondegenerate ground state—consequence of the fact Eq. (C1) that N is exponentially larger than N_s.

In order to illustrate the above claim, let us consider as a more realistic example, the system of N_s spins 1/2 on a cubic lattice with ferromagnetic nearest-neighbor exchange interaction and periodic boundary conditions. The Hamiltonian is $\mathcal{H}=-J\Sigma_{\text{NN}}\mathbf{S}_m\cdot\mathbf{S}_n$, where $\mathbf{S}_m$ are vector spin operators, J is the (positive) exchange constant, and NN refers to the summation over the nearest neighbor $\{m,n\}$ pairs. In this case, the ground state has energy $E_{\text{min}}=-\frac{3}{4}JN_s$. It is N_s-fold degenerate because all states with total spin $\frac{1}{2}N_s$ have this energy. The excited states have a character of spin waves. Yet these spin waves are gapped by the finite linear size of the system $(\sqrt[3]{N_s})$, i.e., $E_2-E_{\text{min}} \sim J/\sqrt[3]{N_s} \gg |E_{\text{min}}|/N$. As far as the ground-state degeneracy is concerned, one can imagine that any even unrealistically small stray magnetic field would lift this degeneracy with the energy splitting that would still be exponentially larger than $|E_{\text{min}}|/N$. (It should not be difficult to extend the result of this work to the theoretical case of degenerate ground state.)

APPENDIX D: CONDENSATION INTO THE LOWEST LEVEL OF MACROSCOPIC SYSTEM

When condition (30) is not fulfilled, volume $V_k(p_k)$ does not decay exponentially fast. The possible alternatives are (i) that it changes slowly—decreases or increases, or (ii) it has a sharp Gaussian-like maximum at $p_k=p_{k0}$ somewhere between 0 and 1, in which case $\langle p_k\rangle \approx p_{k0}$. In the both cases, $\langle p_k\rangle$ would be a significant fraction of 1.

The first of the above cases may be realizable in numerical studies when $N \gg 1$, but $\log N$ is not too large. In this case, several low-lying levels may exhibit large values of $\langle p_k\rangle$.

I now show that in the macroscopic system, of the type described in Sec. II E, it is the second of the above cases that is realized and that the significant average occupation builds only for the lowest-lying level, while all other levels continue exhibiting occupations $\langle p_k \rangle \ll 1$ describable by formula (21).

The subtlety of the present part is that it requires one to find a correction to a very accurate approximation (31). In doing so, one needs to go back and forth between the scale of $|E_{\rm min}|$ and the scale of the level spacing between the lowest two levels.

I begin with several general observations, which are applicable to both cases (i) and (ii).

(1) Let us denote as I_1, the sum over the populations of those exceptional low-lying levels not describable by formulas (19) and (21) and exhibiting large average occupations $\langle p_k \rangle$. As mentioned in Sec. II D, there can exist only a relatively small number of these levels. Therefore, their energies should all be close to $E_{\rm min}$.

All other levels—in particular those surrounding the dominant peak in the density of states $\nu(E)$—would have "regular" values of $\langle p_k \rangle$ given by formula (21). Given the overall normalization (22), the total occupation of regular levels, to be denoted as I_2, is

$$I_2 = 1 - I_1. \tag{D1}$$

I can now use the energy condition (23) and the fact that the occupations of the exceptional levels are peaked around $E_{\rm min}$, while the integrand $\nu(E)/[1-\lambda(E-E_{\rm av})]$ is also peaked around $E_C \approx 0$ [see Eq. (C11) and its derivation] to obtain

$$(E_{\rm min} - E_{\rm av})I_1 - \frac{E_{\rm av}}{1-\lambda E_{\rm av}} I_2 = 0, \tag{D2}$$

which, in combination with Eq. (D1) and approximation (34) for λ gives

$$I_1 \approx \frac{E_{\rm av}}{E_{\rm min}}, \tag{D3}$$

$$I_2 \approx \frac{E_{\rm min} - E_{\rm av}}{E_{\rm min}}. \tag{D4}$$

(2) When the general formula (33) is used, one has to remember that manifold M_k exists and its volume V_k has nonzero value, only when $E'_{\rm min} \le E_{\rm av} \le E'_{\rm max}$, where $E'_{\rm min}$ and $E'_{\rm max}$ are the minimum and the maximum value among all energies excluding E_k. This means that the argument of $\lambda[E]$ should also stay within the same limits, which, in turn imposes cutoff on $V_k(p_k)$ as a function of p_k when the upper integration limit in Eq. (33) reaches $E'_{\rm max}$ or $E'_{\rm min}$. Beyond this cutoff, $V_k(p_k)=0$.

Here I am primarily concerned with the exceptional low-lying levels (and also exclude the case $E_{\rm av} < E_2$), which translates into constraint

$$E_{\rm av} - \frac{(E_k - E_{\rm av})p_k}{1-p_k} \le E_{\rm max}. \tag{D5}$$

This results in the upper maximum value for p_k:

$$p_{k[\rm max]} = \frac{E_{\rm max} - E_{\rm av}}{E_{\rm max} - E_k}. \tag{D6}$$

One can establish a stronger effective cutoff for p_k, beyond which $V_k(p_k)$ is guaranteed to exhibit sharp exponential decay (for $E_k < E_{\rm av}$). This cutoff corresponds to

$$E_{\rm av} - \frac{(E_k - E_{\rm av})p_k}{1-p_k} = 0, \tag{D7}$$

which translates into the cutoff value

$$p_{kC} = \frac{E_{\rm av}}{E_k}. \tag{D8}$$

The above cutoff originates from the following argument. When $V_k(p_k)$ given by Eq. (33) decays slowly or increases at small p_k, it happens because the increasing value of integral in Eq. (33) nearly compensates or outweighs the decreasing value of the preceding logarithmic term. I note now that $\lambda[E]$ becomes negative above $E=0$ (see Fig. 1). Therefore, once p_k reaches the value given by Eq. (D7), the integration extends into positive E and the integral starts decreasing. After that, it is certain that nothing any longer can slow the fast exponential decay—hence cutoff (D8).

(3) Cutoff (D8) can now be used to show that as $E_{\rm av}$ decreases, the value of $E_\lambda[E_{\rm av}]$ cannot always stay below $E_{\rm min}$. In principle, the estimate [Eq. (C11)] already indicates this, but it could have happened that it signified only E_λ approaching $E_{\rm min}$ within $O(1/N)$ from below and never crossing it.

If the latter possibility were to be realized, the derivative of $V_1(p_1)$ would remain negative or zero for $0 \le p_1 \le 1$ with rapid exponential drop above p_{1C} given by Eq. (D8). This would, in turn, imply that

$$\langle p_1 \rangle < \frac{1}{2} p_{1C} + O(1/N) = \frac{1}{2}\frac{E_{\rm av}}{E_{\rm min}} + O(1/N). \tag{D9}$$

Given inequality (41), $\langle p_2 \rangle \ll 1$ for $E_\lambda < E_{\rm min}$. Therefore, the only "exceptional" level in this case would be the lowest one. That is, $I_1 = \langle p_1 \rangle$, where $\langle p_1 \rangle$ is given by Eq. (D9), which contradicts to Eq. (D3). Thus the estimate [Eq. (C11)] indicated correctly that E_λ crossing $E_{\rm min}$ corresponds to $E_{\rm av} = E_C \ll E_{\rm min}$.

(4) When $E_\lambda > E_{\rm min}$, the volume $V_1(p_1)$ increases at small p_1; then it reaches a maximum at the value of p_1 to be denoted at p_{10} and, finally, decays to zero at $p_1=1$.

Below I locate p_{10} and show that it corresponds to a δ-function-like maximum:

$$V_1(p_1) \sim \exp\left[-\frac{(p_1 - p_{10})^2}{2\sigma_1^2}\right], \tag{D10}$$

where $\sigma_1 \ll 1$, which implies

$$\langle p_1 \rangle \approx p_{10}. \tag{D11}$$

Requiring the derivative of the exponent in Eq. (33) with respect to p_k to be equal to zero, I obtain for $k=1$:

$$1 + \lambda\left[E_{\rm av} - \frac{(E_{\rm min} - E_{\rm av})p_{10}}{1-p_{10}}\right]\frac{E_{\rm min} - E_{\rm av}}{1-p_{10}} = 0. \tag{D12}$$

Making in Eq. (D12) substitution

$$\lambda[E] = \frac{1}{E - E_\lambda[E]}, \tag{D13}$$

I obtain after some manipulation:

$$E_\lambda\left[E_{\mathrm{av}} - \frac{(E_{\min} - E_{\mathrm{av}})p_{10}}{1 - p_{10}}\right] = E_{\min}. \tag{D14}$$

Therefore, according to the definition of E_C given by Eq. (32),

$$E_{\mathrm{av}} - \frac{(E_{\min} - E_{\mathrm{av}})p_{10}}{1 - p_{10}} = E_C. \tag{D15}$$

As a result,

$$p_{10} = \frac{E_C - E_{\mathrm{av}}}{E_C - E_{\min}} \approx \frac{E_{\mathrm{av}}}{E_{\min}}. \tag{D16}$$

The transition to the approximate value above follows from inequality (40).

The approximate value in Eq. (D16) is equal to the effective cutoff value p_{1C} given by Eq. (D8), where the derivative of $V_k(p_k)$ is supposed to be strongly negative. There is, however, no contradiction here. The accurate value of p_{10} given by the middle expression in Eq. (D16) is smaller than p_{1C}, and, as shown below, the width of the maximum σ_1 is much smaller than the difference between p_{1C} and p_{10}.

The value of σ_1 can now be obtained from

$$\frac{1}{\sigma_1^2} = -\left.\frac{d^2 \log V_1(p_1)}{dp_1^2}\right|_{p_1=p_{10}} = -\frac{(N-3)}{(1-p_{10})^2}\left.\frac{dE_\lambda[E]}{dE}\right|_{E=E_C}. \tag{D17}$$

Condition $-dE_\lambda[E]/dE|_{E=E_C} \gg 1/N$ would then be sufficient to justify $\sigma_1 \ll 1$.

By differentiating the accurate version of conditions (D1) and (D2) and using formula (33) for $V_1(p_1)$ to calculate $I_1 = \langle p_1\rangle$, I was able to obtain

$$-\left.\frac{dE_\lambda[E]}{dE}\right|_{E=E_C} \approx \frac{2}{\pi}\frac{E_{\min}^2}{\sigma_s^2} \sim N_s \gg 1, \tag{D18}$$

which guarantees the validity of Eq. (D9) with p_{10} approximated by Eq. (D16)—hence

$$\langle p_1\rangle \approx \frac{E_{\mathrm{av}}}{E_{\min}}. \tag{D19}$$

Finally, I observe that Eqs. (D3) and (D19) imply that

$$\langle p_1\rangle \approx I_1. \tag{D20}$$

The approximate values (D3) and (D19) for I_1 and $\langle p_1\rangle$ were obtained under the same assumption $E_C \approx 0$. In fact, Eq. (D20) also holds when E_C is not neglected.

Equation (D20) indicates that $\langle p_1\rangle$ exhausts or almost exhausts the total occupation I_1 of all exceptional levels, whose respective Hilbert-space volumes depart significantly from formula (19).

One can further rule out the possibility "almost exhausts." It would require that $E_\lambda[E_{\mathrm{av}}]$ reaches at least the second lowest-energy level E_2. If this were to happen at $E_{\mathrm{av}} = E_{C2}$, then $V_2(p_2)$ would acquire maximum at

$$p_{20} = \frac{E_{C2} - E_{\mathrm{av}}}{E_{C2} - E_{\min}} \tag{D21}$$

for all $E_{\mathrm{av}} < E_{C2}$. This maximum, sharp or not, would then lead to $\langle p_1\rangle + \langle p_2\rangle$ becoming significantly greater than $E_{\mathrm{av}}/E_{\min}$ for most of the range $E_{\mathrm{av}} < E_{C2}$ in contradiction to Eq. (D3).

Therefore, E_λ is always sufficiently smaller than E_2 to justify the use of formula (21) for all $k \geq 2$.

APPENDIX E: DERIVATION OF EQS. (73)–(76) FOR THE DENSITY MATRIX OF A SUBSYSTEM IN A MACROSCOPIC ENVIRONMENT

It follows from inequality (40) that $E_\lambda[E]$ has the following approximate property:

$$\text{if } E_\lambda[E] < E_{\min}, \text{ then } E \approx E_P \tag{E1}$$

and

$$\text{if } E_{\min} < E < E_P, \text{ then } E_\lambda[E] \approx E_{\min}, \tag{E2}$$

where E_P is the position of the sharp maximum of $\nu(E)$. It was also obtained in Appendix D that

$$E_\lambda[E] < E_2, \quad \forall\ E < E_P, \tag{E3}$$

where E_2 is the energy of the second lowest level.

The key assumption of the present calculation is that the above conditions apply to both sets of energies $\{E_a\}$ and $\{E_b\}$ with the appropriate insertion of subscripts a and b. The densities of states $\nu_a(E)$ and $\nu_b(E)$ corresponding to these two sets are characterized by the respective peak positions:

$$E_{Pa} = E_{S\alpha}, \tag{E4}$$

$$E_{Pb} = -\frac{E_{S\alpha}}{N_1 - 1}. \tag{E5}$$

Each energy set also has a respective minimum value $E_{a\,\min}$ and $E_{b\,\min}$. The outcome of the calculation now simply depends on whether $E_{a\,\min}$ is smaller or larger than $E_{b\,\min}$.

Case I: $\alpha \geq 2$.

In this case:

$$E_{a\,\min} = E_{S\alpha} + E_{E\,\min} \tag{E6}$$

and

$$E_{b\,\min} = E_{S\,\min} + E_{E\,\min} \equiv E_{\min}, \tag{E7}$$

which implies that $E_{a\,\min} > E_{b\,\min}$.

Given conditions (E3) and (72), I can further constrain

$$E_{\lambda_b} < E_{b2} \lesssim E_{a\,\min}. \tag{E8}$$

This condition applies to $E_{\lambda_b}[E]$ independently of its argument. Therefore,

$$E_{\lambda_a}\left[E_{\text{av}}+\frac{E_A}{\rho_\alpha}\right] < E_{a\,\text{min}}. \tag{E9}$$

Thus, according to Eq. (E1),

$$E_{\text{av}}+\frac{E_A}{\rho_\alpha} \approx E_{Pa} = E_{S\alpha}. \tag{E10}$$

One can then solve the pair of Eqs. (69) and (E10) with respect to E_A and ρ_α to obtain

$$\rho_\alpha = \frac{1}{N_1}\frac{E_{\text{av}}-E_{\lambda_a}\left[E_{\text{av}}+\dfrac{E_A}{\rho_\alpha}\right]}{E_{S\alpha}-E_{\lambda_a}\left[E_{\text{av}}+\dfrac{E_A}{\rho_\alpha}\right]}. \tag{E11}$$

Now, in order to find $E_{\lambda_a}[E_{\text{av}}+E_A/\rho_\alpha]$, one is helped by the inequality

$$E_{\text{av}} < E_{Pa}, E_{Pb}, \tag{E12}$$

which is the consequence of the earlier assumption (71) that $|E_{\text{av}}| \gg E_{S\alpha}, \forall\ \alpha$. Equations (E10) and (E12) now require that $E_A > 0$. As a result,

$$E_{\text{av}} - \frac{E_A}{1-\rho_\alpha} < E_{\text{av}} < E_{Pb}, \tag{E13}$$

which, according to Eq. (E2), implies that

$$E_{\lambda_b}\left[E_{\text{av}} - \frac{E_A}{1-\rho_\alpha}\right] = E_{b\,\text{min}}. \tag{E14}$$

Therefore, according to Eqs. (70) and (E7)

$$E_{\lambda_a}\left[E_{\text{av}}+\frac{E_A}{\rho_\alpha}\right] = E_{\text{min}}. \tag{E15}$$

The substitution of Eq. (E15) into Eq. (E11) yields

$$\rho_\alpha = \frac{1}{N_1}\frac{E_{\text{av}}-E_{\text{min}}}{E_{S\alpha}-E_{\text{min}}}. \tag{E16}$$

Given inequality (71), the leading order approximation of Eq. (E16) is

$$\rho_\alpha = \frac{1}{N_1}\left(1-\frac{E_{\text{av}}}{E_{E\,\text{min}}}\right). \tag{E17}$$

Case II: $\alpha=1$.

Now

$$E_{a\,\text{min}} = E_{S\,\text{min}} + E_{E\,\text{min}} \equiv E_{\text{min}} \tag{E18}$$

and

$$E_{b\,\text{min}} = E_{S2} + E_{E\,\text{min}}, \tag{E19}$$

implying $E_{a\,\text{min}} < E_{b\,\text{min}}$.

One can obtain using condition (72) that $E_{b\,\text{min}} - E_{a\,\text{min}} = E_{S2} - E_{S\,\text{min}} \geq E_{E2} - E_{E\,\text{min}} = E_{a2} - E_{a\,\text{min}}$. The resulting inequality together with condition (E3) implies that

$$E_{\lambda_a} < E_{a2} \leq E_{b\,\text{min}}. \tag{E20}$$

Inequality (E20) applies to any argument of $E_{\lambda_a}[E]$ including $E_{\text{av}}+E_A/\rho_1$. Using this fact together with Eq. (70), I obtain

$$E_{\lambda_b}\left[E_{\text{av}} - \frac{E_A}{1-\rho_1}\right] < E_{b\,\text{min}}. \tag{E21}$$

Thus, according to Eq. (E1),

$$E_{\text{av}} - \frac{E_A}{1-\rho_1} \approx E_{Pb} = -\frac{E_{S\,\text{min}}}{N_1-1}. \tag{E22}$$

Given inequality (E12), Eq. (E22) implies that $E_A < 0$. As a result,

$$E_{\text{av}} + \frac{E_A}{\rho_1} < E_{\text{av}} < E_{Pa}, \tag{E23}$$

and thus, according to Eq. (E2),

$$E_{\lambda_a}[E_{\text{av}} + E_A/\rho_1] = E_{\text{min}}. \tag{E24}$$

After Eq. (E24) is substituted into Eq. (69) and the resulting equation is solved jointly with Eq. (E22) with respect to ρ_1 and E_A, I obtain

$$\rho_1 = \frac{E_{\text{av}}\left(1-\dfrac{1}{N_1}\right) + \dfrac{E_{S\,\text{min}}}{N_1-1} + \dfrac{E_{\text{min}}}{N_1}}{\dfrac{E_{S\,\text{min}}}{N_1-1} + E_{\text{min}}}. \tag{E25}$$

Given the condition $|E_{S\,\text{min}}| \ll |E_{\text{av}}|, |E_{E\,\text{min}}|$, the leading order approximation of Eq. (E25) is

$$\rho_1 = \frac{E_{\text{av}}}{E_{E\,\text{min}}} + \frac{1}{N_1}\left(1-\frac{E_{\text{av}}}{E_{E\,\text{min}}}\right). \tag{E26}$$

It is clear from the derivation that formulas (E16) and (E25) describe a broader range of mostly abstract possibilities beyond the physical assumptions used so far.

One can, in particular, consider relaxing the condition $|E_{S\alpha}| \ll |E_{\text{av}}|, |E_{E\,\text{min}}|$. In this case, however, on needs to be concerned with the validity of conditions (E1) and (E2) for the energy set $\{E_b\}$. For example, if the spectrum of $\{E_{S\alpha}\}$ consists of only a few far separated levels, then $\nu_b(E)$ loses the single peak structure and hence conditions (E1) and (E2). However, when $N_1 \gg 1$, and the spectrum of energies $\{E_{S\alpha}\}$ has a sharply-peaked Gaussian-like density of states, then conditions (E1) and (E2) are recovered.

In the latter case, one also needs to examine what happens when E_{av} falls between E_{Pa} and E_{Pb}. In this case, the system of Eqs. (69) and (70) with approximations (E1) and (E2) generates two more solutions, in addition to the one already found. These two solutions correspond to the possibility that both $E_{\text{av}}+E_A/\rho_\alpha$ and $E_{\text{av}}-E_A/(1-\rho_\alpha)$ become approximately equal to E_{Pa} and E_{Pb}, respectively. One solution would then correspond to positive values and the other one to the negative values of λ_a, λ_b. They are expected to be a maximum and a minimum located close to each other in the plane of variables (E_A, ρ_α). The additional maximum should presumably have a smaller value, in comparison to the one found earlier, because it has a larger value of ρ_α and therefore stronger suppressed by term containing $\log(1-\rho_\alpha)$ in Eq. (64).

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